Mathematical Aspects of the BCS Theory of Superconductivity and Related Theories

Dissertation
der Mathematisch-Naturwissenschaftlichen Fakultät
der Eberhard Karls Universität Tübingen
zur Erlangung des Grades eines
Doktors der Naturwissenschaften
(Dr. rer. nat.)

vorgelegt von
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aus Zürich/Schweiz

Tübingen 2014

Tag der mündlichen Qualifikation:	15.09.2014
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Danksagung

Allen voran danke ich meinem Hauptbetreuer, Prof. Dr. Christian Hainzl. Ein besserer Doktorvater wäre schwer zu finden gewesen. Dies nicht nur im wissenschaftlichen Sinne – ich durfte mit ihm auch einige unvergesslichen Stunden bei geselligen und sportlichen Unternehmungen teilen.

Mein besonderer Dank gilt auch meinem externen Gutachter, Prof. Dr. Robert Seiringer am IST Austria für die Co-Autorenschaft bei Publikationen und für wichtige wissenschaftliche Anregungen, sowie meinem zweiten Betreuer Prof Dr. Stefan Teufel für zahlreiche wertvolle Diskussionen.

Ferner richte ich einen spezieller Dank an Andreas Deuchert, Dennis Zelle sowie meinen Vater, Reinhold Bräunlich für das Korrekturlesen der Dissertation.

Sehr fördernd für das Gelingen der Arbeit war die angenehme und produktive Arbeitsatmosphäre, für welche meine Arbeitskollegen stets gesorgt haben. Dafür danke ich meinen ersten Kollegen in meiner Tübinger Zeit: Andreas Wöhr, Hans Stiepan und Marco Schreiber, sowie Max Lein, der lange Zeit mein Zimmergenosse war. Ausserdem danke ich Falk Anger als Ansprechpartner für experimental-physikalische Fragen, Carla Cederbaum für wertvolle Tipps zu meinen wissenschaftlichen Bewerbungen, Sebastian Egger, Johannes von Keler, Sebastian Debrelli-Boelzle, Jonas Lampart, Stefan Haag, Pascal Kilian, Silvia Freund, Wolfgang Gaim, Tim Tsanatheas, Stefan Keppeler und Frank Loose.

Contents

1 Zusammenfassung

Die vorliegende Arbeit beginnt mit einer Einführung in die der Supraleitung und Superfluidität zugrunde liegenden BCS-Theorie. Der Hauptteil besteht aus einer Zusammenfassung von drei Publikationen [BHS14c; BHS13; BHS14b] und einem Beitrag zu einem Tagungsband [BHS14a]. Die Einführung (Kapitel 1) beinhaltet einen kurzen historischen Rückblick auf die Forschung im Gebiet der Supraleitung und der Superfluidität, beginnend mit den Umständen, die dazu führten, dass Kamerlingh Onnes im Jahr 1911 die Supraleitung entdeckte. Abgeschlossen wird der erste Teil mit einem kurzen Überblick über die technischen Anwendungen der Supraleitung. Kapitel 2 beginnt mit einer Zusammenfassung der bekannten Konzepte aus der Quantenmechanik und der Quantenstatistik, auf die die BCS-Theorie aufbaut. Dazu werden unter anderem die Quasifreien Zustände eingeführt und die zu ihnen assoziierten Einteilchen-Dichtematrizen. Der Hauptteil dieses Kapitels ist die Herleitung des BCS-Funktionals aus der Quantenstatistik. Dabei wird auf alle verwendeten Näherungen eingegangen. Das resultierende Funktional

$$\begin{aligned} \mathcal{F}_T(\Gamma) &= \int_{\mathbb{R}^3} (p^2+\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p - TS(\Gamma) + \int_{\mathbb{R}^3} |\alpha(r)|^2 V(r)\,\mathrm{d}^3r, \\ S(\Gamma) &= -\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\big(\Gamma(p)\ln(\Gamma(p))\big)\,\mathrm{d}^3p \end{aligned} \tag{1.1}$$

liefert zu einem gegebenen Zustand $\Gamma = \begin{pmatrix} \hat{\gamma} & \hat{\alpha} \\ \bar{\hat{\alpha}} & 1-\hat{\gamma} \end{pmatrix}$ den negativen, thermodynamischen Druck eines Systems im chemischen Potential μ und der Temperatur T, in welchem die Fermionen über das effektive Potential V wechselwirken. $S(\Gamma)$ bezeichnet dabei die Entropie des Zustandes Γ, welcher sich aus der Einteilchen-Dichteverteilung γ und der Cooper-Paar-Wellenfunktion α zusammensetzt. Ziel der BCS-Theorie ist es unter anderem zu den Daten des Systems (μ, T, V) den Minimierer Γ des Funktionals $\mathcal{F}_T$ zu finden. Man stellt fest, dass unter gewissen Umständen – abhängig von den Parametern des Systems – eine Temperatur T_c existiert, oberhalb welcher der α-Anteil des Minimierers verschwindet. Auf diese Art kann mit Hilfe der BCS-Theorie der Phasenübergang eines Normalleiters zu einem Supraleiter durch Bildung von Cooper-Paaren modelliert werden. Die Temperatur T_c wird als Sprungtemperatur bezeichnet.

Kapitel 3 erklärt die Ergebnisse aus den oben erwähnten Publikationen. In der Arbeit [BHS14c] wird die Gültigkeit einer Näherung bei der Herleitung des BCS-Funktionals untersucht. Es handelt sich dabei um die Vernachlässigung des so genannten *exchange term*

$$A_{\mathrm{ex}}(\Gamma) = -\int_{\mathbb{R}^3} |\gamma(r)|^2 V(r)\, \mathrm{d}^3 r$$

und des *direct term*

$$A_{\mathrm{dir}}(\Gamma) = 2[\gamma(0)]^2 \int_{\mathbb{R}^3} V(r)\, \mathrm{d}^3 r$$

in der vollständigen Form

$$\begin{aligned} \mathcal{F}_T^V(\Gamma) = &\int_{\mathbb{R}^3} (p^2+\mu)\widehat{\gamma}(p)\, \mathrm{d}^3 p + T \int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left(\widehat{\Gamma}(p)\ln(\widehat{\Gamma}(p))\right) \mathrm{d}^3 p \\ &+ \int_{\mathbb{R}^3} |\alpha(r)|^2 V(r)\, \mathrm{d}^3 r + A_{\mathrm{ex}}(\Gamma) + A_{\mathrm{dir}}(\Gamma) \end{aligned} \tag{1.2}$$

des Funktionals (1.1). Bei Berücksichtigung dieser beiden Terme ist die Charakterisierung oder gar Definition einer Sprungtemperatur viel schwieriger als im Fall von (1.1). Die Situation vereinfacht sich, wenn man sich auf kurzreichweitige Wechselwirkungspotentiale V_ℓ beschränkt, bei denen die Fermionen nur mit anderen Fermionen im Abstand von höchstens $\ell \ll 1$ wechselwirken. Dieser Sachverhalt wurde schon in der Physik-Literatur [Leg80] heuristisch motiviert mit dem Argument, dass für kurzreichweitige Potentiale der einzige Effekt der vernachlässigten Terme eine Renormierung des chemischen Potentials ist. Diese Behauptung wird in [BHS14c] auf einer mathematisch rigorosen Basis gerechtfertigt. Darüber hinaus wird durch die so genannte *effektive Gap-Gleichung* eine Definition und Charakterisierung einer Sprungtemperatur ermöglicht. Diese Gleichung,

$$-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\tilde{\mu}}^{0,\Delta}} - \frac{1}{p^2} \right) \mathrm{d}^3 p \tag{1.3}$$

findet sich auch in [Leg80] wieder. Hier bezeichnet a die Streulänge des Potentials V,

$$\Delta(p) = \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q)\hat{\alpha}(q)\, \mathrm{d}^3 q$$

die spektrale Energie-Lücke Δ und die Grösse $K_{T,\mu}^{\gamma,\Delta}$ ist definiert durch

$$K_{T,\mu}^{\gamma,\Delta}(p) = \frac{E_{\mu}^{\gamma,\Delta}(p)}{\tanh\left(\frac{E_{\mu}^{\gamma,\Delta}(p)}{2T}\right)},$$
$$E_{\mu}^{\gamma,\Delta}(p) = \sqrt{(\varepsilon^{\gamma}(p) - \tilde{\mu}^{\gamma})^2 + |\Delta(p)|^2}.$$

Die Gleichung (1.3) ist im Limes $\ell \to 0$ (Punktwechselwirkung) gültig und stellt die zu einem Minimierer gehörende spektrale Energie-Lücke Δ in Beziehung zur Streulänge. Dies ermöglicht im Limes $\ell \to 0$ eine Definition der kritischen Temperatur T_c. Dazu nutzt man aus, dass ab der Temperatur T_c die Cooper-Paar-Wellenfunktion α und somit auch die spektrale Energie-Lücke verschwinden. Fordert man $\Delta = 0$ in (1.3), so erhält man zusammen mit dem Ausdruck für das renormierte chemische Potential $\tilde{\mu}$ ein Gleichungssystem für T_c und $\tilde{\mu}$,

$$-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{\tanh\left(\frac{p^2-\tilde{\mu}}{2T_c}\right)}{p^2-\tilde{\mu}} - \frac{1}{p^2}\right)\mathrm{d}^3p\,,$$
$$\tilde{\mu} = \mu - \frac{2\mathcal{V}}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\frac{1}{1+\mathrm{e}^{\frac{p^2-\tilde{\mu}}{T_c}}}\,\mathrm{d}^3p\,,$$

wobei $\mathcal{V} = \lim_{\ell\to 0}\hat{V}_\ell(0)$.

Eine echte Renormierung $\tilde{\mu} \neq \mu$ erhält man allerdings nur für Potentiale mit $\mathcal{V} \neq 0$. Eines der einfachsten Beispiele zur Approximation von Punktwechselwirkungen, nämlich die Methode aus [Alb+88], liefert hier keine echte Renormierung. Diese Methode startet mit einem Referenz-Potential V und skaliert dieses gemäss

$$V_\ell(x) = \lambda(\ell)\ell^{-2}V(\tfrac{x}{\ell}), \qquad \lambda(0) = 1,\ \lambda(\ell) < 1 \text{ for } \ell > 0. \tag{1.4}$$

Die Funktion λ bestimmt dabei die Streulänge im Limes $\ell \to 0$. Nach Konstruktion gilt hier $\mathcal{V} = 0$. Es muss eine allgemeinere Klasse von Familien $\{V_\ell\}_{\ell>0}$ herangezogen werden, um $\mathcal{V} \neq 0$ zu erreichen. Ein Beispiel wird in [BHS14c] konstruiert.

Familien der Art (1.4) approximieren Punktwechselwirkungen. In der Quantenmechanik in drei Dimensionen werden diese durch selbst-adjungierte Erweiterungen des Laplace-Operators $-\Delta|_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}$ beschrieben

(Punktwechselwirkung im Punkt 0). Eine wichtige Aussage in [Alb+88] ist, dass der Schrödingeroperator $-\Delta + V_\ell$ im Norm-Resolventen-Sinn gegen eine durch die Streulänge $a = \lim_{\ell \to 0} a(V_\ell)$ bestimmte, selbst-adjungierte Erweiterung konvergiert. Da Punktwechselwirkungen in der Physik eine wichtige Rolle spielen, wurde eine eigene Arbeit [BHS13] verfasst, deren Inhalt es ist, zu zeigen, dass auch Familien V_ℓ mit $\mathcal{V} \neq 0$ auf die selbe Art zur Approximation von Punktwechselwirkungen herangezogen werden können.

In einer letzten Arbeit [BHS14b] wird der Zusammenhang mit der Gross-Pitaevskii-Theorie untersucht. Seit den 80er Jahren ist bekannt [Leg80; NSR85], dass aus der fermionischen, mikroskopischen BCS-Theorie die bosonische makroskopische Gross-Pitaevskii-Theorie hergeleitet werden kann. Falls man nämlich genügend starke Paar-Wechselwirkungen V betrachtet, bilden die Fermionen bosonische Zwei-Atomige Moleküle, die sich zu einem Bose-Einstein-Kondensat verdichten können. In [HS12; HS13] wurde diese Herleitung auf eine mathematisch rigorose Basis gestellt. Die Arbeit [BHS14b] kommt bei einem anderen Systemaufbau zum selben Schluss. Ausgangspunkt ist ein System von N Fermionen bei Temperatur $T = 0$, eingeschränkt durch ein externes Potential W. Die Paar-Wechselwirkung der Fermionen wird durch ein Potential V vermittelt, welches stark genug ist um zweiatomige, gebundene Zustände zu bilden. Zusätzlich wird angenommen, dass die Skala des externen Potentials W viel grösser ist als die Skala von V und dass die Dichte des Systems sehr klein ist. Diesen Gegebenheiten wird mathematisch Rechnung getragen, indem ein kleiner Parameter h eingeführt wird, mit dem das Verhältnis der beiden Skalen eingestellt werden kann. W übernimmt dabei die Rolle eines Referenzpotentials, welches gemäss $W(x) \to W(hx)$ skaliert wird. Gleichzeitig wird mit h die Teilchenzahl N gemäss $N \to N/h$ angepasst und die Stärke des externen Potentials mit h^2 skaliert. Da auf diese Art das Volumen des Systems wie h^{-3} skaliert, führt dies auf eine Teilchen-Dichte, der Grössenordnung h^2. Unter diesen Annahmen kann gezeigt werden, dass die Grundzustandsenergie gemäss dem translations-varianten BCS-Funktional in makroskopischen Variablen ($x_h = hx$, $y_h = hy$, $\alpha_h(x, y) = h^{-3}\alpha(\frac{x}{h}, \frac{y}{h})$,

$\gamma_h(x,y) = h^{-3}\gamma(\frac{x}{h}, \frac{y}{h}))$

$$\begin{aligned} \mathcal{E}^{\mathrm{BHF}}(\Gamma) = \operatorname{tr}(-h^2\Delta + h^2 W)\gamma &+ \frac{1}{2}\int_{\mathbb{R}^6} V\Big(\frac{x-y}{h}\Big)|\alpha(x,y)|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y \\ &- \frac{1}{2}\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\ &+ \int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y) V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y, \end{aligned} \tag{1.5}$$

zur führenden Ordnung in h durch die Bindungsenergie der Fermion-Paare $E_b \frac{N}{2h}$ gegeben ist. In der nächsten Ordnung (die makroskopische Dichtefluktuation) taucht dann das Gross-Pitaevskii-Potential

$$\mathcal{E}^{\mathrm{GP}}(\psi) = \int_{\mathbb{R}^3} \left(\frac{1}{4}|\nabla\psi(x)|^2 + W(x)|\psi(x)|^2 + g|\psi(x)|^4\right)\mathrm{d}^3x$$

auf. Dabei wird der Parameter g durch Grössen aus dem BCS-Funktional bestimmt. Die Funktion ψ geht aus der Cooper-Paar-Wellenfunktion α des Grundzustands von (1.5) hervor und beschreibt die räumlichen Fluktuationen der Fermion-Paare. Im Gegensatz zu [HS12] wird hier der *direct term* und der *exchange term* (die letzten beiden Summanden in (1.5)) berücksichtigt. Auch unterscheiden sich die zugrunde liegenden Systeme. Während in [HS12] ein unendlich ausgedehntes, in alle drei Raum-Richtungen periodisches System betrachtet wird, ist in [BHS14b] das System in dem externen Potential W eingeschlossen und es sind keine periodischen Randbedingungen nötig.

2 List of Publications in the Thesis

2.1 Accepted Papers

[BHS13] G. Bräunlich, C. Hainzl, and R. Seiringer. *On contact interactions as limits of short-range potentials*. Methods Funct. Anal. Topology **19**.4 (2013), pp. 364–375.

URL: http://mfat.imath.kiev.ua/html/papers/2013/4/bra-ha-se/art.pdf.

[BHS14a] G. Bräunlich, C. Hainzl, and R. Seiringer. *On the BCS gap equation for superfluid fermionic gases. Mathematical Results in Quantum Mechanics: Proceedings of the QMath12 Conference*. World Scientific, Singapore, 2014, pp. 127–137.

URL: http://www.worldscientific.com/worldscibooks/10.1142/9250.

[BHS14c] G. Bräunlich, C. Hainzl, and R. Seiringer. *Translation invariant quasi-free states for fermionic systems and the BCS approximation*. Reviews in Mathematical Physics **26**.7 (2014), p. 1450012.

DOI: 10.1142/S0129055X14500123.

URL: http://www.worldscientific.com/doi/abs/10.1142/S0129055X14500123.

2.2 Ready for Submission Manuscripts

[BHS14b] G. Bräunlich, C. Hainzl, and R. Seiringer. *The Bogolubov-Hartree-Fock theory for strongly interacting fermions in the low density limit*. 2014.

3 Personal Contribution

All the publications [BHS14c; BHS13; BHS14b; BHS14a] are joint work with Prof. Dr. Christian Hainzl and Prof. Dr. Robert Seiringer. The problems are a continuation of prior works of Hainzl, Seiringer and coworkers. The analysis was worked out by the author. Both Prof. Dr. Christian Hainzl and Prof. Dr. Robert Seiringer were available for discussions and helped to find and partially to fix some gaps and errors in the arguments. They also simplified the proofs and polished the manuscript.

Chapter 1

History and Applications of Superconductivity and Superfluidity

1.1 History of Superconductivity and Superfluidity[1]

Discovery of Superconductivity Before 1910, the dependence of electrical resistance on temperature was unexplored at low temperatures. James Dewar, John Ambrose Fleming and other experimental physicists have been collecting measurement data on many different metals down to the temperature of boiling liquid oxygen ($-200°C$) [KOGG91, p. xix.]. The extrapolation of the data raised hope that the resistance of metals could vanish at absolute zero or even at finite temperatures. However, theorists such as Lord Kelvin (William Thomson, 1824-1907) suggested [Kel02, § 27., p. 272 and § 30., p. 274] that the electrons should start to condensate onto their parent atoms at temperatures close to absolute zero, thus making electron movement impossible. For that reason, he expected the following dependence of resistance from temperature: Resistance should first decrease with falling temperature, then reach a minimum and increase again, diverging to infinity at absolute zero where the electrons are immobile. It is remarkable that both predictions could be verified. Semiconductors exhibit the behaviour predicted by Lord Kelvin, while superconductors reach zero resistance at temperatures $T > 0\,\mathrm{K}$. However, what physicists at that time did not expect was the abrupt transition from a finite resistance to zero resistance at a material specific temperature, the so called critical temperature. Additionally, normal conductors

[1] This section is based on [Rei04; DK10]

where observed, for which the resistance converges to a constant value as the temperature reaches absolute zero.

This was the situation when Heike Kamerlingh Onnes (Figure 1.1) was appointed 1882 to the Chair of Experimental Physics and Meteorology. The sentence

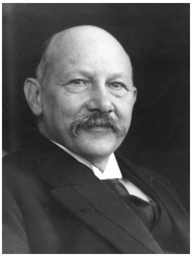

Figure 1.1: Kamerlingh Onnes (Copyright is by Museum Boerhaave)

> But the character of laws of nature becomes apparent only when one varies the measurable quantities through the entire range of possible values.

in his inaugural lecture in Leiden on the 11 November [Lae02, p. 270.] pretty well describes, what he dealt with for the next decade. He built a cryogenic laboratory, which became the most sophisticated in the world at this time. He was the first one who liquefied helium, for which he received the Nobel Prize for Physics in 1913. Although he announced in his inaugural lecture that he would focus on molecular physics and that he would promote the convergence of physics and chemistry, he also was aware of the measurements of the resistance of metals at low temperatures. In fact he supported Kelvin's suggestion [KO04, pp. 27-28; 55-56]. He started to investigate the electrical conductivity of platinum and gold. He soon turned to mercury which could be purified better. Due to its fluid state at room temperatures, it could be distilled repeatedly. This lead him to the discovery of superconductivity on the 26 October 1911. According to an anecdote, his team could not believe the abrupt jump to zero (see Figure 1.2) in the

resistance. They repeated the measurement several times to exclude an electrical short circuit when finally the "blue-boy"[2], controlling the vapor pressure in the cryostat fell asleep. This caused an increase in the pressure and the temperature raised again over the critical temperature. Suddenly the resistance attained its previous value. However, the notebook entry [KO] only reads: "At 4.00 [K] not yet anything to notice of rising resistance.

[2] To construct the complex apparatus for his laboratory, Kamerlingh Onnes founded the Leidse Instrumentmakersschool (Leiden School for Instrument Makers). The term "blue-boys" school is called after the color of the overalls of the mechanics, machinists, and glassblowers, trained there.

At 4.05 [K] not yet either. At 4.12 [K] resistance begins to appear."[DK10] not mentioning the "blue boy".

Discovery of Superfluidity It is remarkable that the Leiden team at the same time observed the phase transition of fluid helium to its superfluid state but without being aware of it. This also is recorded in the notebook [KO]. It took until 1928 that Keesom and Wolfke [KW28] postulated, that there was a phase transition at 2.18 K. They introduced the terms He I and He II for the two phases. The next discovery was made in 1932, when Keesom and Clusius [KC32] measured a jump in the specific heat. For the following development, John Cunningham McLennan, head of the Department of Physics at the University of Toronto played an important role. Importing the know-how of Kamerlingh Onnes, he built up the second low temperature laboratory in the world capable of liquefying ^{4}He. In 1932 he noted [MSW32] that the bubble formation appearing at 4.2 K abruptly disappears at the transition temperature and below. Among others John F. Allen and Austin Donald Misener were graduate students in his cryogenic lab. After finishing his Ph.D., Allen successfully applied for a position in Cambridge and worked with Peter Kapitza who came from the Soviet Union as a graduate student under Rutherford. With the help of funds Rutherford got from the Royal Society, he built the Mond Laboratory (named after Dr. Ludwig Mond, in recognition of his bequest to the Royal Society) including a new helium liquefier with a new innovative design in 1933. At the time when Allen arrived in Cambridge, Kapitza was put under house arrest on one of his regular family visits. He was provided with a huge funding to build a new lab in Moscow. With the permission of Rutherford and the acting Director of the Mond Lab he got assistance from Cambridge by two senior technicians and research equipment. From that point on, Kapitza continued his research in Moscow. In the mean time, Allen took root in Cambridge and effectively became the leader of the research group. Misener, still in Toronto, fin-

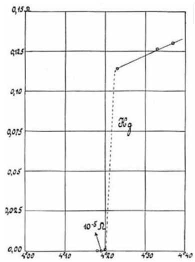

Figure 1.2: Historic plot of resistance [Ω] versus temperature [K] for mercury from the 26 October 1911 experiment (research notebook of Kamerlingh Onnes [KO]).

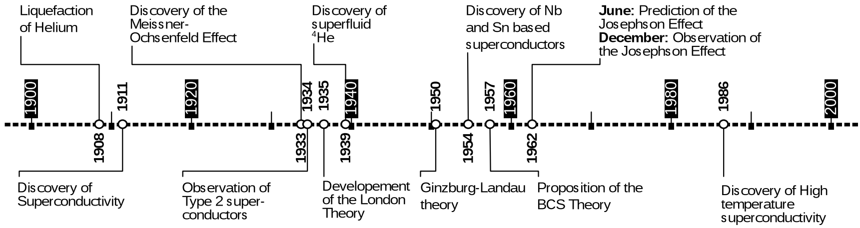

Figure 1.3: Timeline

ished his M.Sc. and continued his research by measuring [Bur35] the shear viscosity of liquid Helium just below the transition temperature of 2.18 K. Later he followed Allen to Cambridge to do his doctorate. Together they studied the flow of liquid Helium in thin capillaries. On 8 January 1938 a paper by Allen and Misener [AM38] as well as another one by Kaptza [Kap38] was published in Nature, presenting the same result. Using different methods, they found, that below 2.18 K, the viscosity of liquid helium almost vanishes. The two parties did not collaborate. Kapitza rather had a rivaling attitude to Misener and Allen who used his liquefier.

Discovery of Type-II Superconductors In the period following the discovery of superconductivity, liquid helium became available in several other laboratories as Toronto, Oxford and Kharkov. This enabled the discovery of superconductivity of many other materials even at higher critical temperatures T_c The search for superconductive materials has since been promoted during hundred years to the present days (see Figures 1.3, 1.4, 1.5 and Table 1.1).

Material	T_c [K]	Discovery	References
Hg	4.154	26.10.1911	[Rob76]
Pb	7.196	31.05.1913	[Rob76; Onn14]
Nb	9.25	08.07.1930	[Rob76; MF30]
NbN	13	01.01.1941	[BK07; HS68]
V_3Si	17.1	30.12.1952	[BK07; Rob76; Col53; HH54]

Continued on next page

Material	T_c [K]	Discovery	References
Nb_3Sn	18.05	10.06.1954	[BK07; Rob76; Mat+54]
NbTi	9.8	19.04.1961	[Rob76; HB61]
$SrTiO_3$	0.28	06.03.1964	[SHC64]
AlGeNb	20	05.05.1967	[Mat+67]
$La_{2-x}Ba_xCuO_4$	30	17.04.1968	[BM86]
Nb_3Ge	23.2	12.07.1973	[BK07; Gav73]
$CeCu_2Si_2$	1.5	10.08.1979	[BK07; Ste+79]
Ube_{13}	0.85	14.03.1983	[BK07; Ott+83]
UPt_3	1.5	24.10.1983	[BK07; Ste+84]
$YBa_2Cu_3O_7$	93	06.02.1987	[BK07; Rob76; Wu+87]
$Ba_{1-x}K_xBiO_3$	35	30.10.1987	[BK07; MGJ88]
$BiSrCaCu_2O_x$	105	22.01.1988	[Mae+88]
$Tl_2Ba_2CaCu_3O_8$	119	09.02.1988	[Rob76; SH88]
$Tl_2Ba_2Ca_2Cu_3O_{10}$	128	22.02.1988	[Rob76; Haz+88]
K_3C_{60}	18	26.03.1991	[Heb+91]
$RbCsC_{60}$	33	25.06.1991	[Tan+91]
UPd_2Al_3	2	01.12.1991	[BK07; Gei+91]
$HgBa_2CaCu_3O_8$	133	14.04.1993	[BK07; Rob76; Sch+93]
$HgBa_2CaCu_3O_8$(150kbar)	153	18.08.1993	[Chu+93]
YPd_2B_2C	23	04.03.1994	[BK07; Fuj+94]
HgTlBaCaCuO	138	18.06.1994	[Sun+94]
Cs_3C_{60}(15kbar)	40	04.10.1994	[Pal+95]
$CeCoIn_5$	2.3	29.03.2000	[Pet+01]
MgB_2	39	01.01.2001	[BK07]
Li(500kbar)	20	11.06.2002	[BK07; LD86; Shi+02]
$PuCoGa_5$	18.5	02.09.2002	[Sar+02]
$PuRhGa_5$	18.2	12.11.2002	[Was+03]
Diamond	4	19.04.2004	[Eki+04]
CaC_6	11.5	18.03.2005	[Wel+05]
YbC_6	6.5	18.03.2005	[Wel+05]
LaOFeP	4	15.05.2006	[Kam+06]

Continued on next page

Material	T_c [K]	Discovery	References
$LaO_{1-x}F_xFeAs$	26	23.02.2008	[Kam+08]
SmFeAsO	55	16.04.2008	[Ren+08]

Table 1.1: Table of selected superconductors

It was discovered, that not only metals exhibit superconductivity but also intermetallic compounds such as Nb_3Sn ($T_c = 18\,K$) or metal oxides such as TiO ($T_c = 1\,K$). However, not long after the discovery of the superconductivity, it was observed that starting at a critical current density superconductivity brakes down. This was related to the discovery of the Meissner-Ochsenfeld effect in 1933, named after Walther Meissner and Robert Ochsenfeld. External applied magnetic fields are expelled completely from the inside, as long as they don't exceed a critical magnetic field H_c. Stronger magnetic fields destroy the effect of superconductivity. At this time all the materials studied exhibited values for H_c fainting the prospects of implementing superconductivity in technical purposes such as the generation of large magnetic fields. In 1936, Schubnikow et al. [Shu+08] found the appearance of a new type of superconductivity. There exist materials for which an external magnetic field, starting at a certain value H_{c1} but not exceeding another critical value H_{c2}, penetrates the conductor without breaking its superconductivity. Below H_{c1}, the material shows the Meissner-Ochsenfeld effect and above H_{c2} the superconductivity breaks down, while in between the magnetic field lowers the critical temperature (see Figure 1.6 (b)). The current understanding of this range is that the magnetic field penetrates the superconductor in form of non-superconducting tubes of magnetic flux, passing through the material, surrounded by a circulating supercurrent. As the external magnetic field increases more and more of these vortices enter, until at H_{c2}, they fill the whole conductor and prevent superconductivity.

Such materials are nowadays referred to as *tpye-II superconductors*. Although it took until 1961 for most of the physicists to recognize this discovery (in principle type-II superconductors already showed up in the Ginzburg-Landau theory from 1950), this kind of superconductors allowed much higher magnetic fields and are therefore in use in many technical applications today.

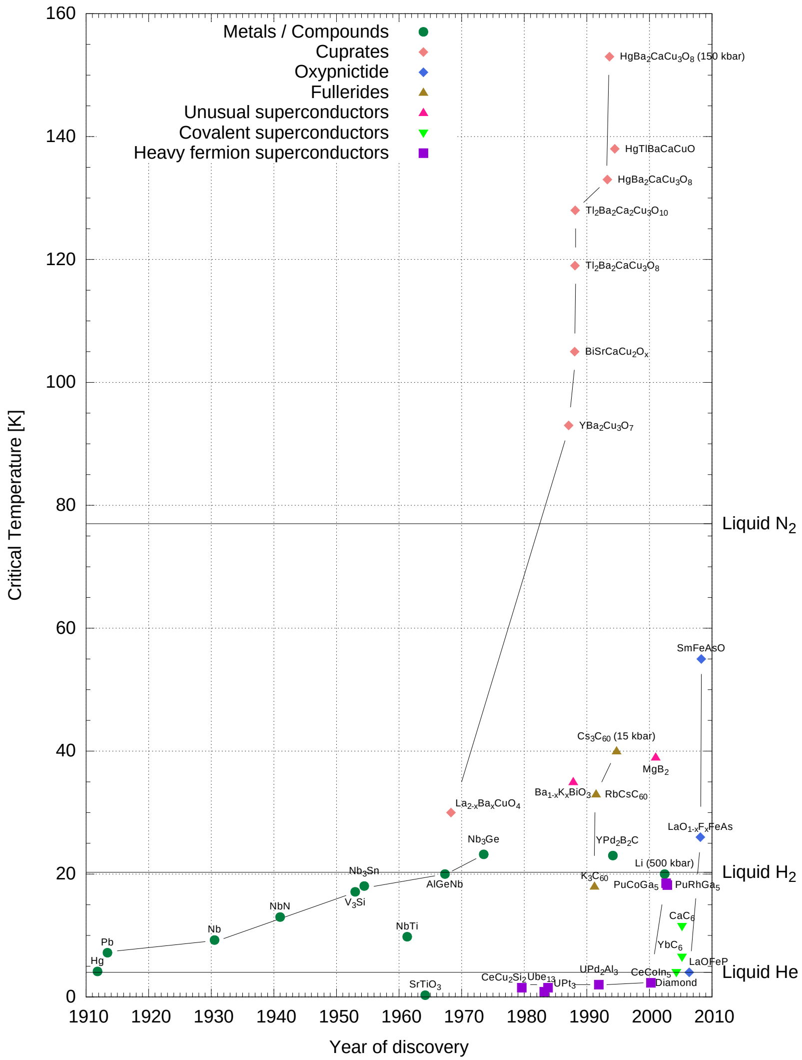

Figure 1.4: Critical temperature plotted against discovery dates of some selected superconductors. See Table 1.1 for the underlying references.

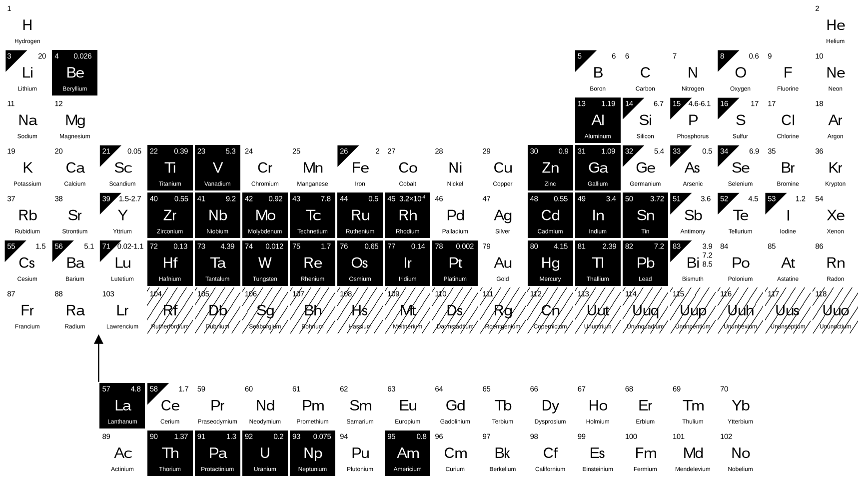

Figure 1.5: Periodic table of the elements with period number and critical temperature [K]. Black: Superconducting element, Black top left corner: Superconducting element under pressure, White: Non-superconducting, Hatched: Not yet studied. Values taken from [BK07].

Discovery of High Temperature Superconductivity In 1975, Arthur W. Sleight at DuPont found [SGB75] that the ceramic compound $BaPb_{1-x}Bi_xO_3$ became superconducting below $T_c = 13\,K$. This and other works in the field of solid state physics lead Johannes Georg Bednorz und Karl Alexander Müller at the IBM Zurich Research Laboratory to start experiments with perovskite structures in 1983. In 1986 they measured a critical temperature $T_c = 35\,K$ for the substance $Ba_xLa_{5-x}Cu_5O_{5(3-y)}$. More precisely, they found an abrupt decrease by up to three orders of magnitude starting at 35 K (so called T_c onset) and reaching zero resistance at 13 K. Bednorz and Müller received the Nobel Price in Physics already one year later. Currently, the superconductor with the highest transition temperature is mercury barium calcium copper oxide with a substitution of Tl for Hg ($Tl_{0.2}Hg_{0.8}Ba_2Ca_2Cu_3O_8$) at around 138 K [Sun+94].

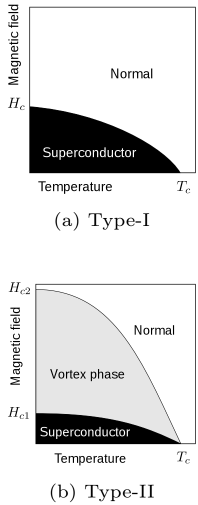

Figure 1.6: Temperature versus magnetic field phase diagram of a type-I and type-II superconductor

Developement of the Underying Theory In the mean time, theorists developed the first explanations for superconductivity. The first phenomenological theory was developed by the London brothers Fritz and Heinz in 1935. By means of a set of two equations, they succeeded in explaining the Meissner-Ochsenfeld effect. In 1950, Ginzburg and Landau put up their theory [GL50] to explain the macroscopic properties of superconductors. They took a Schrödinger-like equation as a basis and could distinguish between the two types of superconductors. Finally, in 1957 Bardeen, Cooper and Schrieffer [BCS57] proposed the first microscopic theory for superconductivity. Later, it could be extended to the context of superfluidity [Leg80; NSR85] and in 1959, Lev Gor'kov [Gor59] (formally) demonstrated the connection to the Ginzburg-Landau theory. Close to the critical temperature, the BCS theory reduces to the Ginzburg-Landau theory. The remarkable finding was, that it concerned a relationship between a macroscopic and a microscopic theory.

1.2 Applications

Creation of Strong Magnetic Fields Strong magnetic fields are very important in today's world. Even physicist are impressed by it's capabilities (see Figure 1.7).

Figure 1.7: A live frog levitates inside a 32 mm diameter vertical bore of a Bitter solenoid in a magnetic field of about 16 T at the Nijmegen High Field Magnet Laboratory. The frog, as many other animals, consists mainly of water which as a diamagnetic substance repels a magnetic field. Permission granted for this photo to be licensed under the GNU-type license by Lijnis Nelemans, High Field Magnet Laboratory, Radboud University Nijmegen.

Superconducting coils can generate very strong magnetic fields while they don't dissipate any energy aside from the power consumed by the refrigeration equipment to cool down the coil below the critical temperature. In 2007, a collaboration between the National High Magnetic Field Laboratory in Tallahassee, Florida and industry partner SuperPower Inc. built a magnet with windings of the high temperature superconductor YBCO and achieved a world record critical field of 26.8 T [Mag]. Though it is possible to construct resistive electromagnets (normal conductors) reaching even higher field strengths, such magnets consume huge amounts of power and require cooling water circulating through pipes. In 2010 the National High Magnetic Field Laboratory established a new record for the world's strongest resistive magnet. The system had a maximum field strength of 36.2 T and consisted of hundreds of separate so called "Bitter plates". It consumes 19.6 MW of electric power [Flu]. Therefore, in practical applications superconducting magnets are preferred. At the Large Hadron Collider, CERN (Geneva, Switzerland) NbTi superconductors are used as magnets (see Figure 1.8) to hold the particles on the ring [EB08]. They are cooled down below 2 K using superfluid helium and operate at fields above 8 T.

However, the largest consumer of superconducting materials is high-field magnetic resonance imaging (MRI) [HS11]. There also NbTi is most widely used. Another material frequently used for magnets is Nb_3Sn. It

Figure 1.8: Views of the LHC tunnel sector 3-4. by Maximilien Brice from `http://cds.cern.ch/record/1211045`, licensed under Creative Commons Attribution-ShareAlike 4.0 license: `http://creativecommons.org/licenses/by-sa/4.0/`

can withstand higher magnetic fields than NbTi but is also more expensive.

Measurement of Extremely Weak Magnetic Fields Superconductors are as well in use for precision measurements. A SQUID (for superconducting quantum interference device, see Figure 1.9) utilizes the fact, that in a superconducting ring placed in a magnetic field, the enclosed magnetic flux is quantized and has to be an integer multiple of the magnetic flux quantum $\Phi_0 = \frac{h}{2e} \approx 2.067833758(46) \times 10^{-15}$ Vs. This is caused by a circular current through the ring, whose contribution to the total magnetic flux exactly compensates the deviation of the flux of the magnetic field to the next integer multiple of Φ_0. This way, by changing the external electric field, the current changes its direction every time the flux is increased by a half of the magnetic flux quantum Φ_0. Inserting two Josephson junctions (insulating barrier or a short section of non-superconducting metal) into the superconducting ring, it is possible to exploit the so called Josephson effect, to measure the circular current and thus also the flux of the external magnetic field. A SQUID is sensitive enough to measure field changes as low as $5 \cdot 10^{-18}$ T [Ran04, p. 26] and is used in medicine for measuring ion current caused waves in the brain (magnetoencephalography).

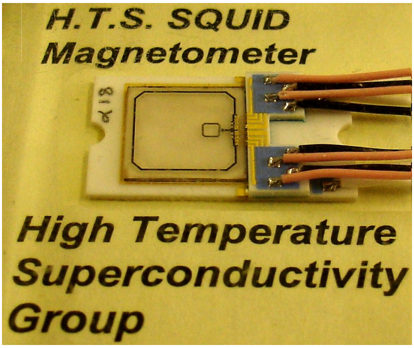

Figure 1.9: A SQUID by Zureks (Own work) [CC-BY-SA-3.0 (http://creativecommons.org/licenses/by-sa/3.0) or GFDL (http://www.gnu.org/copyleft/fdl.html)], via Wikimedia Commons http://commons.wikimedia.org/wiki/File%3ASQUID_by_Zureks, source: http://upload.wikimedia.org/wikipedia/commons/9/98/SQUID_by_Zureks

Chapter 2

Physical Background: The BCS Theory

In this chapter, the BCS theory is recapitulated, which was introduced in 1957 by Bardeen, Cooper, and Shrieffer [BCS57] to describe superconductivity. It is a microscopic description of fermionic gases with local pair interactions at low temperatures. It acts on the assumption that the physical environment and/or the inter particle forces create an effective pair interaction between the fermions. The pairing mechanism is realized by a two body interaction potential V. Given such a potential V, the BCS theory provides an expression for thermodynamic grand potential for the fermionic gas, depending besides the temperature T and the chemical potential μ on the interaction potential V, the momentum distribution γ and the Cooper pair wave function α. The BCS theory was later extended to the context of superfluidity [Leg80; NSR85] and connections to the theory of Bose-Einstein condensates (BEC) [Leg80; NSR85; PS03] where established. Thus, the theory covers the whole spectrum of the so called BCS-BEC crossover [Ran96], where the system smoothly changes from a superfluid state of delocalized Cooper pairs for weak interactions to a BEC of bosonic-like diatomic molecules for strong interactions. For both the regime, where the attraction is weak as well as the regime, where the attraction is strong, the BCS theory could be linked to an older theory, limited only to the particular regime. In the case of the former, this concerns the Ginzburg-Landau theory and in the case of the latter, the Gross-Pitaevskii equation. Both theories could be derived from the BCS theory by Gor'kov [Gor59], and Leggett, Noziéres and Schmitt-Rink [Leg80; NSR85] respectively - at least formally. Mathematical rigorous derivations were given in [Fra+08] and [HS12; HS13] respectively.

In the following sections we will deduce the BCS theory from quantum physics in two steps. First, by restricting the allowed states of the system to quasi-free states and second by assuming translation invariance and $SU(2)$ rotation invariance. We start with an brief overview of quantum mechanics.

2.1 Quantum Mechanics

Physical States The states of a quantum mechanical system Σ (for example a finite number of atomic nuclei and electrons in a region $\Lambda \subseteq \mathbb{R}^3$) are given by *unit rays* $[\psi] = \{z\psi | z \in \mathbb{C}, |z| = 1\}$ for $\|\psi\| = 1$ in a Hilbert space $\mathcal{H}_\Sigma$. Depending on the system Σ one wants to describe, the Hilbert space has to be chosen appropriately. In the following we will refer to a state as a representative of $[\psi]$. We denote by $\langle \cdot, \cdot \rangle$ the scalar product in the Hilbert space and as usual by $\|\psi\| = \sqrt{\langle \psi, \psi \rangle}$ the norm of $\mathcal{H}_\Sigma$. For the scalar product, we use the convention, where $\langle \cdot, \cdot \rangle$ is anti-linear in the first argument and linear in the second argument.

Physical Observables Physical observables are realized by self-adjoint linear operators $A : \mathcal{H}_\Sigma \to \mathcal{H}_\Sigma$. The set of possible values for measurements of the observable is then given by the spectrum $\sigma(A)$ of the operator A. Let $a \in \sigma(A)$ be the result of a measurement of the observable corresponding to A in the state $\psi \in \mathcal{H}_\Sigma$. If $A = \int_{\sigma(A)} \lambda \mathrm{d}E_\lambda$ is the spectral decomposition of A, then

$$P(a \in S) = \langle \psi, \int_S \mathrm{d}E_\lambda \psi \rangle$$

is the probability that the value a lies in the set $S \subseteq \sigma(A)$. The expectation value of the result is therefore given by

$$E(a) = \langle \psi, A\psi \rangle.$$

Mixed States in Statistical Mechanics Since we will be interested in solid state physics where we have to deal with a huge number of particles it is hopeless to keep the view of the exact state of the whole system. Instead we will change to a statistical description of the system, namely to the framework of statistical mechanics. There the concept of a state (pure state) is generalized to mixed states, i.e. a statistical ensemble of several pure quantum states. A *mixed state* on the Hilbert space $\mathcal{H}_\Sigma$ is defined as a *density matrix*[1], that is a positive trace class operator ρ, with $\operatorname{tr}(\rho) = 1$. The expectation value of a measurement of the observable A in the state ρ in this case is

$$\langle A \rangle_\rho := \operatorname{tr}(\rho A)$$

and pure states $\psi \in \mathcal{H}_\Sigma$ correspond to $\rho = P_\psi := \psi\langle\psi, \cdot\,\rangle$. Using the spectral decomposition of ρ,

$$\rho = \sum_{k=1}^{\infty} w_k P_{\psi_k}$$

with $w_1 \geq w_2 \geq \ldots \geq 0$, $\sum_{k=1}^{\infty} w_k = 1$ and pairwise orthogonal ψ_k, we see, that each density matrix is a convex combination of pure states P_{ψ_k}.

Fock Space In statistical mechanics, there are situations where the particle number changes. Even more radical, the constraint of a fixed particle number is dropped. As a consequence, mathematics simplifies in some situations. Therefore, for the Hilbert space $\mathcal{H}_\Sigma$ we choose a special one, providing the structure to deal with more than just one particle. It is based on an abstract Hilbert space $\mathcal{H}$ describing the states of a single fermion. The corresponding Hilbert space describing a system consisting of n identical fermions is constructed by $\mathcal{H}^{(n)} = \bigwedge^n \mathcal{H}$. A *simple vector* in $\mathcal{H}^{(n)}$ is of the form

$$\psi_1 \wedge \cdots \wedge \psi_n := \sum_{\sigma \in S_n} (-1)^\sigma \psi_{\sigma(1)} \otimes \cdots \otimes \psi_{\sigma(n)}, \qquad \text{for } \psi_i \in \mathcal{H},$$

where S_n denotes the set of all permutations of n elements, i.e. the symmetric group, where $(-1)^\sigma$ is the sign of a permutation σ and $\otimes$ is the tensor product. An arbitrary vector in $\mathcal{H}^{(n)}$ then is a (possibly infinite) linear combination of simple vectors.

[1] In [BLS94] a mixed state is a linear map $\rho : \mathcal{L}(\mathcal{H}_\Sigma) \to \mathbb{C}$, with the properties

$$\rho(\mathbb{1}) = 1, \qquad \rho(A^* A) \geq 0.$$

Here $\mathcal{L}(\mathcal{H}_\Sigma)$ denotes the set of all linear operators on $\mathcal{H}_\Sigma$ and A^* the adjoint of A.
However, the assignment $\rho_P(A) := \operatorname{tr}(PA)$ yields a one to one correspondence between density matrices P and linear mappings ρ_P.

However, the n-particle space $\mathcal{H}^{(n)}$ still can't describe systems consisting of a changing or undetermined number of fermions. Therefore, we introduce the so called Fock space

$$\mathcal{F}_{\mathcal{H}} := \bigoplus_{n=0}^{\infty} \mathcal{H}^{(n)},$$

where $\mathcal{H}^{(0)} := \mathbb{C}\Omega$ and Ω is the vacuum state with $\langle \Omega, \Omega \rangle := 1$. Note that $\mathcal{F}_{\mathcal{H}}$ is a Hilbert space on its own with the natural scalar product induced by the vector space sum. In particular sectors of different particle numbers are orthogonal to each other. To any vector $\phi \in \mathcal{H}$ in the one-particle Hilbert space, we associate a creation operator $a^\dagger(\phi) : \mathcal{F}_{\mathcal{H}} \to \mathcal{F}_{\mathcal{H}}$ and an annihilation operator $a(\phi) : \mathcal{F}_{\mathcal{H}} \to \mathcal{F}_{\mathcal{H}}$. We define the creation operator $a^\dagger(\psi)$ for a vector $\psi = (\psi^{(0)}, \psi^{(1)}, ...) \in \mathcal{F}_{\mathcal{H}}$, $\psi^{(n)} \in \mathcal{H}^{(n)}$ by

$$\big(a^\dagger(\phi)\psi\big)^{(n+1)} := (n+1)^{-1/2} \phi \wedge \psi^{(n)},$$

where $\phi \wedge \Omega = \phi$. The annihilation operator $a(\psi)$ is defined to be the adjoint operator of $a^\dagger(\psi)$ and acts as follows: If $\psi^{(n)} = \psi_1 \wedge \cdots \wedge \psi_n$ is the part in the n-particle space $\mathcal{H}^{(n)}$ of ψ, then

$$\big(a(\phi)\psi\big)^{(n-1)} = \sqrt{n} \sum_{i=1}^{n} (-1)^{i-1} \langle \phi, \psi_i \rangle \psi_1 \wedge \cdots \wedge \widehat{\psi_i} \wedge \cdots \wedge \psi_n,$$

where the hat indicates that ψ_i is omitted in the wedge product. Note that $a(\phi)|_{\mathcal{H}^{(0)}} \equiv 0$. By this construction, the creation and annihilation operators fulfill the canonical anti-commutation relations

$$\{a(\phi), a^\dagger(\psi)\} = \langle \phi, \psi \rangle \mathbb{1}_{\mathcal{F}_{\mathcal{H}}}$$
$$\{a(\phi), a(\psi)\} = \{a^\dagger(\phi), a^\dagger(\psi)\} = 0,$$

where $\{A, B\} = AB + BA$ is the anti-commutator.

Bogoliubov Transformations A *Bogoliubov transformation* of $\mathcal{F}_{\mathcal{H}}$ is a unitary operator $W : \mathcal{F}_{\mathcal{H}} \to \mathcal{F}_{\mathcal{H}}$ such that there exists linear operators $v, w : \mathcal{H} \to \mathcal{H}$ of such that for $\psi \in \mathcal{H}$, we have

$$W a^\dagger(\psi) W^* = a^\dagger(v\psi) + a(\overline{w\psi}),$$

where $\overline{\psi}(x) = \overline{\psi(x)}$ is the complex conjugation[2]. As a unitary operator, W leaves invariant the canonical anticommutation relations, i.e. $Wa^\dagger(\psi)W^*$ and $Wa(\psi)W^*$ satisfy the canonical anticommutation relations. This in turn is equivalent to

$$U := \begin{pmatrix} v & \overline{w} \\ w & \overline{v} \end{pmatrix} : \mathcal{H} \oplus \mathcal{H} \to \mathcal{H} \oplus \mathcal{H}$$

being unitary, where $\overline{T}\psi := \overline{T\overline{\psi}}$ for an arbitrary operator $T : \mathcal{H} \to \mathcal{H}$.

Quasi-free States Since it is still very difficult to describe the system with pure quantum statistics, in the BCS theory only so called quasi-free states are considered. The idea behind comes from thermodynamics. There one is interested in equilibrium states, i.e. states which remain invariant under time evolution. In quantum statistics such states are called Gibbs states and are of the form $\rho = Z^{-1}\exp(-\beta H)$, where H is a Hamiltonian on the Fock space and $Z = \operatorname{tr}\big(\exp(-\beta H)\big) < \infty$. As it turns out, Gibbs states are a special case of quasi-free states. A mixed state ρ is a *quasi-free state* if the following "Wick's Theorem" holds.

$$\langle a_1^\# a_2^\# \cdots a_{2n}^\# \rangle_\rho = \sum_{\sigma \in S_n'} (-1)^\sigma \langle a_{\sigma(1)}^\# a_{\sigma(2)}^\# \rangle_\rho \cdots \langle a_{\sigma(2n-1)}^\# a_{\sigma(2n)}^\# \rangle_\rho$$
$$\langle a_1^\# a_2^\# \cdots a_{2n+1}^\# \rangle_\rho = 0,$$

where each $\#$ can stand for $\dagger$ or nothing and where S_n' is the subset of S_n containing the permutations σ which satisfy $\sigma(1) < \sigma(3) < \ldots < \sigma(2n-1)$ and $\sigma(2j-1) < \sigma(2j)$ for all $1 \leq j \leq n$.

One-particle Density Matrices To each quasi-free state we associate a self-adjoint operator $\Gamma : \mathcal{H} \oplus \mathcal{H} \to \mathcal{H} \oplus \mathcal{H}$, called the *one-particle density*

[2] We could have chosen a different antiunitary map $C : \mathcal{H} \to \mathcal{H}$. instead of the complex conjugation. In this case the linear map w also has to be adjusted. This dependence on the antiunitary map comes from the antilinearity of the annihilation operator. If we would define the annihilation operator to accept as its argument an element of $\mathcal{H}^*$ instead of $\mathcal{H}$ (i.e. if we replace a by $\widetilde{a}$, where $\widetilde{a}(J\psi) = a(\psi)$ with $J : \mathcal{H} \to \mathcal{H}^*$ being the conjugate linear map such that $(J\psi)(\phi) = \langle \psi, \phi \rangle$) then the antilinearity would be naturally absorbed in J This is basically the approach of [Sol].

matrix of ρ defined by

$$\langle(\phi_1,\phi_2),\Gamma(\psi_1,\psi_2)\rangle = \rho\big([a^\dagger(\psi_1)+a(\overline{\psi_2})][a(\phi_1)+a^\dagger(\overline{\phi_2})]\big). \tag{2.1.1}$$

Again, this definition depends on the choice of the antiunitary map C which we here specified to be the ordinary complex conjugation.

The operator Γ for fermions has an important property. Namely,

$$0 \le \Gamma \le 1$$

as an operator. This is seen as follows. Let $(\phi,\psi)\in\mathcal{H}\oplus\mathcal{H}$ with $\|\phi\|^2+\|\psi\|^2=1$. Then

$$\langle(\phi,\psi),\Gamma(\phi,\psi)\rangle = \rho\big([a(\phi)+a^\dagger(\overline{\psi})]^*[a(\phi)+a^\dagger(\overline{\psi})]\big)\ge 0.$$

Moreover, by using the anti-commutation rules for a and $a^\dagger$, we obtain

$$[a(\phi)+a^\dagger(\overline{\psi})]^*[a(\phi)+a^\dagger(\overline{\psi})] = \|\phi\|^2+\|\psi\|^2-[a(\overline{\phi})+a^\dagger(\psi)][a(\overline{\phi})+a^\dagger(\psi)]^*$$

and we conclude

$$\langle(\phi,\psi),\Gamma(\phi,\psi)\rangle \le 1.$$

2.2 Derivation of the BCS Functional

We start with a quantum mechanical system Σ consisting of an indefinite number of spin $\frac{1}{2}$ fermions in a cubic box $\Lambda\subset\mathbb{R}^3$ of side length L, with periodic boundary conditions. The interaction between the fermions is defined by a two-body potential $V\in L^1(\Lambda)$. Moreover, the system shall be exposed to external electric and magnetic fields, $W(x)$ and $B(x)=\operatorname{curl}A(x)$. We then aim to take the limit $\Lambda\to\mathbb{R}^3$ and to find the state minimizing the grand potential Φ_G. In the following we will specify the Hilbert space for the system Σ under consideration and define the physical observable corresponding to the grand potential.

Hilbert Space We consider the Hilbert space $\mathcal{H}_\Sigma=\mathcal{F}_\mathcal{H}$, where the underlying one-particle Hilbert space consists of vector valued wave functions and is given by

$$\mathcal{H}=L^2_{\mathrm{per}}(\Lambda)\oplus L^2_{\mathrm{per}}(\Lambda)\cong L^2_{\mathrm{per}}(\Lambda)\otimes\mathbb{C}^2,$$

where we choose an orthonormal basis $\{e_\uparrow, e_\downarrow\}$ for $\mathbb{C}^2$.

Vectors in $\mathcal{H}^{(n)}$ are totally antisymmetric wave functions

$$\psi(z_1, \dots, z_n),$$

where $z_i = (x_i, \sigma_i) \in \Lambda \times \mathbb{C}^2$ denotes a space-spin variable for one particle.

Observables The grand potential of thermodynamics is given by $\Phi_G = \mathcal{U} - T\mathcal{S} - \mu\mathcal{N}$, where $\mathcal{U}$ is the internal energy, T is the temperature, $\mathcal{S}$ is the entropy, μ is the chemical potential and $\mathcal{N}$ is the particle number. The quantities T and μ are scalars and can be interpreted as Lagrange multiplicators, i.e. if we minimize Φ_G, we actually minimize $\mathcal{U}$ under the constraint that $\mathcal{S}$ and $\mathcal{N}$ are constant. We are interested in a quantum statistical description for Φ_G. Thus, we have to define quantum mechanical expressions for for $\mathcal{U}$, $\mathcal{S}$ and $\mathcal{N}$. The internal energy $\mathcal{U}$ corresponds to the energy observable, i.e. the (densely defined) Hamiltonian which is given by

$$H = T + U_V + U_W,$$

$$T|_{\mathcal{H}^{(n)}} = \sum_{j=1}^{n} \big(-i\nabla_{x_j} + A(x_j)\big)^2,$$

$$U_V|_{\mathcal{H}^{(n)}} = \frac{1}{2} \sum_{\substack{j,k=1 \\ j\neq k}}^{n} V(x_j - x_k),$$

$$U_W|_{\mathcal{H}^{(n)}} = \sum_{j=1}^{n} W(x_j),$$

The quantum mechanical counterpart to $\mathcal{N}$ is the particle number operator N, defined by $N|_{\mathcal{H}^{(n)}} = n\mathbb{1}$. Finally, we describe $\mathcal{S}$ by the *von-Neumann entropy* of a state ρ, which is given by

$$S(\rho) = -\operatorname{tr}\big(\rho \ln(\rho)\big).$$

The quantum mechanical grand potential of a state ρ then is

$$\Phi_G(\rho) = \langle H\rangle_\rho - TS(\rho) - \mu\langle N\rangle_\rho.$$

2.2.1 Step 1: Restriction to Quasi-free States

As a first simplification, we restrict the grand potential Φ_G to quasi-free states (see the corresponding paragraph in Section 2.1). $\Phi_G(\rho)$ then reduces to expressions in the operators $\gamma, \alpha : \mathcal{H} \to \mathcal{H}$, defined by

$$\begin{aligned} \langle \phi, \gamma\psi \rangle &= \langle a^\dagger(\psi) a(\phi) \rangle_\rho \\ \langle \phi, \alpha\psi \rangle &= \langle a(\bar{\psi}) a(\phi) \rangle_\rho. \end{aligned} \tag{2.2.1}$$

This is easy to see for a so called 1-*body operator* like T, U_W, and N, i.e. an operator $A : \mathcal{F}_\mathcal{H} \to \mathcal{F}_\mathcal{H}$ of the form

$$A|_{\mathcal{H}^{(n)}} = \sum_{j=1}^{n} \left(\bigotimes_{k=1}^{j-1} \mathbb{1} \right) \otimes A^{(1)} \otimes \left(\bigotimes_{k=j+1}^{n} \mathbb{1} \right),$$

for some operator $A^{(1)} : \mathcal{H} \to \mathcal{H}$. Let $\{\varphi_j\}_{j\in\mathbb{N}}$ be an orthonormal basis of $\mathcal{H}$. Then such operators can be expressed in terms of the creation and annihilation operators $a^\dagger(\varphi_j)$ and $a(\varphi_j)$ according to

$$A = \sum_{j,k\in\mathbb{N}} \langle \varphi_j, A^{(1)} \varphi_k \rangle a^\dagger(\varphi_j) a(\varphi_k).$$

Consequently, expectation values are given by

$$\langle A \rangle_\rho = \langle \varphi_j, A^{(1)} \varphi_k \rangle \langle \varphi_k \gamma \varphi_j \rangle = \mathrm{tr}_\mathcal{H}(A^{(1)}\gamma).$$

An analogous procedure can be given for 2-*body operators*, like U_V. By means of Wick's Theorem, which for quartic monomials in the creation and annihilation operators, reduces to

$$\langle a_1^\# a_2^\# a_3^\# a_4^\# \rangle_\rho = \langle a_1^\# a_2^\# \rangle_\rho \langle a_3^\# a_4^\# \rangle_\rho - \langle a_1^\# a_3^\# \rangle_\rho \langle a_2^\# a_4^\# \rangle_\rho + \langle a_1^\# a_4^\# \rangle_\rho \langle a_2^\# a_3^\# \rangle_\rho,$$

a similar computation using

$$U_V = \sum_{j,k,l,m\in\mathbb{N}} \langle \varphi_j \otimes \varphi_k, V(x-y) \varphi_l \otimes \varphi_m \rangle a^\dagger(\varphi_j) a^\dagger(\varphi_k) a(\varphi_m) a(\varphi_l)$$

shows

$$
\begin{aligned}
\langle U_V \rangle_\rho = \frac{1}{2} \sum_{\sigma,\tau\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} |\alpha(x,\sigma,y,\tau)|^2 V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
- \frac{1}{2} \sum_{\sigma,\tau\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} |\gamma(x,\sigma,y,\tau)|^2 V(y-x)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
+ \frac{1}{2} \sum_{\sigma,\tau\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} \gamma(x,\sigma,x,\sigma)\gamma(y,\tau,y,\tau) V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y,
\end{aligned}
$$

where $\gamma(x,\sigma,y,\tau)$ and $\alpha(x,\sigma,y,\tau)$ are the integral kernels of γ and α respectively.

Another calculation (see Appendix 2.A) shows that in terms of Γ, the entropy functional $S(\rho)$ can be expressed as

$$
S(\Gamma) = -\operatorname{tr}_{\mathcal{H}\oplus\mathcal{H}}\big(\Gamma\ln(\Gamma)\big).
$$

Thus we obtain for the grand potential the functional

$$
\begin{aligned}
\Phi_G(\Gamma) = \operatorname{tr}_{\mathcal{H}}\big(((-i\nabla + A)^2 + \mu + W)\gamma\big) - TS(\Gamma) \\
+ \frac{1}{2} \sum_{\sigma,\tau\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} |\alpha(x,\sigma,y,\tau)|^2 V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
- \frac{1}{2} \sum_{\sigma,\tau\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} |\gamma(x,\sigma,y,\tau)|^2 V(y-x)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
+ \frac{1}{2} \sum_{\sigma,\tau\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} \gamma(x,\sigma,x,\sigma)\gamma(y,\tau,y,\tau) V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y.
\end{aligned}
\tag{2.2.2}
$$

We define the BCS functional as the formal infinite volume limit

$$
\mathcal{F}_{\mathrm{BCS}}(\Gamma) := \lim_{\Lambda\to\mathbb{R}^3} \Phi_G(\Gamma), \tag{2.2.3}
$$

i.e. we replace Λ by $\mathbb{R}^3$ in the expression for $\Phi_G(\Gamma)$.

The BCS theory studies the minimizers of $\mathcal{F}_{\mathrm{BCS}}$. The term $\operatorname{tr}_{\mathcal{H}}\big((-i\nabla + A)^2\gamma\big)$ corresponds to the kinetic energy and S is the entropy. The term involving the Cooper pair wave function α is the pairing energy of the Cooper pairs. If this pairing energy lowers the BCS energy, i.e. if the minimizer of $\mathcal{F}_{\mathrm{BCS}}$ has a non-vanishing α, then we say that the system exhibits a Cooper pair condensate and has a *superfluid* or *superconducting phase*. If the minimizer Γ_0 of $\mathcal{F}_{\mathrm{BCS}}$ has $\alpha \equiv 0$, the system is said to be in a *normal state*. The last two summands of (2.2.2) are referred to as direct and exchange term, respectively. They correspond to density-density interactions between the fermions and are in general difficult to handle. Therefore they are being neglected usually.

The reason behind the interpretation of α as the Cooper pair wave function is that the system displays macroscopically coherent behavior as soon as $\alpha \neq 0$. To see that, we examine the correlation function of a pair at x and a pair at y, formally given by $\langle a^\dagger_{x,\uparrow} a^\dagger_{x,\downarrow} a_{y,\downarrow} a_{y,\uparrow} \rangle_\rho$. We will see later, that for $SU(2)$ invariant states ρ, the operators γ and α satisfy

$$\begin{aligned}\gamma(x,\sigma,y,\tau) &= \delta_{\sigma\tau}\widetilde{\gamma}(x,y),\\ \alpha(x,\sigma,y,\tau) &= (1-\delta_{\sigma\tau})\widetilde{\alpha}(x,y),\end{aligned}$$

for some reduced operators $\widetilde{\gamma}$ and $\widetilde{\alpha}$. In this case, $\langle a^\dagger_{x,\uparrow} a^\dagger_{x,\downarrow} a_{y,\downarrow} a_{y,\uparrow} \rangle_\rho = |\widetilde{\gamma}(x,y)|^2 + \overline{\widetilde{\alpha}(x,x)}\widetilde{\alpha}(y,y)$. If in addition the system is translation invariant, i.e. $\widetilde{\gamma}(x,y) = \widetilde{\gamma}(x+\delta,y+\delta)$ and $\widetilde{\gamma}(x,y) = \widetilde{\gamma}(x+\delta,y+\delta)$, the expression for the correlation reduces to

$$|\widetilde{\alpha}(0,0)|^2 + |\widetilde{\gamma}(x-y,0)|^2.$$

For far apart x and y, $|\widetilde{\gamma}(x-y,0)|^2$ converges to 0 whereas $|\widetilde{\alpha}(0,0)|^2$ stays constant. Therefore the pairs stay correlated over large distances, which is referred to as *long range order*.

2.2.2 Step 2: Assuming $SU(2)$ Invariance

We denote vectors $\psi \in \mathcal{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \cong L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ by

$$\psi = (\psi_\uparrow, \psi_\downarrow).$$

For example, if $\phi \in L^2(\mathbb{R}^3)$ then the state $\psi = \phi \otimes e_\uparrow \in \mathcal{H}$ is given by $\psi = (\phi, 0)$. In other words, we think of ψ as an element of $L^2(\mathbb{R}^3, \mathbb{C}^2)$

such that $\psi(x) \in \mathbb{C}^2$. Rotating the spin space is described by a matrix $S \in SU(2)$ which acts on $\mathcal{H}$ according to

$$(S\psi)(x) = S\psi(x).$$

On the fock space $\mathcal{F}_{\mathcal{H}}$ the action of $S \in SU(2)$ is given by the Bogoliubov transformation $W_S \in \mathcal{L}(\mathcal{F}_{\mathcal{H}})$, which transforms the creation and annihilation operators according to

$$\begin{aligned} W_S a^\dagger(\psi) W_S^* &= a^\dagger(S\psi) \\ W_S a(\psi) W_S^* &= a(S\psi). \end{aligned}$$

A state ρ is said to be invariant under spin rotations or shortly $SU(2)$ invariant if

$$\langle W_S A W_S^* \rangle_\rho = \langle A \rangle_\rho. \tag{2.2.4}$$

In the following, we will restrict $\mathcal{F}_{\mathrm{BCS}}$ to $SU(2)$ invariant states. The reason behind this approximation is that we know that a pure state $\psi \in \mathcal{H}$, minimizing some Hamiltonian H which is $SU(2)$ invariant, i.e. $[H, W_S] = 0$ has to be $SU(2)$ invariant itself, i.e. $W_S\psi = \psi$. In our case, H is in fact $SU(2)$ invariant but Φ_G also contains the non-linear entropy functional S. Therefore it is apriori not clear if the minimizer(s) of Φ_G are $SU(2)$ invariant and the restriction is an approximation.

For quasi-free states the condition to be $SU(2)$ invariant, translates to a transformation law for the operators α, γ via (2.2.1), i.e.

$$\begin{aligned} \gamma &\mapsto S^*\gamma S \\ \alpha &\mapsto S^*\alpha \overline{S}. \end{aligned}$$

If a matrix $M \in \mathbb{C}^{2\times 2}$ has the property $S^*MS = M$ for all $S \in SU(2)$, then M must be a multiple of $\mathbb{1}$. Analogously if $S^*M\bar{S} = M$, then $M = \lambda\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$.

Therefore, for a quasi-free $SU(2)$ invariant state the operators γ, α must have the form

$$\begin{aligned} \gamma &= \widetilde{\gamma} \otimes \mathbb{1} \\ \alpha &= \widetilde{\alpha} \otimes \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right), \end{aligned}$$

for corresponding, reduced operators $\widetilde{\gamma}, \widetilde{\alpha} : L(\mathbb{R}^3) \to L(\mathbb{R}^3)$ satisfying

$$\widetilde{\gamma}^* = \widetilde{\gamma}, \qquad \widetilde{\alpha}^T = \widetilde{\alpha}.$$

We will now show, that the BCS functional $\mathcal{F}_{\mathrm{BCS}}$ for $SU(2)$ invariant states only depends on the reduced one-particle density matrix

$$\widetilde{\Gamma} = \begin{pmatrix} \widetilde{\gamma} & \widetilde{\alpha} \\ \widetilde{\alpha}^* & 1 - \overline{\widetilde{\gamma}} \end{pmatrix}.$$

To see this, we use the notation $(\phi \otimes v, \psi \otimes v) = (\phi, \psi) \otimes v$, such that we have the relations

$$\begin{aligned} \Gamma[(\phi, \psi) \otimes v_1] &= [\widetilde{\Gamma}(\phi, \psi)] \otimes v_1 \\ \Gamma[(\phi, \psi) \otimes v_2] &= [\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right) \widetilde{\Gamma}(\phi, \psi) \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)] \otimes v_2, \end{aligned}$$

where $v_1 = \frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 1 \\ i \end{smallmatrix}\right)$ and $v_2 = \frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 1 \\ -i \end{smallmatrix}\right)$ are the eigenvectors of $\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$. We conclude that $0 \leq \widetilde{\Gamma} \leq 1$ as an operator and

$$S(\Gamma) = \operatorname{tr}_{\mathcal{H} \oplus \mathcal{H}} \big(\Gamma \ln(\Gamma)\big) = 2 \operatorname{tr}_{L^2(\mathbb{R}^3)} \big(\widetilde{\Gamma} \ln(\widetilde{\Gamma})\big) =: 2 \widetilde{S}(\widetilde{\Gamma}).$$

Therefore, the grand potential becomes

$$\begin{aligned} \widetilde{\Phi_G}(\widetilde{\Gamma}) := \frac{1}{2} \Phi_G(\Gamma) &= \operatorname{tr}_{L^2(\mathbb{R}^3)} \big(((-i\nabla + A)^2 + \mu + W)\widetilde{\gamma}\big) - T \widetilde{S}(\widetilde{\Gamma}) \\ &+ \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} |\widetilde{\alpha}(x, y)|^2 V(x - y) \, \mathrm{d}^3 x \, \mathrm{d}^3 y \\ &- \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} |\widetilde{\gamma}(x, y)|^2 V(y - x) \, \mathrm{d}^3 x \, \mathrm{d}^3 y \\ &+ \int_{\mathbb{R}^3 \times \mathbb{R}^3} \widetilde{\gamma}(x, x) \widetilde{\gamma}(y, y) V(x - y) \, \mathrm{d}^3 x \, \mathrm{d}^3 y, \end{aligned} \tag{2.2.5}$$

The functional

$$\mathcal{F}_{\mathrm{BCS}}(\widetilde{\Gamma}) = \widetilde{\Phi_G}(\widetilde{\Gamma})$$

is the starting point in many papers [BHS14b; HS13; Fra+08] (usually again discarding the last two summands, i.e. the direct and the exchange term).

2.2.3 Step 3: Assuming Translation Invariance

We start with the $SU(2)$ invariant functional $\mathcal{F}_{\rm BCS}(\widetilde{\Gamma})$ from above with finite volume Λ, i.e. we don't yet perform the formal limit $\Lambda \to \infty$. We will work with the reduced quantities $\widetilde{\Gamma}$, $\widetilde{\alpha}$, $\widetilde{\gamma}$, and $\widetilde{S}$ but we will drop the "$\widetilde{\ }$". For the same reason for which we have restricted to $SU(2)$ invariant states we will make another approximation.

The translation of a state $\psi \in L^2(\mathbb{R}^3)$ is given by

$$(T_\delta \psi)(x) = \psi(x+\delta).$$

On the Fock space $\mathcal{F}_{L^2(\mathbb{R}^3)}$, this translates to a Bogoliubov transformation defined by $W_\delta a^{\#}(\psi) W_\delta^* = a^{\#}(T_\delta \psi)$. Translation invariant states ρ are again characterized by

$$\langle W_\delta A W_\delta^* \rangle_\rho = \langle A \rangle_\rho.$$

Again, $[H, W_\delta] = 0$, which motivates the restriction to translation invariant states. For quasi-free states the one-particle density matrix Γ obtains the property

$$\Gamma(x,y) = \Gamma(x-\delta, y-\delta) \Leftrightarrow \Gamma(x,y) = \widetilde{\Gamma}(x-y) = \begin{pmatrix} \widetilde{\gamma}(x-y) & \widetilde{\alpha}(x-y) \\ \overline{\widetilde{\alpha}(y-x)} & 1 - \overline{\widetilde{\gamma}(x-y)} \end{pmatrix}.$$

Like in the case of the $SU(2)$ invariance, the BCS functional $\mathcal{F}_{\rm BCS}$ only depends on the reduced one-particle density matrix $\widetilde{\Gamma}(x-y)$: On the orthonormal basis $\psi_k(x) = \frac{\mathrm{e}^{ikx}}{\sqrt{|\Lambda|}}$ the operators γ, α are diagonal, namely

$$\gamma \psi_k = \widehat{\gamma}(k) \psi_k, \qquad \alpha \psi_k = \widehat{\alpha}(k) \psi_k,$$

$$\widehat{\gamma}(k) = \int_\Lambda \widetilde{\gamma}(x) \mathrm{e}^{-ikx}\, \mathrm{d}^3 x, \qquad \widehat{\alpha}(k) = \int_\Lambda \widetilde{\alpha}(x) \mathrm{e}^{-ikx}\, \mathrm{d}^3 x.$$

Therefore the entropy S becomes

$$S(\Gamma) = - \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \mathrm{tr}_{\mathbb{C}^2} \left(\widehat{\Gamma}(k) \ln(\widehat{\Gamma}(k)) \right),$$

for

$$\widehat{\Gamma}(p) = \begin{pmatrix} \widehat{\gamma}(p) & \widehat{\alpha}(p) \\ \overline{\widehat{\alpha}(p)} & 1 - \widehat{\gamma}(-p) \end{pmatrix}, \qquad 0 \leq \widehat{\Gamma}(p) \leq 1.$$

The grand potential per volume (without external electromagnetic field) now reads

$$\frac{1}{2|\Lambda|}\Phi_G(\Gamma) = \frac{1}{|\Lambda|}\sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3}(p^2+\mu)\widehat{\gamma}(p) + T\frac{1}{|\Lambda|}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3}\mathrm{tr}_{\mathbb{C}^2}\left(\widehat{\Gamma}(k)\ln(\widehat{\Gamma}(k))\right)$$
$$+\frac{1}{2}\int_\Lambda |\widetilde{\alpha}(r)|^2 V(r)\,\mathrm{d}^3 r$$
$$-\frac{1}{2}\int_\Lambda |\widetilde{\gamma}(r)|^2 V(r)\,\mathrm{d}^3 r + [\widetilde{\gamma}(0)]^2\int_\Lambda V(r)\,\mathrm{d}^3 r.$$

Taking the limit $\Lambda \to \mathbb{R}^3$ and defining $\alpha := (2\pi)^{3/2}\widetilde{\alpha}, \gamma := (2\pi)^{3/2}\widetilde{\gamma}$ to have the convention

$$\widehat{f}(p) = (2\pi)^{-3/2}\int_{\mathbb{R}^3} f(x)\mathrm{e}^{-ipx}\,\mathrm{d}^3 x,$$

we obtain

$$\begin{aligned}\mathcal{F}_{\mathrm{BCS}}(\Gamma) &:= \lim_{\Lambda\to\mathbb{R}^3}\frac{(2\pi)^3}{2|\Lambda|}\Phi_G(\Gamma)\\ &= \int_{\mathbb{R}^3}(p^2+\mu)\widehat{\gamma}(p)\,\mathrm{d}^3 p + T\int_{\mathbb{R}^3}\mathrm{tr}_{\mathbb{C}^2}\left(\widehat{\Gamma}(p)\ln(\widehat{\Gamma}(p))\right)\mathrm{d}^3 p\\ &+\frac{1}{2}\int_{\mathbb{R}^3}|\alpha(r)|^2 V(r)\,\mathrm{d}^3 r\\ &-\frac{1}{2}\int_{\mathbb{R}^3}|\gamma(r)|^2 V(r)\,\mathrm{d}^3 r + [\gamma(0)]^2\int_{\mathbb{R}^3} V(r)\,\mathrm{d}^3 r.\end{aligned} \tag{2.2.6}$$

Again the first term comes from the kinetic energy. The second term

$$\int_{\mathbb{R}^3}\mathrm{tr}_{\mathbb{C}^2}\left(\widehat{\Gamma}(p)\ln(\widehat{\Gamma}(p))\right)\mathrm{d}^3 p$$

is the negative entropy, which is minimal for $\alpha \equiv 0$. It therefore competes the pairing energy of the Cooper pairs, $\frac{1}{2}\int_{\mathbb{R}^3}|\alpha(r)|^2 V(r)\,\mathrm{d}^3 r$, which can lower $\mathcal{F}_{\mathrm{BCS}}$ if $\alpha \neq 0$. Therefore, if T is lowered, possibly the effect of pairing energy may exceed the one of the entropy. In this case, the system undergoes a phase transition. Like in the previous functionals, the last two summands, i.e. the direct and the exchange term, respectively are being neglected usually.

2.3 The Simplified Translation Invariant BCS Functional

In this section, we study the translation invariant and $SU(2)$ invariant BCS functional. For simplicity, we also drop the direct and the exchange term. In [BHS14c] we attempt to extend the following results, including these terms. An overview over the results obtained is given in Section 3.1

The first investigation concerns the existence of a minimizer of the BCS functional

$$\begin{aligned}\mathcal{F}_T(\Gamma) &= \int_{\mathbb{R}^3} (p^2+\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p - TS(\Gamma) + \frac{1}{2}\int_{\mathbb{R}^3} |\alpha(r)|^2 V(r)\,\mathrm{d}^3r,\\ S(\Gamma) &= -\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left(\Gamma(p)\ln(\Gamma(p))\right)\mathrm{d}^3p.\end{aligned} \tag{2.3.1}$$

Proposition 2.1 (Existence of minimizers). *Let $\mu \in \mathbb{R}$, $0 \le T < \infty$, and let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ be real-valued. Then $\mathcal{F}_T$ is bounded from below and attains a minimizer Γ on*

$$\mathcal{D} = \left\{ \Gamma(p) = \begin{pmatrix} \widehat{\gamma}(p) & \widehat{\alpha}(p) \\ \overline{\widehat{\alpha}(p)} & 1-\widehat{\gamma}(-p) \end{pmatrix} \;\middle|\; \substack{\widehat{\gamma}\in L^1\left(\mathbb{R}^3,(1+p^2)\,\mathrm{d}^3p\right),\\ \alpha\in H^1(\mathbb{R}^3,\,\mathrm{d}^3x),} \quad 0 \le \Gamma \le \mathbb{1}_{\mathbb{C}^2} \right\}.$$

Proof (taken from [Hai+08]). We first show that $\mathcal{F}_T$ dominates both the $L^1(\mathbb{R}^3, (1+p^2)\,\mathrm{d}^3p)$ norm of $\widehat{\gamma}$ and the $H^1(\mathbb{R}^3, \mathrm{d}^3x)$ norm of α. Hence any minimizing sequence will be bounded in these norms. We have

$$\mathcal{F}_T(\Gamma) \ge C_1 + \frac{3}{4}\int_{\mathbb{R}^3} (p^2-\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p + \frac{1}{2}\int_{\mathbb{R}^3} |\alpha(x)|^2 V(x)\,\mathrm{d}^3x\,,$$

where

$$C_1 = \inf_{\Gamma\in\mathcal{D}}\left[\frac{1}{4}\int_{\mathbb{R}^3}(p^2-\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p - TS(\Gamma)\right] = -T\int_{\mathbb{R}^3} \ln(1+e^{-\frac{p^2-\mu}{4T}})\,\mathrm{d}^3p\,.$$

Since $V \in L^{3/2}$ by assumption, it is relatively bounded with respect to $-\Delta$ (in the sense of quadratic forms), and hence $C_2 = \inf\mathrm{spec}\,(p^2/4+V)$ is finite. Using $|\widehat{\alpha}(p)|^2 \le \widehat{\gamma}(p)$, we thus have that

$$\frac{1}{4}\int_{\mathbb{R}^3} p^2\widehat{\gamma}(p)\,\mathrm{d}^3p + \frac{1}{2}\int_{\mathbb{R}^3} V(x)|\alpha(x)|^2\,\mathrm{d}^3x \ge C_2\int_{\mathbb{R}^3}\widehat{\gamma}(p)\,\mathrm{d}^3p\,.$$

Using again that $|\widehat{\alpha}(p)|^2 \leq \widehat{\gamma}(p) \leq 1$, it follows that

$$\mathcal{F}_T(\Gamma) \geq -A + \frac{1}{8}\|\alpha\|^2_{H^1(\mathbb{R}^3,\,\mathrm{d}^3x)} + \frac{1}{8}\|\widehat{\gamma}\|_{L^1(\mathbb{R}^3,(1+p^2)\,\mathrm{d}^3p)}\,, \tag{2.3.2}$$

where

$$A = -C_1 - \int_{\mathbb{R}^3} \left[p^2/4 - 3\mu/4 - 1/4 + C_2\right]_- \,\mathrm{d}^3p\,,$$

with $[\,\cdot\,]_- = \min\{\,\cdot\,,0\}$ denoting the negative part.

To show that a minimizer of $\mathcal{F}_T$ exists in $\mathcal{D}$, we pick a minimizing sequence $\Gamma_n(p) = \begin{pmatrix} \widehat{\gamma_n}(p) & \widehat{\alpha_n}(p) \\ \overline{\widehat{\alpha_n}(p)} & 1-\widehat{\gamma_n}(-p) \end{pmatrix} \in \mathcal{D}$, with $\mathcal{F}_T(\Gamma_n) \leq 0$. From (2.3.2) we conclude that $\|\alpha_n\|^2_{H^1} \leq 8A$, and hence we can find a subsequence that converges weakly to some $\widetilde{\alpha} \in H^1$. Since $V \in L^{3/2}(\mathbb{R}^3)$, this implies that

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} V(x)|\alpha_n(x)|^2\,\mathrm{d}^3x = \int_{\mathbb{R}^3} V(x)|\widetilde{\alpha}(x)|^2\,\mathrm{d}^3x$$

[LL01, Thm. 11.4].

It remains to show that the remaining part of the functional,

$$\mathcal{F}_T^0(\Gamma) = \int_{\mathbb{R}^3} (p^2-\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p - TS(\Gamma)\,, \tag{2.3.3}$$

is weakly lower semicontinuous. Note that $\mathcal{F}_T^0$ is convex in Γ, and that its domain $\mathcal{D}$ is a convex set. We already know that $\alpha_n \rightharpoonup \widetilde{\alpha}$ weakly in $H^1(\mathbb{R}^3)$. Moreover, since $\widehat{\gamma}_n$ is uniformly bounded in $L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we can find a subsequence such that $\widehat{\gamma}_n \rightharpoonup \widetilde{\widehat{\gamma}}$ weakly in $L^p(\mathbb{R}^3)$ for some $1 < p < \infty$. We can then apply Mazur's theorem [LL01, Theorem 2.13] to construct a new sequence as convex combinations of the old one, which now converges *strongly* to $(\widetilde{\widehat{\gamma}}, \widetilde{\alpha})$ in $L^p(\mathbb{R}^3)\times L^2(\mathbb{R}^3)$. By going to a subsequence, we can also assume that $\Gamma_n \to \Gamma$ pointwise [LL01, Theorem 2.7]. Because of convexity of $\mathcal{F}_T^0$, this new sequence is again a minimizing sequence.

Note that the integrand in (2.3.3) is bounded from below independently of γ and α by $-T\ln(1+e^{-(p^2-\mu)/T})$. Since this function is integrable, we can apply Fatou's Lemma [LL01, Lemma 1.7], together with the pointwise convergence, to conclude that $\liminf \mathcal{F}_T^0(\Gamma_n) \geq \mathcal{F}_T^0(\widetilde{\Gamma})$.

We have thus shown that

$$\mathcal{F}_T(\widetilde{\Gamma}) \leq \liminf_{n\to\infty} \mathcal{F}_T(\Gamma_n)\,.$$

It is easy to see that $\widetilde{\Gamma} \in \mathcal{D}$, hence it is a minimizer. This proves the claim. □

Now that we know about the existence of a minimizer, we want to characterize it. We therefore have a look at the Euler-Lagrange equation.

Lemma 2.1 (Euler-Lagrange and gap equation)**.** *The Euler-Lagrange equations for a minimizer* $\Gamma(p) = \begin{pmatrix} \widehat{\gamma}(p) & \widehat{\alpha}(p) \\ \overline{\widehat{\alpha}(p)} & 1-\widehat{\gamma}(-p) \end{pmatrix} \in \mathcal{D}$ *of* $\mathcal{F}_T$ *are of the form*

$$\widehat{\gamma}(p) = \frac{1}{2} - \frac{p^2 - \mu}{2K^{\Delta}_{T,\mu}(p)} \tag{2.3.4a}$$

$$\widehat{\alpha}(p) = \frac{1}{2}\Delta(p)\frac{\tanh\left(\frac{E^{\Delta}_{\mu}(p)}{2T}\right)}{E^{\Delta}_{\mu}(p)}, \tag{2.3.4b}$$

where we use the abbreviations

$$\Delta = \widehat{V\alpha} \tag{2.3.5a}$$

$$K^{\Delta}_{T,\mu}(p) = \frac{E^{\Delta}_{\mu}(p)}{\tanh\left(\frac{E^{\Delta}_{\mu}(p)}{2T}\right)}, \tag{2.3.5b}$$

$$E^{\Delta}_{\mu}(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}\,, \tag{2.3.5c}$$

In particular, the function Δ *satisfies the BCS gap equation*

$$\frac{1}{2(2\pi)^{3/2}} \int_{\mathbb{R}^3} \widehat{V}(p-q)\frac{\Delta(q)}{K^{\Delta}_{T,\mu}(q)}\,\mathrm{d}^3q = -\Delta(p) \tag{2.3.6}$$

We note that the BCS gap equation (2.3.6) can equivalently be written as

$$(K^{\Delta}_{T,\mu} + V/2)\widehat{\alpha} = 0,$$

where $K^{\Delta}_{T,\mu}$ is interpreted as a multiplication operator in Fourier space, and V as multiplication operator in configuration space. This form of the equation will turn out to be useful later on.

Taken from [BHS14c]. We first restrict our attention to $T > 0$. A minimizer Γ of $\mathcal{F}_T$ fulfills the inequality

$$0 \leq \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathcal{F}_T\big(\Gamma + t(\widetilde{\Gamma} - \Gamma)\big) \tag{2.3.7}$$

for arbitrary $\widetilde{\Gamma} \in \mathcal{D}$. Here we may assume that Γ stays away from 0 and 1 by arguing as in [Hai+08, Proof of Lemma 1]. A simple calculation using

$$S(\Gamma) = -\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}(\Gamma \ln \Gamma)\,\mathrm{d}^3p = -\frac{1}{2}\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\big(\Gamma \ln(\Gamma) + (1-\Gamma)\ln(1-\Gamma)\big)\,\mathrm{d}^3p$$

shows that

$$\begin{aligned}&\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathcal{F}_T\big(\Gamma + t(\widetilde{\Gamma} - \Gamma)\big)\\ &\qquad = \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left[H_\Delta(\widetilde{\Gamma} - \Gamma) + T(\widetilde{\Gamma} - \Gamma)\ln\left(\frac{\Gamma}{1-\Gamma}\right)\right]\mathrm{d}^3p,\end{aligned}$$

with

$$H_\Delta = \begin{pmatrix} p^2 - \mu & \Delta \\ \bar{\Delta} & -(p^2 - \mu) \end{pmatrix},$$

using the definition $\Delta = \widehat{V\alpha}$. Separating the terms containing no $\widetilde{\Gamma}$ and moving them to the left side in (2.3.7), we obtain

$$\begin{aligned}&\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left(H_\Delta\big(\Gamma - \left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)\big) + T\,\Gamma\ln\left(\frac{\Gamma}{1-\Gamma}\right)\right)\mathrm{d}^3p\\ &\quad \leq \int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left(H_\Delta\big(\widetilde{\Gamma} - \left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)\big) + T\,\widetilde{\Gamma}\ln\left(\frac{\Gamma}{1-\Gamma}\right)\right)\mathrm{d}^3p.\end{aligned}$$

Note that $\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\big(H_\Delta\Gamma\big)\,\mathrm{d}^3p$ is not finite but $\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\Big(H_\Delta\big(\widetilde{\Gamma} - \left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)\big)\Big)\,\mathrm{d}^3p$ is. Since $\widetilde{\Gamma}$ was arbitrary, Γ also minimizes the linear functional

$$\widetilde{\Gamma} \mapsto \int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left(H_\Delta\big(\widetilde{\Gamma} - \left(\begin{smallmatrix}0&0\\0&1\end{smallmatrix}\right)\big) + T\,\widetilde{\Gamma}\ln\left(\frac{\Gamma}{1-\Gamma}\right)\right)\mathrm{d}^3p, \tag{2.3.8}$$

whose Euler-Lagrange equation is of the simple form

$$0 = H_\Delta + T\ln\left(\frac{\Gamma}{1-\Gamma}\right), \tag{2.3.9}$$

which is equivalent to

$$\Gamma = \frac{1}{1+\mathrm{e}^{\frac{1}{T}H_\Delta}}.$$

This in turn implies (2.3.4a) and (2.3.4b). Indeed,

$$\Gamma = \frac{1}{1+\mathrm{e}^{\frac{1}{T}H_\Delta}} = \frac{1}{2} - \frac{1}{2}\tanh\left(\tfrac{1}{2T}H_\Delta\right).$$

For the simple reason, that $\frac{\tanh(x)}{x} = g(x^2)$ is an even function and $H_\Delta^2 = [E_\mu^\Delta]^2\,\mathbb{1}_{\mathbb{C}^2}$, the expression simplifies to

$$\Gamma = \frac{1}{2} - \frac{1}{2}H_\Delta \frac{\tanh\left(\frac{E_\mu^\Delta}{2T}\right)}{E_\mu^\Delta} = \frac{1}{2} - \frac{1}{2K_{T,\mu}^\Delta}H_\Delta = \begin{pmatrix} \frac{1}{2} - \frac{p^2-\mu}{2K_{T,\mu}^\Delta} & -\frac{\Delta}{2K_{T,\mu}^\Delta} \\ -\frac{\bar{\Delta}}{2K_{T,\mu}^\Delta} & \frac{1}{2} + \frac{p^2-\mu}{2K_{T,\mu}^\Delta} \end{pmatrix}.$$

We now turn to $T = 0$. By inspecting (2.3.8), we note that there are no critical points in the interior of $\mathcal{D}$. We thus have to impose the additional (pointwise) condition $\Gamma(p) = 0$ or $\Gamma(p) = 1$ on Γ. This is equivalent to $\Gamma(1-\Gamma) = 0$ which holds if and only if $\operatorname{tr}_{\mathbb{C}^2}\big(\Gamma(1-\Gamma)\big) = 0$ and either $\widehat{\gamma}(p) = \widehat{\gamma}(-p)$ or $\widehat{\alpha}(p) = 0$. It will turn out, that already imposing the condition on the trace suffices to find a critical point which also has the symmetry $\widehat{\gamma}(p) = \widehat{\gamma}(-p)$ or $\widehat{\alpha}(p) = 0$. We thus minimize

$$\int_{\mathbb{R}^3} (p^2+\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p + \frac{1}{2}\int_{\mathbb{R}^3} |\alpha(r)|^2 V(r)\,\mathrm{d}^3r + \lambda\operatorname{tr}_{\mathbb{C}^2}\big(\Gamma(1-\Gamma)\big),$$

with the Lagrange multiplicator λ. Varying this functional with respect to Γ, yields for the critical point Γ

$$H_\Delta = \lambda(1-2\Gamma).$$

Using the constraint $\Gamma(1-\Gamma) = 0$, we obtain $\lambda = E_\mu^\Delta$ and solving for Γ yields

$$\Gamma = \frac{1}{2} - \frac{1}{2E_\mu^\Delta}H_\Delta.$$

Performing the convolution with $\widehat{V}$ on both sides of (2.3.4b) and using the relation $\Delta = (2\pi)^{-3/2}\widehat{V} * \widehat{\alpha}$ gives the BCS-gap equation (2.3.6). □

Clearly, the minimizer of the *non-interacting* case $V = 0$ which is given by

$$\Gamma_0(p) = \frac{1}{1 + \mathrm{e}^{\frac{1}{T}H_0(p)}} = \begin{pmatrix} \gamma_0(p) & 0 \\ 0 & 1 - \gamma_0(-p) \end{pmatrix}$$

solves the Euler-Lagrange equation, where

$$\gamma_0(p) = \frac{1}{1 + \mathrm{e}^{\frac{1}{T}(p^2-\mu)}}, \qquad H_0 = \begin{pmatrix} p^2 - \mu & 0 \\ 0 & -(p^2 - \mu) \end{pmatrix}.$$

We will refer to this state as the *normal state.* The key question, which will decide if the system is superfluid is whether the BCS functional has a minimum at the normal state or just a saddle point. In order to examine that we need the second variation of the BCS functional.

Lemma 2.2 (Second variation of the BCS functional)**.** *Let* $\Gamma = \begin{pmatrix} \widehat{\gamma} & \widehat{\alpha} \\ \overline{\widehat{\alpha}} & 1-\widehat{\gamma} \end{pmatrix}$ *be a critical point of* $\mathcal{F}_T$*, i.e.* Γ *satisfies the Euler-Lagrange equations* $\Gamma = \frac{1}{1+\mathrm{e}^{\frac{1}{T}H_\Delta}}$*. Let* $G = \begin{pmatrix} \rho & \varphi \\ \overline{\varphi} & -\rho \end{pmatrix}$*, for* φ *in the domain of* $K^\Delta_{T,\mu} + V/2$ *and*

$$\rho = \begin{cases} \frac{\alpha\overline{\varphi}+\overline{\alpha}\varphi}{1-2\widehat{\gamma}}, & \alpha(p) \neq 0 \\ 0, & \alpha(p) = 0. \end{cases}$$

Then

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0} \mathcal{F}_T\left(\Gamma + tG\right) = 2\langle\varphi, (K^\Delta_{T,\mu} + V/2)\varphi\rangle + 2\langle\rho, K^\Delta_{T,\mu}\rho\rangle. \qquad (2.3.10)$$

Proof. By taking the second derivative, only the entropy term and the α term survive. The second derivative of the latter is simply $\langle\varphi, V\varphi\rangle$. For the entropy term, we introduce $s(z) = \frac{1}{2}\big(z\ln(z) + (1-z)\ln(1-z)\big)$, such that

$$-S(\Gamma) = \int_{\mathbb{R}^3} \operatorname{tr}_{\mathbb{C}^2}\left(s(\Gamma)\right)\mathrm{d}^3p.$$

As an initial point, we take the first derivative of the integrand

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{tr}_{\mathbb{C}^2}\left(s(\Gamma + tG)\right) &= \operatorname{tr}_{\mathbb{C}^2}\left(s'(\Gamma + tG)G\right) \\ &= \frac{1}{2\pi i}\operatorname{tr}_{\mathbb{C}^2}\left[\int_C s'(z)\frac{1}{z - (\Gamma + tG)}G\,\mathrm{d}z\right],\end{aligned}$$

where C is a closed curve enclosing the interval $(0,1)$. We have to differentiate this expression a second time at $t=0$. The definition of ρ is constructed, such that Γ and G satisfy the anti-commutation relation $\{\Gamma, G\} = G$. Therefore,

$$\left\{G, \frac{1}{z-\Gamma}\right\} = \frac{1}{z-\Gamma}\{G, z-\Gamma\}\frac{1}{z-\Gamma} = (2z-1)\frac{1}{z-\Gamma}G\frac{1}{z-\Gamma}$$
$$= (2z-1)\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\frac{1}{z-(\Gamma+tG)}$$

and we obtain

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0}\operatorname{tr}_{\mathbb{C}^2}\big(s'(\Gamma+tG)G\big) = \frac{1}{2\pi i}\operatorname{tr}_{\mathbb{C}^2}\left[\int_C \frac{s'(z)}{2z-1}\left\{\frac{1}{z-\Gamma}, G\right\}G\,\mathrm{d}z\right].$$

We use the cyclicity of the trace to conclude that

$$\frac{1}{2}\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0}\operatorname{tr}_{\mathbb{C}^2}\big(s(\Gamma+tG)\big) = \frac{1}{2\pi i}\operatorname{tr}_{\mathbb{C}^2}\left[\int_C \frac{s'(z)}{2z-1}\frac{1}{z-\Gamma}G^2\,\mathrm{d}z\right]$$
$$= \operatorname{tr}_{\mathbb{C}^2}\left[\frac{s'(\Gamma)}{2\Gamma-1}G^2\right].$$

Now note that

$$\left.\frac{s'(z)}{2z-1}\right|_{z=\frac{1}{1+e^x}} = \frac{1}{2}\frac{x}{\tanh(x)}$$

and that $\Gamma = \frac{1}{1+\mathrm{e}^{\frac{1}{T}H_0}}$. Therefore,

$$\frac{s'(\Gamma)}{2\Gamma-1} = \frac{K^{\Delta}_{T,\mu}}{2T},$$

which implies

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0}\operatorname{tr}_{\mathbb{C}^2}\big(s(\Gamma+tG)\big) = \frac{K^{\Delta}_{T,\mu}}{T}\operatorname{tr}_{\mathbb{C}^2}(G^2).$$

Inserted into the expression for $\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0} - TS(\Gamma+tG)$, this finishes the proof. □

This observation together with the Euler-Lagrange and gap equation may be combined in the following theorem

Theorem 2.1. *Let $V \in L^{3/2}(\mathbb{R}^3)$, $\mu \in \mathbb{R}$, and $0 \leq T < \infty$. Then the following statements are equivalent:*

(i) The normal state Γ_0 is unstable under pair formation, i.e.,

$$\inf_{\Gamma \in \mathcal{D}} \mathcal{F}_T(\Gamma) < \mathcal{F}_T(\Gamma_0).$$

(ii) There exists $\Gamma \in \mathcal{D}$, with $\alpha = 0$, such that $\Delta = \widehat{V\alpha}$ satisfies the BCS gap equation

$$\Delta = \frac{1}{2(2\pi)^{3/2}} \widehat{V} * \frac{\Delta}{K^{\Delta}_{T,\mu}}.$$

(iii) The linear operator

$$K^0_{T,\mu} + V/2, \qquad K^0_{T,\mu}(p) = \frac{\tanh(\frac{p^2-\mu}{T})}{p^2 - \mu},$$

has at least one negative eigenvalue.

Proof. **(i) ⇒ (ii)**: Assumption (i) together with the existence of a minimizer (Proposition 2.1) immediately implies the existence of a minimizer with $\alpha \neq 0$, which has to satisfy the Euler-Lagrange equation and thus also the gap equation.
(ii) ⇒ (iii): Let us observe now that

$$x \mapsto K^x_{T,\mu}(p)$$

is a monotone increasing function for all p. Therefore, as we can bring the gap equation into the form

$$(K^{\Delta}_{T,\mu} + V/2)\widehat{\alpha} = 0,$$

as soon as $\alpha \neq 0$,

$$\langle \alpha, (K^0_{T,\mu} + V/2)\alpha \rangle < 0,$$

because $K^{\Delta}_{T,\mu}(p) > K^{0}_{T,\mu}(p)$ for all p where $\Delta(p) \neq 0$, which is the same set where $\widehat{\alpha}(p) \neq 0$.
(iii) $\Rightarrow$ **(i)**: This is Lemma 2.2 applied to the normal state Γ_0 with

$$G = \begin{pmatrix} 0 & \varphi(p) \\ \overline{\varphi(p)} & 0 \end{pmatrix}.$$

We obtain

$$\left.\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right|_{t=0} \mathcal{F}_T\left(\Gamma_0 + tG\right) = 2\langle\varphi, (K^0_{T,\mu} + V/2)\varphi\rangle,$$

which implies that though the normal state is a critical point, it is not a minimizer. □

Theorem 2.1 enables a precise definition of the critical temperature, by

$$T_c(V) := \inf\{T | K^0_{T,\mu} + V/2 \geq 0\}. \tag{2.3.11}$$

Expressed differently, the critical temperature T_c is given by the value T, such that $K^0_{T_c,\mu} + V/2$ has 0 as lowest eigenvalue. The uniqueness of the critical temperature follows from the fact that the symbol $K^0_{T,\mu}(p)$ is point-wise monotone in T. This implies that for any potential V , there is a critical temperature $0 \leq T_c(V) < \infty$ that separates a superfluid phase for $0 \leq T \leq T_c(V)$ from a normal phase for $T_c(V) \leq T < \infty$. Note that $T_c(V) = 0$ means that there is no superfluid phase at all for V. Using the linear criterion (2.3.11) we can classify the potentials for which $T_c(V) > 0$, and simultaneously we can evaluate the asymptotic behavior of $T_c(V)$ in certain limits. For example, in [Fra+07; HS08] the *weak coupling limit* is studied, i.e. the asymptotic behaviour of $T_c(\lambda V)$ for small $\lambda > 0$. Another interesting case is the *low density limit*, considered in [HS12]. Here, the behaviour of $T_c(V)$ subject to $\mu \to 0$ is treated. Finally, in [BHS14c; BHS14a] the *short range limit* is examined, where basically the range $\ell = \mathrm{diam}(\mathrm{supp}(V))$ becomes small at a fixed scattering length a.

Appendix

2.A Expression for the Entropy for Quasi-free States

Throughout the calculations, we will use the following orthonormal basis for $\mathcal{F}_{\mathcal{H}}$. Given an orthonormal basis $\{\varphi_i\}_{i\in\mathbb{N}}$ of $\mathcal{H}$, we construct the orthonormal basis $\{\varphi_J\}_{\substack{J\subset\mathbb{N}\\ |J|<\infty}}$ of $\mathcal{F}_{\mathcal{H}}$ by

$$\varphi_J = \frac{1}{\sqrt{|J|!}} \bigwedge_{j\in J} \varphi_j, \tag{2.A.1}$$

where $|J|$ denotes the number of elements of the set J. We also introduce the projectors

$$P_{JK} := \langle \varphi_J, \cdot \rangle \varphi_K. \tag{2.A.2}$$

Lemma 2.3. *Let ρ be a quasi-free state with one-particle density matrix Γ. Then*

$$S(\rho) = -\operatorname{tr}_{\mathcal{F}_{\mathcal{H}}}\big(\rho\ln(\rho)\big) = -\operatorname{tr}_{\mathcal{H}\oplus\mathcal{H}}\big(\Gamma\ln(\Gamma)\big).$$

In the proof of this equation, the following characterization of quasi-free states is useful:

Lemma 2.4. *For each quasi-free state ρ there is an orthonormal basis $\{\varphi_i\}_{i\in\mathbb{N}}$ of $\mathcal{H}$ and a Bogoliubov transformation W, such that*

$$W^*\rho W = \frac{1}{\operatorname{tr}_{\mathcal{F}_{\mathcal{H}}}\big(P\exp(Q)\big)} P\exp(Q), \tag{2.A.3}$$

$$Q = \sum_{i\in I} q_i a^\dagger(\varphi_i) a(\varphi_i),$$

where the q_i satisfy

$$\frac{\mathrm{e}^{q_j}}{1-\mathrm{e}^{q_j}} = \langle a^\dagger(\varphi_j)a(\varphi_j)\rangle_{W^*\rho W},$$

$I = \{j \in \mathbb{N} | \langle a^\dagger(\varphi_j)a(\varphi_j)\rangle_{W^*\rho W} \neq 0\}$ *and where as above* $P = \sum_{J\subseteq I} P_{JJ}$ *is the projection onto* $\ker\big(\sum_{i\in\mathbb{N}\setminus I} a^\dagger(\varphi_i)a(\varphi_i)\big) \subset \mathcal{F}_\mathcal{H}$.

Proof. Following [BLS94, Proof of Theorem 2.3], we first find an orthonormal basis $\{\varphi_i\}_{i\in\mathbb{N}}$ of $\mathcal{H}$, such that the basis $(\varphi_i, 0)$, $(0, \varphi_i)$ diagonalizes the one-particle density matrix Γ of ρ. Note that $\operatorname{tr}\big(\Gamma(1-\Gamma)\big) < \infty$, because $\operatorname{tr}(\gamma)$ is finite. Hence, there is an orthonormal basis of eigenvectors of $\Gamma(1-\Gamma)$. If ψ is an eigenvector of $\Gamma(1-\Gamma)$ to the eigenvalue μ, then so is $\Gamma\psi$. Since $\Gamma^2\psi = \Gamma\psi - \mu\psi$, it follows, that Γ leaves invariant the subspace $\{\psi, \Gamma\psi\}$, which is at most 2-dimensional. We conclude, that there is an orthonormal basis of $\mathcal{H}\oplus\mathcal{H}$ of eigenvectors of Γ. If $\psi = (\phi_1, \phi_2)$ is an eigenvector of Γ with eigenvalue λ, then using the properties of Γ, we find that $\widetilde{\psi} = (\overline{\phi_2}, \overline{\phi_1})$ is an eigenvector of Γ with eigenvalue $(1-\lambda)$. Thus we can find a unitary transformation U of $\mathcal{H}\oplus\mathcal{H}$, such that

$$U^*\Gamma U(\varphi_i, 0) = \lambda_i(\varphi_i, 0)$$
$$U^*\Gamma U(0, \varphi_i) = (1-\lambda_i)(0, \varphi_i).$$

U corresponds to a Bogoliubov transformation W on $\mathcal{F}_\mathcal{H}$ (see [BLS94, Proof of Theorem 2.3]) and we end up with $U^*\Gamma U$ being the one-particle density matrix of $W^*\rho W$.

Next, we show that $\rho_Q = \frac{1}{\operatorname{tr}_{\mathcal{F}_\mathcal{H}}\big(P\exp(Q)\big)} P\exp(Q)$ equals $W^*\rho W$ for q_i chosen such that

$$\frac{\mathrm{e}^{q_j}}{1+\mathrm{e}^{q_j}} = \lambda_j$$

and $I = \{n \in \mathbb{N} | \lambda_n \neq 0\}$. In order to do that we show that

$$\langle \varphi_J, W^*\rho W\varphi_K\rangle = \langle \varphi_J, \rho_Q\varphi_K\rangle, \tag{2.A.4}$$

with respect to the orthonormal basis $\{\varphi_J\}_{\substack{J\subset\mathbb{N}\\|J|<\infty}}$ defined in (2.A.1). It is easy to compute the right hand side of (2.A.4). As a first step we find

$$\langle \varphi_J, P\exp(Q)\varphi_K\rangle = \begin{cases} \delta_{JK}\prod_{j\in J}\mathrm{e}^{q_j}, & \text{if } J\subseteq I \\ 0, & \text{else} \end{cases}$$

and consequently

$$\operatorname{tr}_{\mathcal{F}_{\mathcal{H}}}\big(P\exp(Q)\big) = \sum_{J\subseteq I}\prod_{j\in J} \mathrm{e}^{q_j} = \prod_{i\in I}(1+\mathrm{e}^{q_i}). \tag{2.A.5}$$

Combining the last two expressions, we end up with

$$\begin{aligned}\langle\varphi_J, \rho_Q\varphi_K\rangle &= \begin{cases}\delta_{JK}\prod_{j\in J}\frac{\mathrm{e}^{q_j}}{1+\mathrm{e}^{q_j}}\prod_{j\in I\setminus J}\frac{1}{1+\mathrm{e}^{q_j}}, & J\subseteq I\\ 0, & \text{else}\end{cases}\\ &= \delta_{JK}\prod_{j\in J}\lambda_j\prod_{j\in I\setminus J}(1-\lambda_j).\end{aligned} \tag{2.A.6}$$

To compute the matrix elements on the left hand side of (2.A.4), note that $\langle\varphi_J, W^*\rho W\varphi_K\rangle = \langle P_{JK}\rangle_{W^*\rho W}$, where $P_{JK} := \langle\varphi_J,\cdot\rangle\varphi_K$. We then express P_{JK} in terms of the creation and annihilation operators.

$$P_{JK} = \frac{\sqrt{|K|!}}{\sqrt{|J|!}}\left(\prod_{j\in J}a^\dagger(\varphi_j)\right)\left(\prod_{k\in K}a(\varphi_k)\right)\prod_{j\in\mathbb{N}\setminus K}(1-a^\dagger(\varphi_j)a(\varphi_j)).$$

This formal expression[3] allows us to apply Wick's theorem, defining quasi-

[3] The expression is the weak limit of the sequence of operators

$$P_{JK}^{(n)} = \frac{\sqrt{|K|!}}{\sqrt{|J|!}}\left(\prod_{j\in J}a^\dagger(\varphi_j)\right)\left(\prod_{k\in K}a(\varphi_k)\right)\prod_{j\in\{1,\dots,n\}\setminus K}(1-a^\dagger(\varphi_j)a(\varphi_j)).$$

For the following calculation, we want to argue that

$$\langle P_{JK}\rangle_{W^*\rho W} = \lim_{n\to\infty}\langle P_{JK}^{(n)}\rangle_{W^*\rho W}.$$

Indeed, this is possible by noting that the series elements $|\langle\varphi_L, W^*\rho W P_{JK}^{(n)}\varphi_L\rangle|$ are monotone decreasing because every additional factor $(1-a^\dagger(\varphi_j)a(\varphi_j))$ either leaves invariant the vector φ_L or maps it to 0. Thus monotone convergence applies.

free states

$$\begin{aligned}\langle P_{JK}\rangle_{W^*\rho W} &= \delta_{JK}\prod_{j\in J}\langle a^\dagger(\varphi_j)a(\varphi_j)\rangle_{W^*\rho W}\times\\ &\qquad\times\lim_{n\to\infty}\prod_{j\in I\cap(\{1,\dots,n\}\setminus J)}\langle 1-a^\dagger(\varphi_j)a(\varphi_j)\rangle_{W^*\rho W}\\ &= \delta_{JK}\prod_{j\in J}\lambda_i\prod_{j\in I\cap(\{1,\dots,n\}\setminus J)}(1-\lambda_i).\end{aligned}$$

Note that all matrix elements where $J\neq K$ vanish. This is the same expression as in (2.A.6), which proves the lemma. □

Proof of Lemma 2.3. By Lemma 2.4, we find a unitary transform U of $\mathcal{H}\oplus\mathcal{H}$ with corresponding Bogoliubov transform W, such that $U^*\Gamma U$ is the one-particle density function of

$$W^*\rho W=\rho_Q,$$

where ρ_Q is the expression on the right hand side of (2.A.3). We start with

$$-S(\rho)=\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(\rho\ln(\rho)\big)=\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(W^*\rho W\ln(W^*\rho W)\big)=\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(\rho_Q\ln(\rho_Q)\big).$$

Substituting the expression from (2.A.3), we obtain

$$\begin{aligned}-S(\rho)&=\frac{1}{\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(P\mathrm{e}^Q\big)}\,\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(P\mathrm{e}^Q\ln(P\mathrm{e}^Q)\big)-\ln\big(\mathrm{tr}_{\mathcal{F}_\mathcal{H}}(P\mathrm{e}^Q)\big)\\ &=\frac{1}{\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(P\mathrm{e}^Q\big)}\,\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\big(P\mathrm{e}^Q Q\big)-\ln\big(\mathrm{tr}_{\mathcal{F}_\mathcal{H}}(P\mathrm{e}^Q)\big).\end{aligned}\tag{2.A.7}$$

With respect to the orthonormal basis $\{\varphi_J\}_{\substack{J\subset\mathbb{N}\\|J|<\infty}}$ defined in (2.A.1), the factor $\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\left(P\mathrm{e}^{Q}Q\right)$ becomes

$$\begin{aligned}\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\left(P\mathrm{e}^{Q}Q\right) &= \sum_{J\subseteq I}\langle\varphi_J, \mathrm{e}^{Q}Q\varphi_J\rangle\\ &= \sum_{J\subseteq I}\left(\prod_{j\in J}\mathrm{e}^{q_j}\right)\sum_{i\in J}q_i\\ &= \sum_{i\in I}\sum_{J\subseteq I\setminus\{i\}}\left(\prod_{j\in J}\mathrm{e}^{q_j}\right)\mathrm{e}^{q_i}q_i\\ &= \sum_{i\in I}\left(\prod_{j\in I\setminus\{i\}}(1+\mathrm{e}^{q_j})\right)\mathrm{e}^{q_i}q_i.\end{aligned}$$

To see the step, where the two sums are interchanged, note that there is a bijective map between $\{(J,i)|J\subseteq I, i\in J\}$ and $\{(J,i)|i\in I, J\subseteq I\setminus\{i\}\}$ given by $(J,i)\mapsto(J\setminus\{i\},i)$. Comparing to (2.A.5), we see that

$$\mathrm{tr}_{\mathcal{F}_\mathcal{H}}\left(P\mathrm{e}^{Q}Q\right) = \mathrm{tr}_{\mathcal{F}_\mathcal{H}}(P\mathrm{e}^{Q})\sum_{i\in I}\frac{\mathrm{e}^{q_i}}{1+\mathrm{e}^{q_i}}q_i.$$

Inserting into (2.A.7) and again using (2.A.5) yields

$$\begin{aligned}-S(\rho) &= \sum_{i\in I}\frac{\mathrm{e}^{q_i}}{1+\mathrm{e}^{q_i}}q_i - \sum_{i\in I}\ln\left(1+\mathrm{e}^{q_i}\right)\\ &= \sum_{i\in I}\lambda_i\ln\left(\frac{\lambda_i}{1-\lambda_i}\right) + \sum_{i\in I}\ln(1-\lambda_i)\\ &= \sum_{i\in I}\lambda_i\ln(\lambda_i) + \sum_{i\in I}(1-\lambda_i)\ln(1-\lambda_i),\end{aligned}$$

where $\lambda_i = \langle a^\dagger(\varphi_j)a(\varphi_j)\rangle_{W^*\rho W} = \langle(\varphi_i,0), U^*\Gamma U(\varphi_i,0)\rangle$. That is

$$-S(\rho) = \mathrm{tr}_{\mathcal{H}\oplus\mathcal{H}}\left(U^*\Gamma U\ln(U^*\Gamma U)\right) = \mathrm{tr}_{\mathcal{H}\oplus\mathcal{H}}\left(\Gamma\ln(\Gamma)\right),$$

which finishes the proof. □

Chapter 3

Results

This chapter documents the results of the doctoral research. Its foundation is the theoretical framework explained in Chapter 2.

3.1 The Full Translation Invariant BCS Functional

We consider the translation invariant and $SU(2)$ invariant BCS functional

$$
\begin{aligned}
\mathcal{F}_T^V(\Gamma) = &\int_{\mathbb{R}^3} (p^2+\mu)\widehat{\gamma}(p)\,\mathrm{d}^3p + T\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left(\widehat{\Gamma}(p)\ln(\widehat{\Gamma}(p))\right)\mathrm{d}^3p \\
&+ \int_{\mathbb{R}^3} |\alpha(r)|^2 V(r)\,\mathrm{d}^3r \\
&- \int_{\mathbb{R}^3} |\gamma(r)|^2 V(r)\,\mathrm{d}^3r + 2[\gamma(0)]^2\int_{\mathbb{R}^3} V(r)\,\mathrm{d}^3r,
\end{aligned}
\tag{3.1.1}
$$

derived in Section 2.2.3, (2.2.6). Note that we replaced V by $2V$ to avoid the factors of $\frac{1}{2}$.

In the physics literature, usually the last two terms – referred to as the *direct term*, the *exchange term* respectively – are neglected. Section 2.3 gives a summary of the basic properties of the BCS functional if these terms are absent. A heuristic justification of this approximation was given for example in [Leg80; Leg08]. The author argues, that for suitably short ranged interactions, the direct and exchange terms only gives rise to a renormalization of the chemical potential.

It turns out, that this heuristic justification can be made rigorous which is the result of [BHS14c]. Some basic properties of the original functional can be carried over to the extended case taking into account the two terms.

However, the interaction potential V has to satisfy some requirements in order that the energy is bounded from below. In contrast to Proposition 2.1, we need $\|\widehat{V}\|_\infty \leq 2\widehat{V}(0)$ in addition.

Proposition 3.1 (Existence of minimizers [BHS14c]). *Let $\mu \in \mathbb{R}$, $0 \leq T < \infty$, and let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ be real-valued with $\|\widehat{V}\|_\infty \leq 2\widehat{V}(0)$. Then $\mathcal{F}_T^V$ is bounded from below and attains a minimizer (γ, α) on*

$$\mathcal{D} = \left\{ \Gamma = \begin{pmatrix} \widehat{\gamma} & \widehat{\alpha} \\ \overline{\widehat{\alpha}} & 1-\widehat{\gamma} \end{pmatrix} \;\middle|\; \begin{smallmatrix} \widehat{\gamma} \in L^1\left(\mathbb{R}^3, (1+p^2)\,\mathrm{d}^3p\right), \\ \alpha \in H^1(\mathbb{R}^3,\, \mathrm{d}^3x), \end{smallmatrix} \quad 0 \leq \Gamma \leq \mathbf{1}_{\mathbb{C}^2} \right\}.$$

Moreover, the function

$$\Delta(p) = \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q)\widehat{\alpha}(q)\,\mathrm{d}^3q \tag{3.1.2}$$

satisfies the BCS gap equation

$$\boxed{\frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \widehat{V}(p-q)\frac{\Delta(q)}{K_{T,\mu}^{\gamma,\Delta}(q)}\,\mathrm{d}^3q = -\Delta(p)} \tag{3.1.3}$$

A further observation is, that in all expressions involved, the chemical potential μ gets replaced by a renormalized version $\widetilde{\mu}^\gamma$, depending on the one-particle density γ. In the following, we denote, for general γ,

$$\varepsilon^\gamma(p) = p^2 - \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left(\hat{V}(p-q) - \hat{V}(0)\right)\hat{\gamma}(q)\,\mathrm{d}^3q\,, \tag{3.1.4}$$

$$\tilde{\mu}^\gamma = \mu - \frac{2}{(2\pi)^{3/2}}\widehat{V}(0) \int_{\mathbb{R}^3} \widehat{\gamma}(p)\,\mathrm{d}^3p\,, \tag{3.1.5}$$

$$K_{T,\mu}^{\gamma,\Delta}(p) = \frac{E_\mu^{\gamma,\Delta}(p)}{\tanh\left(\frac{E_\mu^{\gamma,\Delta}(p)}{2T}\right)}, \tag{3.1.6}$$

$$E_\mu^{\gamma,\Delta}(p) = \sqrt{(\varepsilon^\gamma(p) - \tilde{\mu}^\gamma)^2 + |\Delta(p)|^2}\,, \tag{3.1.7}$$

As a consequence, the important criterion to characterize the critical temperature T_c, Theorem 2.1 breaks down in general. Indeed, the operator $K_{T,\mu}^{\Delta}$ inherits the dependence on γ and it is no more clear, whether $K_{T,\mu}^{\gamma,\Delta}(p) \geq K_{T,\mu}^{\gamma_0,0}(p)$. This makes impossible the conclusion (ii) $\Rightarrow$ (iii) in

Theorem 2.1. The other two implications, (iii) $\Rightarrow$ (i) and (i) $\Rightarrow$ (ii) remain true [BHS14c, Theorem 1]. In order to state the result, we first have to define a normal state. A *normal state* Γ_0 is a minimizer of the functional (3.1.1) restricted to states with $\alpha = 0$. Any such minimizer can easily be shown to be of the form

$$\widehat{\gamma}_0(p) = \frac{1}{1 + \mathrm{e}^{\frac{\varepsilon^{\gamma_0}(p) - \tilde{\mu}^{\gamma_0}}{T}}}, \tag{3.1.8}$$

Theorem 3.1 (Existence of a superfluid phase)**.** *Let $\mu \in \mathbb{R}$, $0 \leq T < \infty$, and let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ be real-valued with $\|\widehat{V}\|_\infty \leq 2\widehat{V}(0)$. Let $\Gamma_0 = (\gamma_0, 0)$ be a normal state and recall the definition of $K_{T,\mu}^{\gamma_0,0}(p)$ in* (3.1.6)*–*(3.1.7)*.*

(i) If $\inf \operatorname{spec}(K_{T,\mu}^{\gamma_0,0} + V) < 0$*, then Γ_0 is unstable, i.e.,* $\inf_{\Gamma \in \mathcal{D}} \mathcal{F}_T^V(\Gamma) < \mathcal{F}_T^V(\Gamma_0)$*.*

(ii) If Γ_0 is unstable, then there exist $(\gamma, \alpha) \in \mathcal{D}$, with $\alpha \neq 0$, such that Δ defined in (3.1.2) *solves the BCS gap equation* (3.1.3)*.*

However, when restricting to interaction potentials V with short range, it is possible to recover the criterion and thus the definition of a critical temperature. More precisely, we consider a family $\{V_\ell\}_{\ell>0}$ of interaction potentials, where $\ell \ll 1$ measures the range via $\operatorname{supp} V_\ell \subseteq B_\ell(0)$. Moreover we fix the scattering length a in the sense that

$$\lim_{\ell \to 0} a(V_\ell) = a < 0.$$

Here, we use the expression of the scattering length of $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$

$$a(V) = \frac{1}{4\pi} \left\langle |V|^{1/2}, \frac{1}{1+V^{1/2}\frac{1}{p^2}|V|^{1/2}} V^{1/2} \right\rangle,$$

derived in [HS08]. Moreover we impose some additional technical assumptions on V_ℓ summarized all together in the following.

Assumption 3.1. (A1) $V_\ell \in L^1 \cap L^2$

(A2) the range of V_ℓ is at most ℓ, i.e., $\operatorname{supp} V_\ell \subseteq B_\ell(0)$

(A3) the scattering length $a(V_\ell)$ is negative and does not vanish as $\ell \to 0$, i.e., $\lim_{\ell\to 0} a(V_\ell) = a < 0$

(A4) $\limsup_{\ell\to 0} \|V_\ell\|_1 < \infty$

(A5) $\widehat{V_\ell}(0) > 0$ and $\lim_{\ell\to 0} \widehat{V_\ell}(0) = \mathcal{V} \geq 0$

(A6) $\|\widehat{V_\ell}\|_\infty \leq 2\widehat{V_\ell}(0)$

(A7) for small ℓ, $\|V_\ell\|_2 \leq C_1 \ell^{-N}$ for some $C_1 > 0$ and $N \in \mathbb{N}$

(A8) $\exists\, 0 < b < 1$ such that $\inf \operatorname{spec}(p^2 + V_\ell - |p|^b) > C_2 > -\infty$ holds independently of ℓ

(A9) the operator $1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}$ is invertible, and has an eigenvalue e_ℓ of order ℓ, with corresponding eigenvector ϕ_ℓ. Moreover,

$$(1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2})^{-1} (1 - P_\ell)$$

is uniformly bounded in ℓ, where $P_\ell = \langle J_\ell \phi_\ell | \phi_\ell \rangle^{-1} |\phi_\ell\rangle\langle J_\ell \phi_\ell|$ and $J_\ell = \operatorname{sgn}(V_\ell)$

(A10) the eigenvector ϕ_ℓ satisfies $|\langle \phi_\ell | \operatorname{sgn}(V_\ell) \phi_\ell \rangle|^{-1} \langle |V_\ell|^{1/2} | |\phi_\ell| \rangle \leq O(\ell^{1/2})$ for small ℓ.

An example for an admissible family of interaction potentials is given in [Alb+88], where it is used to approximate a contact potential. There, a reference potential $V \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ with a simple zero-energy resonance is scaled via

$$V_\ell(x) = \lambda(\ell) \ell^{-2} V(\tfrac{x}{\ell}), \qquad \lambda(0) = 1,\ \lambda(\ell) < 1 \text{ for } \ell > 0. \tag{3.1.9}$$

However, since $\lim_{\ell\to 0} \int_{\mathbb{R}^3} V_\ell \, \mathrm{d}^3 x = 0$, the resulting renormalized chemical potential in the limit $\ell \to 0$ is just the usual chemical potential. It needs a family V_ℓ with a repulsive core (see Figure 3.1), whose L^1 norm does not vanish in the limit $\ell \to 0$ to obtain a real renormalization.

In the limit $\ell \to 0$, it is possible to bridge the gap in the proof of the equivalence of the three criteria for the characterization of the critical temperature, mentioned above. As an important ingredient an effective gap equation, also appearing in the literature [Leg80] is derived [BHS14c, Theorem 2]

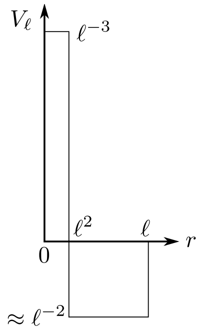

Figure 3.1: Radial run of a family V_ℓ of potentials resulting in a renormalized chemical potential $\widetilde{\mu} \neq \mu$ in the limit $\ell \to 0$.

Theorem 3.2 (Effective Gap equation)**.** *Let $T \geq 0$, $\mu \in \mathbb{R}$, and let $(\widehat{\gamma}_\ell, \widehat{\alpha}_\ell)$ be a minimizer of $\mathcal{F}_T^{V_\ell}$ with corresponding $\Delta_\ell = 2(2\pi)^{-3/2}\hat{V}_\ell * \hat{\alpha}_\ell$. Then there exist $\Delta \geq 0$ and $\hat{\gamma} : \mathbb{R}^3 \to \mathbb{R}_+$ such that $|\Delta_\ell(p)| \to \Delta$ pointwise, $\hat{\gamma}_\ell(p) \to \hat{\gamma}(p)$ pointwise and $\tilde{\mu}^{\gamma_\ell} \to \tilde{\mu}$ as $\ell \to 0$, satisfying*

$$\begin{aligned} \tilde{\mu} &= \mu - \frac{2\mathcal{V}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \widehat{\gamma}(p)\, \mathrm{d}^3p \\ \hat{\gamma}(p) &= \frac{1}{2} - \frac{p^2 - \tilde{\mu}}{2K_{T,\tilde{\mu}}^{0,\Delta}(p)}\,. \end{aligned} \tag{3.1.10}$$

If $\Delta_\ell \neq 0$ for a subsequence of ℓ's going to zero, then, in addition,

$$\boxed{-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\tilde{\mu}}^{0,\Delta}} - \frac{1}{p^2} \right) \mathrm{d}^3p\,.} \tag{3.1.11}$$

For a less complicated version (discarding the direct and exchange term) of this result, see [BHS14a].

The new gap equation motivates the following definition of the critical temperature [BHS14c, Definition 1]

Definition 3.1 (Critical temperature / renormalized chemical potential)**.** Let $\mu > 0$. The *critical temperature* T_c and the *renormalized chemical potential* $\tilde{\mu}$ in the limit of a contact potential with scattering length $a < 0$

and $\lim_{\ell\to 0} \widehat{V_\ell}(0) = \mathcal{V} \geq 0$ are implicitly given by the set of equations

$$\begin{aligned} -\frac{1}{4\pi a} &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{\tanh\left(\frac{p^2-\tilde{\mu}}{2T_c}\right)}{p^2-\tilde{\mu}} - \frac{1}{p^2} \right) \mathrm{d}^3 p\,, \\ \tilde{\mu} &= \mu - \frac{2\mathcal{V}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{1}{1+\mathrm{e}^{\frac{p^2-\tilde{\mu}}{T_c}}} \mathrm{d}^3 p\,. \end{aligned} \tag{3.1.12}$$

Although T_c is only defined in the limit $\ell \to 0$, by the following theorem [BHS14c, Theorem 3], it still serves as a tool to find upper and lower bounds on the critical temperature for small (but non-zero) ℓ.

Theorem 3.3 (Bounds on critical temperature)**.** *Let $\mu \in \mathbb{R}$, $T \geq 0$ and let $(\gamma_\ell^0, 0)$ be a normal state for $\mathcal{F}_T^{V_\ell}$.*

(i) For $T < T_c$, there exists an $\ell_0(T) > 0$ such that for $\ell < \ell_0(T)$, $\inf \operatorname{spec}(K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell) < 0$. Consequently, the system is superfluid.

(ii) For $T > T_c$, there exists an $\ell_0(T) > 0$ such that for $\ell < \ell_0(T)$, $\mathcal{F}_T^{V_\ell}$ is minimized by a normal state. I.e., the system is not superfluid.

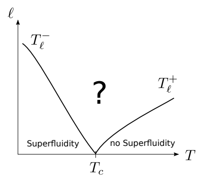

Figure 3.2: Phase diagram: Temperature T versus range ℓ of the interaction potential.

As sketched in Figure 3.2, Theorem 3.3 shows that Definition 3.1 is indeed the correct definition of the critical temperature in the limit $\ell \to 0$. Moreover the equivalence of the criteria (ii) and (iii) in Theorem 2.1 is recovered for small ℓ.

3.1.1 Contact interactions as limits of short-range potentials

In quantum mechanics, a *contact potential* realizes a point interaction, i.e. it is a potential vanishing everywhere except at one point. While it is possible to describe a contact potential in one dimension by a Dirac delta function, in two and three dimensions another approach has to be used. This is because a Hamiltonian involving a Dirac delta distribution would not be well defined. Instead, Hamiltonians modelling point interactions are constructed as the self-adjoint extensions of the Laplacian $-\Delta|_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}$ defined on the punctured configuration space.

A good mathematical reference for the analysis of contact potentials is [Alb+88]. As an important result, the authors show that for potentials of type (3.1.9), the family of Schrödinger operators $-\Delta + V_\ell$ converges in norm resolvent sense to an appropriate self-adjoint extension of the Laplacian determined by the scattering length a [Alb+88, Theorem 1.2.5].

As mentioned above, the method (3.1.9) although yielding a family of potentials satisfying the requirements of Assumption 3.1 does not renormalize the chemical potential μ. To illustrate a situation, where a renormalized chemical potential arises, an example for V_ℓ is constructed in [BHS14c], having the form sketched in Figure 3.1 and satisfying Assumption 3.1 and in addition

$$\lim_{\ell\to 0}\int_{\mathbb{R}^3} V_\ell \, \mathrm{d}^3x > 0.$$

More precisely we consider

$$V_\ell = V_\ell^+ - V_\ell^-, \qquad \begin{array}{rcl} V_\ell^+(x) & = & (k_\ell^+)^2\,\chi_{\{|x|<\epsilon_\ell\}}(x), \\ V_\ell^-(x) & = & (k_\ell^-)^2\,\chi_{\{\epsilon_\ell<|x|<\ell\}}(x), \end{array} \qquad \begin{array}{l} k_\ell^+ = k^+\epsilon_\ell^{-3/2} \\ k_\ell^- = \frac{\frac{\pi}{2}-\ell\omega}{\ell-\epsilon_\ell}, \end{array} \tag{3.1.13}$$

with $\omega > 0$, $k^+ > 0$ and $0 < \epsilon_\ell < c\ell^2$ with $c < 2\omega/\pi$. The function $\chi_A(x)$ denotes the characteristic function of the set A.

For the investigation of the short range limit for the full BCS functional it would be sufficient to know only the scattering length $a(V_\ell)$ as well as the integral $\int_{\mathbb{R}^3} V_\ell \, \mathrm{d}^3x$ in the limit $\ell \to 0$. However, since in physics contact potentials play an important role, we dedicated an own paper [BHS13] to the study of the approximation of contact potentials by short ranged potentials with strong repulsive core in more detail. More precisely, we adapt the result [Alb+88, Theorem 1.2.5], that the Schrödinger-Operator $-\Delta + V_\ell$ converges to a contact potential for potentials of the type (3.1.13). We use the notation $V^{1/2}(x) = \mathrm{sgn}(x)|V(x)|^{1/2}$ and write $V_\ell^\pm$ for the positive and negative part of the potential V_ℓ in the decomposition

$$V_\ell = V_\ell^+ - V_\ell^-, \qquad \mathrm{supp}(V_\ell^+) \cap \mathrm{supp}(V_\ell^-) = \emptyset.$$

For our main theorem [BHS13, Theorem 1], we do not need to obey Assumption 3.1. The following will be sufficient.

Assumption 3.2. (A1) $(V_\ell)_{\ell>0} \in L^{3/2}(\mathbb{R}^3) \cap L^1\big(\mathbb{R}^3, (1+|x|^2)dx\big)$.

(A2) There are sequences $e_\ell, e_\ell^- \in \mathbb{R}$ such that $e_\ell \neq 0$, $\lim_{\ell\to 0} e_\ell = 0$, $e_\ell^- = O(e_\ell)$ and

$$-\Delta + \lambda V_\ell \quad \text{and} \quad -\Delta - \lambda^- V_\ell^-$$

have non-degenerate zero-energy resonances for $\lambda = (1-e_\ell)^{-1}$ and $\lambda^- = (1-e_\ell^-)^{-1}$, respectively. All other $\lambda, \lambda^- \in \mathbb{R}$ for which $-\Delta + \lambda V_\ell$ and $-\Delta - \lambda^- V_\ell^-$ have zero-energy resonances are separated from 1 by a gap of order 1.

(A3) $\|V_\ell\|_{L^1}$ is uniformly bounded in ℓ and $\|V_\ell^-\|_{L^1} = O(e_\ell)$,

(A4) $\int_{\mathbb{R}^3} |V_\ell(x)|\,|x|^2\,\mathrm{d}^3x = O(e_\ell^2)$ and $\int_{\mathbb{R}^3} |V_\ell^-(x)|\,|x|^2\,\mathrm{d}^3x = O(e_\ell^3)$,

(A5) the limit

$$a = \lim_{\ell\to 0} a(V_\ell) = \frac{1}{4\pi} \lim_{\ell \to 0} \big\langle |V_\ell|^{1/2} \big| (1+B_\ell)^{-1} V_\ell^{1/2} \big\rangle \tag{3.1.14}$$

exists and is finite.

Theorem 3.4. *Let $(V_\ell)_{\ell>0}$ be a family of real-valued functions satisfying Assumption 3.2. Then, as $\ell \to 0$,*

$$\frac{1}{-\Delta + V_\ell - k^2} \to \frac{1}{-\Delta - k^2} - \frac{4\pi}{a^{-1} + ik} |g_k\rangle\langle g_k|, \qquad \Im(k) > 0\,,\ k \neq i/a \tag{3.1.15}$$

in norm, where $g_k(x) = \frac{1}{4\pi} \frac{\mathrm{e}^{ik|x|}}{|x|}$.

The resolvent on the right side of (3.1.15) belongs to a Hamiltonian of a special point interaction centered at the origin. More precisely, for $\theta \in [0, 2\pi)$ let $\big(H_\theta, D(H_\theta)\big)$ be the self-adjoint extension of the kinetic energy Hamiltonian

$$-\Delta|_{H_0^{2,2}(\mathbb{R}^3 \setminus \{0\})}$$

with the domain

$$D(H_\theta) = H_0^{2,2}(\mathbb{R}^3 \setminus \{0\}) \oplus \langle \psi_+ + \mathrm{e}^{i\theta} \psi_- \rangle,$$

$$\psi_\pm(x) = \frac{\mathrm{e}^{i\sqrt{\pm i}|x|}}{4\pi|x|}, \qquad x \in \mathbb{R}^3 \setminus \{0\}, \Im(\sqrt{\pm i}) > 0,$$

such that $H_\theta(\psi_+ + \mathrm{e}^{i\theta}\psi_-) = i\psi_+ - i\mathrm{e}^{i\theta}\psi_-$. Then, if θ is chosen such that

$$-a^{-1} = \cos(\pi/4)\big(\tan(\theta/2) - 1\big),$$

we have by [Alb+88, Theorem 1.1.2.] that

$$\frac{1}{H_\theta - k^2} = \frac{1}{p^2 - k^2} - \frac{4\pi}{a^{-1} + ik}|g_k\rangle\langle g_k|. \tag{3.1.16}$$

Hence, Theorem 3.4 implies that the operator $-\Delta + V_\ell$ converges in norm resolvent sense to $\big(H_\theta, D(H_\theta)\big)$.

3.2 The Link to the Gross-Pitaevskii Theory

This section is dedicated to the results obtained in [BHS14b].

It may seem surprising, that the BCS theory, describing fermions is related to the Gross-Pitaevskii theory describing condensates of bosons (Bose-Einstein condensation). The solution to the apparent contradiction is, that we here are interested in pairs of fermions which together behave like a boson. While in the usual BCS setting, the interaction potential V is not strong enough for formation of bound fermion-fermion systems, we here consider strong interactions capable of binding fermions in diatomic molecules. We start with the $SU(2)$ invariant but not translation invariant BCS functional (2.2.5) without external magnetic field at temperature $T = 0$. Instead of using a chemical potential μ, we fix the particle number via $\mathrm{tr}(\gamma) = N$.

$$\begin{aligned}\mathcal{E}^{\mathrm{BHF}}(\Gamma) = \mathrm{tr}\,\big(-\Delta + W\big)\gamma &+ \frac{1}{2}\int_{\mathbb{R}^6} V(x-y)|\alpha(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y \\ &- \frac{1}{2}\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y \\ &+ \int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y)V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y.\end{aligned} \tag{3.2.1}$$

The external potential W serves as confinement for the system of fermions. We are interested in the ground state energy of the system under the assumption, that the scale of W is large compared to the pair interaction

V. We therefore introduce a small scale parameter h, which we will not only use to tune the ratio of scales via $W(x) \to W(hx)$ but also at the same time to tune the strength of W via $W \to h^2 W$ as well as the particle number N via $N \to N/h$ to achieve systems with low density. Note that this way, the volume scales like h^{-3}, yielding a particle density of magnitude h^2. We will express the functional in terms of macroscopic variables $x_h = hx$, $y_h = hy$, $\alpha_h(x,y) = h^{-3}\alpha(\frac{x}{h}, \frac{y}{h})$, $\gamma_h(x,y) = h^{-3}\gamma(\frac{x}{h}, \frac{y}{h})$. In the resulting functional, we now denote by x, y, γ and α the corresponding macroscopic quantities.

$$\begin{aligned}\mathcal{E}^{\mathrm{BHF}}(\Gamma) = {} & \operatorname{tr}(-h^2\Delta + h^2 W)\gamma + \frac{1}{2}\int_{\mathbb{R}^6} V\Big(\frac{x-y}{h}\Big)|\alpha(x,y)|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y \\ & - \frac{1}{2}\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\ & + \int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y) V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y,\end{aligned} \tag{3.2.2}$$

with corresponding ground state energy

$$E^{\mathrm{BHF}}(N,h) = \inf\{\mathcal{E}^{\mathrm{BHF}}(\Gamma) \,|\, 0 \le \Gamma \le 1,\ \operatorname{tr}\gamma = N/h\}. \tag{3.2.3}$$

The main result of [BHS14b] is, that in the limit $h \to 0$, the ground state energy is to leading order in h given by he binding energy $\frac{E_b}{2}\frac{N}{h}$ of the fermion pairs and the next order, i.e. the macroscopic density fluctuations of the pairs, is given by h times the Gross-Pitaevskii potential

$$\mathcal{E}^{\mathrm{GP}}(\psi) = \int_{\mathbb{R}^3} \Big(\frac{1}{4}|\nabla\psi(x)|^2 + W(x)|\psi(x)|^2 + g|\psi(x)|^4\Big)\,\mathrm{d}^3x, \tag{3.2.4}$$

where the parameter $g > 0$ will be determined by the BHF functional and represents the interaction strength among different pairs. The function $\psi(x)$ represents the spatial fluctuation of the pairs and will emerge from the ground state α. Denoting the ground state energy of (3.2.4) by

$$E^{\mathrm{GP}}(g,N) = \inf\{\mathcal{E}^{\mathrm{GP}}(\psi) \,|\, \psi \in H^1(\mathbb{R}^3),\ \|\psi\|_2^2 = N\}, \tag{3.2.5}$$

we can formulate our result [BHS14b, Theorem 1], which acts on the following assumptions.

Assumption 3.3. Let $V \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, with $V(x) = V(-x)$ and such that $-2\Delta + V$ has a ground state α_0 with norm $\|\alpha_0\| = 1$ with corresponding ground state energy $-E_b < 0$.

Assumption 3.4. There exists $U \in L^2(\mathbb{R}^3)$, with positive Fourier transform $\widehat{U} \geq 0$, such that $V - \frac{1}{2}V_+ \geq U$. Here $V_+ = \frac{1}{2}(|V| + V)$ denotes the positive part of V.

Theorem 3.5. *Let $W \in H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Under Assumptions 3.3 and 3.4, we have for small h,*

$$E^{\mathrm{BHF}}(N, h) = -\frac{E_b}{2}\frac{N}{h} + hE^{\mathrm{GP}}(g, N) + O(h^{3/2}), \tag{3.2.6}$$

where g is given by

$$g = \frac{1}{(2\pi)^3} \int |\widehat{\alpha}_0(p)|^4 (2p^2 + E_b)\,\mathrm{d}^3p \\ - \frac{1}{2} \int_{\mathbb{R}^3} |(\overline{\alpha_0} * \alpha_0)(x)|^2\, V(x)\,\mathrm{d}^3x + \int_{\mathbb{R}^3} V(x)\,\mathrm{d}^3x.$$

Moreover, if Γ is an approximate minimizer of $\mathcal{E}^{\mathrm{BHF}}$, in the sense that

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) \leq -\frac{E_b}{2}\frac{N}{h} + h(E^{\mathrm{GP}}(g, N) + \epsilon)$$

for some $\epsilon > 0$, then the corresponding α can be decomposed as

$$\alpha = \alpha_\psi + \xi, \qquad \|\xi\|_2^2 \leq O(h), \tag{3.2.7}$$

where

$$\alpha_\psi(x, y) = h^{-2}\psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big), \tag{3.2.8}$$

and ψ is an approximate minimizer of $\mathcal{E}^{\mathrm{GP}}$ in the sense that

$$\mathcal{E}^{\mathrm{GP}}(\psi) \leq E^{\mathrm{GP}}(g, N) + \epsilon + O(h^{1/2}). \tag{3.2.9}$$

In contrast to [HS12], which states a similar result, we here include the exchange and the direct term. Moreover, the setting in [HS12] assumes a system with periodic boundary conditions in all three spatial directions, which we replace by a system confined in an arbitrary external potential $W \in L^\infty(\mathbb{R}^3)$. Theorem 3.5 also improves the error bounds, it even implies $E^{\mathrm{BHF}}(N, h) = -E_b \frac{N}{2h} + hE^{\mathrm{GP}}(g_{BCS}, N) + O(h^2)$ when discarding the direct term.

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DOI: 10.1007/BFb0120125.

Appendix A

Publications in the Thesis

A.1 Accepted papers

A.1.1 On Contact Interactions as Limits of Short-Range Potentials

Methods of Functional Analysis and Topology
Vol. 19 (2013), no. 4, pp. 364–375

ON CONTACT INTERACTIONS AS LIMITS OF SHORT-RANGE POTENTIALS

GERHARD BRÄUNLICH, CHRISTIAN HAINZL, AND ROBERT SEIRINGER

ABSTRACT. We reconsider the norm resolvent limit of $-\Delta + V_\ell$ with V_ℓ tending to a point interaction in three dimensions. We are mainly interested in potentials V_ℓ modelling short range interactions of cold atomic gases. In order to ensure stability the interaction V_ℓ is required to have a strong repulsive core, such that $\lim_{\ell\to 0}\int V_\ell > 0$. This situation is not covered in the previous literature.

1. Introduction

Quantum mechanical systems with contact interaction, or point interaction, are treated extensively in the physics literature, in connection with problems in atomic, nuclear and solid state physics. In two and three dimensions such point interaction Hamiltonians have to be defined carefully for the simple reason that the Dirac δ-function is not relatively form-bounded with respect to the kinetic energy described by the Laplacian $-\Delta$. Mathematically this can be overcome by removing the point of interaction from the configuration space and extending $-\Delta$ to a self-adjoint operator. This leads to a one-parameter family of extensions in two and three dimensions. One way to pick out the physically relevant extension is by approximating the contact interaction by a sequence of corresponding short range potentials $V_\ell(x)$ such that the range ℓ converges to zero, but the *scattering length* $a(V_\ell)$ has a finite limit $a \in \mathbb{R}$. The corresponding self-adjoint extension is then uniquely determined by this a.

The mathematical analysis of such problems is extensively studied in the book of Albeverio, Gesztesy, Hoegh-Krohn and Holden [1]. Among other things the authors show that $-\Delta + V_\ell$ converges in norm resolvent sense to an appropriate self-adjoint extension of the Laplacian determined by a. As one of their implicit assumptions the L^1-norm of V_ℓ goes to zero in the limit $\ell \to 0$. This assumption can be too restrictive for applications, however, as explained in [3].

Indeed, one major area of physics where contact interactions play a significant role are *cold atomic gases*, see e.g. [11, 12, 3]. The corresponding BCS gap equation has a particularly simple form in this case. However, in order to prevent such a Fermi gas from collapsing and to ensure stability of matter, the contact interaction has to arise from potentials V_ℓ which have a large repulsive core (such that $\lim_{\ell\to 0}\int V_\ell > 0$) in addition to an attractive tail. The strength of the attractive tail depends on the system under consideration, ranging from a weakly interacting superfluid (where $-\Delta + V_\ell \geq 0$) [10, 8] to a strongly interacting gas of tightly bound fermion pairs (where $-\Delta + V_\ell$ typically has one negative eigenvalue) [12, 7, 6].

Having such systems in mind, the present paper is dedicated to the study of contact interactions arising as a limit of short range potentials V_ℓ with large positive core and, in particular, a non-vanishing and positive integral $\int V_\ell$ in the limit $\ell \to 0$. The simplest

2000 *Mathematics Subject Classification.* Primary 46N50, 35J10.
Key words and phrases. Contact interaction, Birman-Schwinger principle, Schrödinger operator.

form of such a V_ℓ we can think of is depicted in Figure 1. We shall generalize a result of [2, 1] and show that for $\Im(k) > 0$

$$\frac{1}{-\Delta + V_\ell - k^2} \overset{\ell\to 0}{\longrightarrow} \frac{1}{-\Delta - k^2} - \frac{4\pi}{a^{-1} + ik}|g_k\rangle\langle g_k|$$

in norm, where $g_k(x) = \frac{1}{4\pi}\frac{e^{ik|x|}}{|x|}$, and $a = \lim_{\ell\to 0} a(V_\ell)$ is the limiting scattering length. The main mathematical obstacle we have to overcome is the fact that the corresponding Birman-Schwinger operators are "very" non-self-adjoint, which requires a refined analysis to get a hand on the corresponding norms. One important ingredient of our analysis is a useful formula for the scattering length $a(V_\ell)$ which was recently derived in [9].

Throughout the paper, we adopt physics notation and use $\langle \cdot | \cdot \rangle$ for the inner product in $L^2(\mathbb{R}^3)$, $|f\rangle\langle f|$ for the rank-one projection in the direction of f, etc.

2. Main Results

In the following, we shall consider a family $(V_\ell)_{\ell>0}$ of real-valued functions in $L^1(\mathbb{R}^3)\cap L^{3/2}(\mathbb{R}^3)$. We use the notation $V^{1/2}(x) = \operatorname{sgn}(x)|V(x)|^{1/2}$ and write $V_\ell^{\pm}$ for the positive and negative part of the potential V_ℓ in the decomposition

$$V_\ell = V_\ell^+ - V_\ell^-, \quad \operatorname{supp}(V_\ell^+) \cap \operatorname{supp}(V_\ell^-) = \emptyset.$$

Further we will abbreviate

$$J_\ell = \begin{cases} 1, & V_\ell \geq 0, \\ -1, & V_\ell < 0, \end{cases} \qquad \text{i.e.} \quad J_\ell(x) = \operatorname{sgn}\big(V_\ell(x)\big),$$

$$X_\ell = |V_\ell|^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}, \quad X_\ell^- = (V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2},$$

so that the Birman-Schwinger operator reads

$$B_\ell := V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2} = J_\ell X_\ell\,. \tag{2.1}$$

For a given real-valued potential $V \in L^1(\mathbb{R}^3)\cap L^{3/2}(\mathbb{R}^3)$, it was shown in [9] that the scattering length can be expressed via

$$a(V) = \frac{1}{4\pi}\Big\langle |V|^{1/2} \Big| \frac{1}{1 + V^{1/2}\frac{1}{p^2}|V|^{1/2}} V^{1/2}\Big\rangle. \tag{2.2}$$

This assumes that $1 + V^{1/2}\frac{1}{p^2}|V|^{1/2}$ is invertible, otherwise $a(V)$ is infinite.

Throughout the paper we will use the notation

$$f = O(g) \Leftrightarrow 0 \leq \limsup_{\ell\to 0}\left|\frac{f(\ell)}{g(\ell)}\right| < \infty.$$

For our main theorem we will need to make the following assumptions.

Assumptions 1. (A1) $(V_\ell)_{\ell>0} \in L^{3/2}(\mathbb{R}^3)\cap L^1\big(\mathbb{R}^3, (1+|x|^2)dx\big)$.

(A2) There are sequences $e_\ell, e_\ell^- \in \mathbb{R}$ such that $e_\ell \neq 0$, $\lim_{\ell\to 0} e_\ell = 0$, $e_\ell^- = O(e_\ell)$ and

$$-\Delta + \lambda V_\ell \quad \text{and} \quad -\Delta - \lambda^- V_\ell^-$$

have non-degenerate zero-energy resonances for $\lambda = (1-e_\ell)^{-1}$ and $\lambda^- = (1 - e_\ell^-)^{-1}$, respectively. All other $\lambda, \lambda^- \in \mathbb{R}$ for which $-\Delta + \lambda V_\ell$ and $-\Delta - \lambda^- V_\ell^-$ have zero-energy resonances are separated from 1 by a gap of order 1.

(A3) $\|V_\ell\|_{L^1}$ is uniformly bounded in ℓ and $\|V_\ell^-\|_{L^1} = O(e_\ell)$,

(A4) $\int_{\mathbb{R}^3} |V_\ell(x)|\,|x|^2\,\mathrm{d}^3x = O(e_\ell^2)$ and $\int_{\mathbb{R}^3} |V_\ell^-(x)|\,|x|^2\,\mathrm{d}^3x = O(e_\ell^3)$,

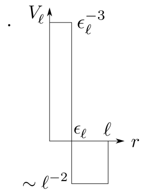

FIGURE 1. Example of a sequence of potentials V_ℓ.

(A5) the limit

$$a = \lim_{\ell\to 0} a(V_\ell) = \frac{1}{4\pi}\lim_{\ell\to 0}\left\langle |V_\ell|^{1/2}\middle|(1+B_\ell)^{-1}V_\ell^{1/2}\right\rangle \tag{2.3}$$

exists and is finite.

Remark 1. Assumption (A2) can be reformulated in terms of the corresponding Birman-Schwinger operators. Recall that $-\Delta + \frac{1}{1-e}V$ has a zero-energy resonance if and only if $1 + V^{1/2}\frac{1}{p^2}|V|^{1/2}$ has an eigenvalue e. Therefore (A2) is equivalent to the following assumption:

(A2)' The lowest eigenvalues e_ℓ and e_ℓ^- of the operators $1 + J_\ell X_\ell$ and $1 - X_\ell^-$, respectively, are non-degenerate, converge to 0 as $\ell \to 0$, with $e_\ell^- = O(e_\ell)$, and all other eigenvalues are isolated from 0 by a gap of order 1.

The fact that $e_\ell \neq 0$ means that $1 + B_\ell$ is invertible. For simplicity, we also assume that the limit in (2.3) is finite. We expect our result to be true also for $a = \infty$, but the proof has to be suitably modified in this case.

We are now ready to state our main theorem.

Theorem 1. *Let $(V_\ell)_{\ell>0}$ be a family of real-valued functions satisfying Assumptions 1. Then, as $\ell \to 0$,*

$$\frac{1}{-\Delta + V_\ell - k^2} \to \frac{1}{-\Delta - k^2} - \frac{4\pi}{a^{-1}+ik}|g_k\rangle\langle g_k|, \quad \Im k > 0, \quad k \neq i/a \tag{2.4}$$

in norm, where $g_k(x) = \frac{1}{4\pi}\frac{e^{ik|x|}}{|x|}$.

Remark 2. The simplest example of potentials satisfying Assumptions 1 is shown in Figure 1.

By simple calculations it is immediate to see that (A1), (A3) and (A4) hold, with $e_\ell = O(\ell)$. By fine tuning the strength of the negative part of V_ℓ, it is possible to meet a resonance condition such that (A2) holds. The corresponding scattering length can be calculated explicitly in this case, verifying (A5). (See [3, Appendix] for such explicit calculations in the case where $\epsilon_\ell \ll \ell$.)

Remark 3. In case $a = 0$, the fraction $(a^{-1} + ik)^{-1}$ has to be interpreted as 0.

Remark 4. One consequence of Theorem 1 is that in the case $0 < a < \infty$ the smallest eigenvalue of $-\Delta + V_\ell$ converges to $-\frac{1}{a^2}$, with the eigenfunction tending to $\sqrt{\frac{2\pi}{a}}g_{i/a}(x)$ in L^2. Moreover, all other eigenvalues necessarily tend to 0.

Remark 5. The resolvent on the right side of (2.4) belongs to a Hamiltonian of a special point interaction centered at the origin. More precisely, for $\theta \in [0, 2\pi)$ let $\big(H_\theta, D(H_\theta)\big)$ be the self-adjoint extension of the kinetic energy Hamiltonian

$$-\Delta|_{H_0^{2,2}(\mathbb{R}^3\setminus\{0\})}$$

with the domain

$$D(H_\theta) = H_0^{2,2}(\mathbb{R}^3 \setminus \{0\}) \oplus \langle \psi_+ + \mathrm{e}^{i\theta}\psi_- \rangle, \quad \psi_\pm(x) = \frac{\mathrm{e}^{i\sqrt{\pm i}|x|}}{4\pi|x|},$$

$$x \in \mathbb{R}^3 \setminus \{0\}, \quad \Im(\sqrt{\pm i}) > 0,$$

such that $H_\theta(\psi_+ + \mathrm{e}^{i\theta}\psi_-) = i\psi_+ - i\mathrm{e}^{i\theta}\psi_-$. Then, if θ is chosen such that

$$-a^{-1} = \cos(\pi/4)\big(\tan(\theta/2) - 1\big),$$

we have by [1, Theorem 1.1.2.] that

$$\frac{1}{H_\theta - k^2} = \frac{1}{p^2 - k^2} - \frac{4\pi}{a^{-1} + ik}|g_k\rangle\langle g_k|. \tag{2.5}$$

Hence Theorem 1 implies that the operator $-\Delta + V_\ell$ converges to $(H_\theta, D(H_\theta))$ in norm resolvent sense.

Remark 6. Let us explain one of the main difficulties arising from potentials with large L^1-core compared to the situation treated in [1], where the $L^{3/2}$-norm of V_ℓ is uniformly bounded and hence the L^1-norm tends to zero. One of the necessary tasks in the proof of Theorem 1 is to bound the inverse of operator $1 + B_\ell$, where B_ℓ denotes the Birman-Schwinger operator defined in (2.1). One way to bound the norm of this non-self-adjoint operator is to use the identity

$$\frac{1}{1 + B_\ell} = 1 - J_\ell X_\ell^{1/2} \frac{1}{1 + X_\ell^{1/2} J_\ell X_\ell^{1/2}} X_\ell^{1/2},$$

which implies for its norm

$$\left\| \frac{1}{1 + B_\ell} \right\| \le 1 + \|X_\ell\| \left\| \frac{1}{1 + X_\ell^{1/2} J_\ell X_\ell^{1/2}} \right\|.$$

The Hardy-Littlewood-Sobolev inequality implies that $\|X_\ell\|$ can be bounded by a constant times $\|V_\ell\|_{L^{3/2}}$, and with $X_\ell^{1/2} J_\ell X_\ell^{1/2}$ being isospectral to $B_\ell = J_\ell X_\ell$ we obtain that

$$\left\| \frac{1}{1 + B_\ell} \right\| \le 1 + C\frac{1}{|e_\ell|} \|V_\ell\|_{L^{3/2}}\,. \tag{2.6}$$

This shows that $\big\|(1 + B_\ell)^{-1}\big\| \le O(|e_\ell|^{-1})$ for sequences V_ℓ used in [1], which turns out to be sufficient. However, in our present situation we are dealing with potentials V_ℓ with strong repulsive core satisfying Assumptions 1, where the corresponding $L^{3/2}$ norm diverges and typically is of the order of $O(1/|e_\ell|)$. Hence the inequality (2.6) only implies a bound of the form

$$\left\| \frac{1}{1 + B_\ell} \right\| \le O\big(|e_\ell|^{-2}\big)\,,$$

which is not good enough for our purpose. To this aim we have to perform a more refined analysis.

Remark 7. For related work on two-scale limits in one-dimensional systems, see, e.g., [4, 5].

The following lemma turns out to be very useful in the proof of Theorem 1.

Lemma 1. *Let* $V = V_+ - V_-$*, where* $V_-, V_+ \geq 0$ *have disjoint support. Denote* $J = \begin{cases} 1, & V \geq 0 \\ -1, & V < 0 \end{cases}$*,* $X = |V|^{1/2} \frac{1}{p^2} |V|^{1/2}$ *and* $X_\pm = V_\pm^{1/2} \frac{1}{p^2} V_\pm^{1/2}$*. Then for any* $\phi \in L^2(\mathbb{R}^3)$*, we have*

$$\sqrt{2}\, \|\phi\|_{L^2} \|(J+X)\phi\|_{L^2} \geq \langle \phi | (X_+ + 1 - X_-)\phi \rangle. \tag{2.7}$$

Proof of Lemma 1. Decompose $\phi = \phi_+ + \phi_-$, such that $\operatorname{supp}(\phi_-) \subseteq \operatorname{supp}(V_-)$ and $\operatorname{supp}(\phi_+) \cap \operatorname{supp}(V_-) = \emptyset$. By applying twice the Cauchy-Schwarz inequality,

$$\begin{aligned} \|(J+X)\phi\|_{L^2} \|\phi_+\|_{L^2} &\geq \Re \langle \phi_+ | (J+X)\phi \rangle \\ &= \langle \phi_+ | (1+X_+)\phi_+ \rangle + \Re \langle \phi_+ | V_+^{1/2} \tfrac{1}{p^2} V_-^{1/2} \phi_- \rangle, \\ \|(J+X)\phi\|_{L^2} \|\phi_-\|_{L^2} &\geq \Re \langle (J+X)\phi | \; -\phi_- \rangle \\ &= \langle \phi_- | (1-X_-)\phi_- \rangle - \Re \langle \phi_+ | V_+^{1/2} \tfrac{1}{p^2} V_-^{1/2} \phi_- \rangle. \end{aligned}$$

We add the two inequalities to get rid of the cross terms

$$\begin{aligned} &\|(J+X)\phi\|_{L^2} \left(\|\phi_+\|_{L^2} + \|\phi_-\|_{L^2} \right) \\ &\quad \geq \langle \phi_+ | (1+X_+)\phi_+ \rangle + \langle \phi_- | (1-X_-)\phi_- \rangle = \langle \phi | (X_+ + 1 - X_-)\phi \rangle. \end{aligned} \tag{2.8}$$

Finally, we use that $\|\phi_+\|_{L^2} + \|\phi_-\|_{L^2} \leq \sqrt{2} \|\phi\|_{L^2}$, which finishes the proof. □

One difficulty in proving Theorem 1 is that the operator $1 + B_\ell$ is not self-adjoint and the norm of its inverse cannot be controlled by the spectrum. One consequence of Lemma 1 and our assumptions is that the norm of $(1+B_\ell)^{-1}$ diverges like $\frac{1}{e_\ell}$. The following statement identifies the divergent term in terms of the projection onto the eigenvector to the lowest eigenvalue of the Birman Schwinger operator.

Consequence 1. *Let* $(V_\ell)_{\ell>0}$ *satisfy (A1)–(A4) in Assumptions 1. Then the operator*

$$(1+B_\ell)^{-1}(1-P_\ell)$$

is uniformly bounded in ℓ*, where*

$$P_\ell = \frac{1}{\langle J_\ell \phi_\ell | \phi_\ell \rangle} |\phi_\ell\rangle \langle J_\ell \phi_\ell| \tag{2.9}$$

with ϕ_ℓ *the eigenvector to the eigenvalue* e_ℓ *of* $1 + B_\ell$*.*

Another consequence of Lemma 1 is the following set of relations, which the proof of Theorem 1 heavily relies on.

Consequence 2. *Let* $(V_\ell)_{\ell>0}$ *be a family of real-valued functions which satisfy (A1)–(A4) in Assumptions 1. Then*

(i) $\int_{\mathbb{R}^3} |x|\, |V_\ell(x)|\, \mathrm{d}^3x = O(e_\ell)$,
(ii) $\langle J_\ell \phi_\ell | \phi_\ell \rangle = -1 + O(e_\ell)$,
(iii) $\langle |V_\ell|^{1/2} | |\phi_\ell| \rangle = O(|e_\ell|^{1/2})$,
(iv) $\int_{\mathbb{R}^3} |x|\, |V_\ell(x)|^{1/2}\, |\phi_\ell(x)|\, \mathrm{d}^3x = O(|e_\ell|^{3/2})$.

The proof of these facts will be given Section 4.

3. Proof of Theorem 1

Let $k \in \mathbb{C}$ with $\Im k > 0$. Following the strategy in [1] our starting point is the identity

$$\frac{1}{p^2 + V_\ell - k^2} = \frac{1}{p^2 - k^2} - \underbrace{\frac{1}{p^2 - k^2} |V_\ell|^{1/2}}_{①} \underbrace{\frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2 - k^2} |V_\ell|^{1/2}}}_{②} \underbrace{V_\ell^{1/2} \frac{1}{p^2 - k^2}}_{③}. \tag{3.1}$$

Note that the operators ① and ③ are uniformly bounded in ℓ. In fact,

$$\Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\Big\| \le \Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\Big\|_2 = \big\|\frac{1}{p^2-k^2}\big\|_{L^2}\|V_\ell^{1/2}\|_{L^2},$$

which is uniformly bounded due to our assumptions on V_ℓ. We will first show in Lemma 2 that $\frac{1}{p^2-k^2}|V_\ell|^{1/2}$ is, up to small errors of $O(|e_\ell|^{1/2})$, equal to the rank one operator $|g_k\rangle\langle|V_\ell|^{1/2}|$. Together with the formula (2.2) for the scattering length this will lead us finally to (2.4).

Lemma 2.

$$\Big\|\Big(\frac{1}{p^2-k^2}|V_\ell|^{1/2} - |g_k\rangle\big\langle|V_\ell|^{1/2}\big|\Big)\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\Big\|_{L^2} = O(|e_\ell|^{1/2}), \tag{3.2a}$$

$$\Big\|\Big(\frac{1}{p^2-k^2}|V_\ell|^{1/2} - |g_k\rangle\big\langle|V_\ell|^{1/2}\big|\Big)\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\Big\| = O(|e_\ell|^{1/2}). \tag{3.2b}$$

Proof. We make use of the decomposition

$$\frac{1}{1+B_\ell} = \frac{1}{e_\ell}P_\ell + \frac{1}{1+B_\ell}(1-P_\ell), \tag{3.3}$$

where we first treat the contribution of the second summand to (3.2a) and (3.2b). This is the easier one thanks to Consequence 1, which tells us that $\frac{1}{1+B_\ell}(1-P_\ell)$ is uniformly bounded in ℓ. Note that the integral kernel of the operator $\frac{1}{p^2-k^2}|V_\ell|^{1/2} - |g_k\rangle\big\langle|V_\ell|^{1/2}\big|$ in (3.2a) and (3.2b) is given by the expression

$$\big(g_k(x-y) - g_k(x)\big)|V_\ell|^{1/2}(y)\,.$$

An explicit computation shows that

$$F_k(y) := \int_{\mathbb{R}^3}\frac{\mathrm{e}^{ik|x|}}{|x|}\frac{\mathrm{e}^{-i\bar{k}|x-y|}}{|x-y|}\,\mathrm{d}^3x = \frac{2\pi}{\Im(k)}\mathrm{e}^{-\Im(k)|y|}\frac{\sin(\Re(k)|y|)}{\Re(k)|y|}\,.$$

From this one easily obtains the bound

$$\int_{\mathbb{R}^3}\big|g_k(x-y)-g_k(x)\big|^2\,\mathrm{d}^3x = \frac{2}{(4\pi)^2}\left(F_k(0)-F_k(y)\right) \le \frac{1}{4\pi}\left(1+\frac{|\Re(k)|}{2|\Im(k)|}\right)|y|\,. \tag{3.4}$$

Hence we infer from Consequence 2(i) that the Hilbert-Schmidt norm of this operator is bounded as

$$\begin{aligned}&\Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2} - |g_k\rangle\big\langle|V_\ell|^{1/2}\big|\Big\|_2\\ &\quad\le\left[\frac{1}{4\pi}\Big(1+\frac{|\Re(k)|}{2|\Im(k)|}\Big)\int_{\mathbb{R}^3}|V_\ell(x)||x|\,\mathrm{d}^3x\right]^{1/2} = O(|e_\ell|^{1/2}).\end{aligned} \tag{3.5}$$

Thus the contribution of the last term in (3.3) to (3.2a) gives a term of order $|e_\ell|^{1/2}$. With $V_\ell^{1/2}\frac{1}{p^2-k^2}$ being a uniformly bounded operator we also infer that the same holds true for (3.2b).

It remains to estimate the contribution coming from the first term on the right side of (3.3). With P_ℓ defined in (2.9), the norm of the corresponding vector in (3.2a) is

$$\begin{aligned}&\frac{1}{|e_\ell|}\Big\|\Big(\frac{1}{p^2-k^2}|V_\ell|^{1/2} - |g_k\rangle\big\langle|V_\ell|^{1/2}\big|\Big)P_\ell|V_\ell^{1/2}\rangle\Big\|_{L^2}\\ &= \left|\frac{\langle|V_\ell|^{1/2}|\phi_\ell\rangle}{e_\ell\langle J_\ell\phi_\ell|\phi_\ell\rangle}\right|\left(\int_{\mathbb{R}^3}\left|\int_{\mathbb{R}^3}|V_\ell|^{1/2}(z)\phi_\ell(z)\big(g_k(z-x)-g_k(x)\big)\,\mathrm{d}^3z\right|^2\mathrm{d}^3x\right)^{1/2}\\ &= \left|\frac{\langle|V_\ell|^{1/2}|\phi_\ell\rangle}{4\pi e_\ell\langle J_\ell\phi_\ell|\phi_\ell\rangle}\right|\left(\int_{\mathbb{R}^6}\Omega_k(z,w)|V_\ell|^{1/2}(z)\phi_\ell(z)|V_\ell|^{1/2}(w)\phi_\ell(w)\,\mathrm{d}^3z\,\mathrm{d}^3w\right)^{1/2},\end{aligned} \tag{3.6}$$

where

$$\begin{aligned}\Omega_k(z,w) &= (4\pi)^2 \int_{\mathbb{R}^3} [g_{\bar{k}}(x-z) - g_{\bar{k}}(x)][g_k(x-w) - g_k(x)]\,\mathrm{d}^3x \\ &= F_k(w-z) + F_k(0) - F_k(w) - F_k(z)\,.\end{aligned}$$

The bound (3.4) implies that

$$|\Omega_k(z,w)| \le \frac{1}{2\pi}\left(1 + \frac{|\Re(k)|}{2|\Im(k)|}\right)(|z|+|w|).$$

Together with Consequence 2(iii) and (iv) we are thus able to estimate (3.6) by $O(|e_\ell|^{1/2})$. This implies (3.2a). In order to get (3.2b) we make use of (3.5) and Consequence 2(iii) and evaluate

$$\begin{aligned}\left\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}|\phi_\ell\rangle\right\|_{L^2} &\le \| |g_k\rangle\langle |V_\ell|^{1/2}|\phi_\ell\rangle \|_{L^2} + \left\|\Big(\frac{1}{p^2-k^2}|V_\ell|^{1/2} - |g_k\rangle\langle |V_\ell|^{1/2}|\Big)|\phi_\ell\rangle\right\|_{L^2} \\ &= |\langle |V_\ell| |\phi_\ell\rangle| + O(|e_\ell|^{1/2}) = O(|e_\ell|^{1/2}).\end{aligned}$$

This completes the proof. □

Since the norm of ② diverges in the limit of small ℓ we need to keep track of precise error bounds. In order to do that, we start by rewriting the term ② in a particularly useful way, which is presented in the following lemma.

Lemma 3.

$$\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2-k^2}|V_\ell|^{1/2}} = \Big(1 - \frac{1}{\frac{4\pi}{ik} + 4\pi a(V_\ell)}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\Big)\frac{1}{1+Q_\ell}\frac{1}{1+B_\ell}, \tag{3.7}$$

where

$$Q_\ell = \frac{1}{1+B_\ell}R_\ell\left(1 - \frac{1}{\frac{4\pi}{ik} + 4\pi a(V_\ell)}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\right) \tag{3.8}$$

and where R_ℓ is the operator with integral kernel

$$R_\ell(x,y) = -\frac{ik}{4\pi}V_\ell^{1/2}(x) r(ik|x-y|)|V_\ell|^{1/2}(y) \tag{3.9}$$

with $r(z) = \dfrac{\mathrm{e}^z - 1 - z}{z}$.

Moreover, Q_ℓ satisfies

$$\|Q_\ell\| = O(|e_\ell|^{1/2}), \tag{3.10a}$$

$$\left\|Q_\ell \frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\right\| = O(|e_\ell|^{1/2}). \tag{3.10b}$$

Proof. The integral kernel of the operator $(p^2-k^2)^{-1}$ is given by $g_k(x-y)$. We expand this function as

$$g_k(x) = \frac{1}{4\pi}\frac{\mathrm{e}^{ik|x|}}{|x|} = \frac{1}{4\pi}\frac{1}{|x|} + \frac{ik}{4\pi} - \frac{ik}{4\pi}r(ik|x|),$$

where $r(z) = \frac{\mathrm{e}^z-1-z}{z}$. We insert this expansion in the expression for ② and thus obtain the identity

$$1 + V_\ell^{1/2}\frac{1}{p^2-k^2}|V_\ell|^{1/2} = 1 + B_\ell + \frac{ik}{4\pi}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}| + R_\ell$$

with R_ℓ defined in (3.9). We further rewrite this expression as

$$(1+B_\ell)\left(1+\frac{1}{1+B_\ell}\left(\frac{ik}{4\pi}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|+R_\ell\right)\right)$$
$$=(1+B_\ell)\left(1+\frac{1}{1+B_\ell}R_\ell\frac{1}{1+\frac{ik}{4\pi}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|}\right)\left(1+\frac{ik}{4\pi}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\right).$$

The inverse of the operator in the last parenthesis can be calculated explicitly, and is given by

$$\left(1+\frac{ik}{4\pi}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\right)^{-1}=1-\frac{1}{\frac{4\pi}{ik}+4\pi a(V_\ell)}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|,$$

at least whenever $a(V_\ell)\neq i/k$, which we can assume for small enough ℓ. Hence (3.7) holds, with Q_ℓ defined in (3.8).

We will now prove (3.10a) and (3.10b). We have

$$\|Q_\ell\|\leq\left\|\frac{1}{1+B_\ell}R_\ell\right\|+\frac{1}{\left|\frac{4\pi}{ik}+4\pi a(V_\ell)\right|}\left\|\frac{1}{1+B_\ell}R_\ell\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\right\|_{L^2}\|V_\ell\|_{L^1}^{1/2},$$
$$\left\|Q_\ell\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\right\|\leq\left\|\frac{1}{1+B_\ell}R_\ell\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\right\|$$
$$+\frac{1}{\left|\frac{4\pi}{ik}+4\pi a(V_\ell)\right|}\left\|\frac{1}{1+B_\ell}R_\ell\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\right\|_{L^2}\left\|\frac{1}{p^2-\bar{k}^2}|V_\ell|^{1/2}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\right\|_{L^2}.$$

The norm $\|V_\ell\|_{L^1}$ is uniformly bounded by assumption, and it follows from Lemma 2 that also $\left\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\right\|_{L^2}$ is uniformly bounded. Hence it suffices to bound the following expressions:

$$\|\frac{1}{1+B_\ell}R_\ell\|, \tag{3.11a}$$

$$\left\|\frac{1}{1+B_\ell}R_\ell\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\right\|_{L^2}, \tag{3.11b}$$

$$\left\|\frac{1}{1+B_\ell}R_\ell\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\right\|. \tag{3.11c}$$

To this aim we again use the decomposition (3.3). For (3.11a) note that

$$\begin{aligned}\|R_\ell\|_2^2&=\frac{|k|^2}{(4\pi)^2}\int_{\mathbb{R}^6}|V_\ell(x)||r(ik|x-y|)|^2|V_\ell(y)|\,\mathrm{d}^3x\,\mathrm{d}^3y\\&\leq\frac{c^2|k|^2}{(4\pi)^2}\int_{\mathbb{R}^6}|V_\ell(x)||x-y|^2|V_\ell(y)|\,\mathrm{d}^3x\,\mathrm{d}^3y\\&\leq\frac{4c^2|k|^2}{(4\pi)^2}\|V_\ell\|_{L^1}\int_{\mathbb{R}^3}|V_\ell(x)|\,|x|^2\,\mathrm{d}^3x=O(e_\ell^2),\end{aligned} \tag{3.12}$$

using $|r(z)|\leq c|z|$ for $\Re z<0$ and some $c>0$, as well as Assumptions (A3) and (A4). Since the last term in (3.3) is uniformly bounded by Consequence 1, $\|\frac{1}{1+B_\ell}(1-P_\ell)R_\ell\|_2=O(e_\ell)$ and $\|R_\ell\frac{1}{1+B_\ell}(1-P_\ell)\|_2=O(e_\ell)$. On the other hand

$$\|P_\ell R_\ell\|=\frac{\|R_\ell^*J_\ell\phi_\ell\|_{L^2}}{|\langle J_\ell\phi_\ell|\phi_\ell\rangle|},$$

where

$$(R_\ell^*J_\ell\phi_\ell)(x)=\frac{i\bar{k}}{4\pi}\int_{\mathbb{R}^3}|V_\ell(x)|^{1/2}r(-i\bar{k}|x-y|)|V_\ell(y)|^{1/2}\phi_\ell(y)\,\mathrm{d}^3y.$$

Using again the above pointwise bound on r, it follows from Consequence 2 that

$$\|P_\ell R_\ell\| = O(|e_\ell|^{3/2})\,. \tag{3.13}$$

Thus (3.11a) $= O(|e_\ell|^{1/2})$.

Finally, we estimate (3.11b) and (3.11c). Proceeding as above one also shows that $\|R_\ell \frac{1}{1+B_\ell}\| = O(|e_\ell|^{1/2})$. Hence, in the decomposition (3.3) for the vector

$$\frac{1}{1+B_\ell} R_\ell \frac{1}{1+B_\ell} |V_\ell^{1/2}\rangle$$

and the operator

$$\frac{1}{1+B_\ell} R_\ell \frac{1}{1+B_\ell} V_\ell^{1/2} \frac{1}{p^2-k^2},$$

we see that the only parts left to estimate are

$$\frac{1}{e_\ell^2} P_\ell R_\ell P_\ell |V_\ell^{1/2}\rangle = \frac{1}{e_\ell^2} \langle J_\ell \phi_\ell | R_\ell \phi_\ell\rangle \frac{\langle |V_\ell|^{1/2} | \phi_\ell\rangle}{|\langle J_\ell\phi_\ell|\phi_\ell\rangle|^2} |\phi_\ell\rangle, \tag{3.14a}$$

$$\frac{1}{e_\ell^2} P_\ell R_\ell P_\ell V_\ell^{1/2} \frac{1}{p^2-k^2} = \frac{1}{e_\ell^2} \langle J_\ell \phi_\ell | R_\ell \phi_\ell\rangle \frac{|\phi_\ell\rangle\langle\phi_\ell| |V_\ell|^{1/2} \frac{1}{p^2-k^2}}{|\langle J_\ell\phi_\ell|\phi_\ell\rangle|^2}. \tag{3.14b}$$

Using again Consequence 2 and the pointwise bound on r we obtain $|\langle J_\ell\phi_\ell|R_\ell\phi_\ell\rangle| = O(e_\ell^2)$. In particular, we conclude that the L^2-norm of the vector in (3.14a) is of order $O(|e_\ell|^{1/2})$. The same argument applies to the operator in (3.14b) after using (3.5). This shows that (3.11b) and (3.11c) are of order $O(|e_\ell|^{1/2})$, and completes the proof. □

The estimates (3.10a) and (3.10b) suggest that for small ℓ we may drop Q_ℓ in ② in (3.1). With the help of the identity (3.7) and the expansion $\frac{1}{1+Q_\ell} = 1 - \frac{1}{1+Q_\ell} Q_\ell$ the second summand on the right side of (3.1) decomposes into two parts, namely

$$-\frac{1}{p^2-k^2} |V_\ell|^{1/2} \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2-k^2} |V_\ell|^{1/2}} V_\ell^{1/2} \frac{1}{p^2-k^2} = \mathrm{I}_\ell + \mathrm{II}_\ell,$$

with

$$\mathrm{I}_\ell = -\frac{1}{p^2-k^2} |V_\ell|^{1/2} \Big(1 - \frac{1}{\frac{4\pi}{ik} + 4\pi a(V_\ell)} \frac{1}{1+B_\ell} |V_\ell^{1/2}\rangle\langle |V_\ell|^{1/2}|\Big) \frac{1}{1+B_\ell} V_\ell^{1/2} \frac{1}{p^2-k^2},$$

$$\mathrm{II}_\ell = \frac{1}{p^2-k^2} |V_\ell|^{1/2} \Big(1 - \frac{1}{\frac{4\pi}{ik} + 4\pi a(V_\ell)} \frac{1}{1+B_\ell} |V_\ell^{1/2}\rangle\langle |V_\ell|^{1/2}|\Big) \times \frac{1}{1+Q_\ell} Q_\ell \frac{1}{1+B_\ell} V_\ell^{1/2} \frac{1}{p^2-k^2}.$$

The term I_ℓ contains the main part, whereas II_ℓ vanishes in operator norm for small ℓ. This is the content of the following lemma, which immediately implies the statement of Theorem 1. Its proof relies heavily on Lemmas 2 and 3.

Lemma 4.

$$\Big\| \mathrm{I}_\ell + \frac{4\pi}{a(V_\ell)^{-1} + ik} |g_k\rangle\langle g_k| \Big\| = O(|e_\ell|^{1/2}), \tag{3.15a}$$

$$\|\mathrm{II}_\ell\| = O(|e_\ell|^{1/2}). \tag{3.15b}$$

Proof. We first show (3.15a). We can write

$$\mathrm{I}_\ell = -\frac{1}{p^2-k^2} |V_\ell|^{1/2} \frac{1}{1+B_\ell} V_\ell^{1/2} \frac{1}{p^2-k^2} + \frac{1}{\frac{4\pi}{ik} + 4\pi a(V_\ell)} \frac{1}{p^2-k^2} |V_\ell|^{1/2} \frac{1}{1+B_\ell} |V_\ell^{1/2}\rangle\langle |V_\ell|^{1/2}| \frac{1}{1+B_\ell} V_\ell^{1/2} \frac{1}{p^2-k^2}.$$

It turns out that both summands converge in operator norm to the projector $|g_k\rangle\langle g_k|$, multiplied by numbers which add up to $-\frac{-4\pi}{a^{-1}+ik}$. More precisely, we are going derive to the following asymptotic behavior

$$\begin{aligned}
&\Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}-4\pi a(V_\ell)|g_k\rangle\langle g_k|\Big\| \\
&= \Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}-|g_k\rangle\big\langle|V_\ell|^{1/2}\big|\frac{1}{1+B_\ell}\big|V_\ell^{1/2}\big\rangle\langle g_k|\Big\| \\
&\le \Big\|\Big(\frac{1}{p^2-k^2}|V_\ell|^{1/2}-|g_k\rangle\big\langle|V_\ell|^{1/2}\big|\Big)\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\Big\| \\
&\quad+\Big\||g_k\rangle\big\langle|V_\ell|^{1/2}\big|\frac{1}{1+B_\ell}\Big(V_\ell^{1/2}\frac{1}{p^2-k^2}-\big|V_\ell^{1/2}\big\rangle\langle g_k|\Big)\Big\| \\
&= O(|e_\ell|^{1/2})
\end{aligned}\tag{3.16a}$$

and

(3.16b)

$$\begin{aligned}
&\Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}-\big(4\pi a(V_\ell)\big)^2|g_k\rangle\langle g_k|\Big\| \\
&\le \Big\|\Big(\frac{1}{p^2-k^2}|V_\ell|^{1/2}-|g_k\rangle\big\langle|V_\ell|^{1/2}\big|\Big)\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\Big\| \\
&\quad+4\pi|a(V_\ell)|\Big\||g_k\rangle\langle|V_\ell|^{1/2}|\frac{1}{1+B_\ell}\Big(V_\ell^{1/2}\frac{1}{p^2-k^2}-\big|V_\ell^{1/2}\big\rangle\langle g_k|\Big)\Big\| \\
&= O(|e_\ell|^{1/2}),
\end{aligned}$$

where we made use of the expression $a(V_\ell)=\frac{1}{4\pi}\big\langle|V_\ell|^{1/2}\big|\frac{1}{1+B_\ell}\big|V_\ell^{1/2}\big\rangle$ for the scattering length. The bounds (3.16a) and (3.16b) are in fact simple consequences of Lemma 2. Eq. (3.16a) follows immediately from (3.2a) and (3.2b). To see (3.16b) we apply (3.2a) twice, once to the first vector in the first term on the right side, and once to the second.

In order to show (3.15b) we simply bound $\mathbb{I}_\ell$ by

$$\begin{aligned}
\|\mathbb{I}_\ell\| \le{}& \Big\|\frac{1}{p^2-k^2}|V_\ell|^{1/2}\Big(1-\frac{1}{\frac{4\pi}{ik}+4\pi a(V_\ell)}\frac{1}{1+B_\ell}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|\Big)\frac{1}{1+Q_\ell}\Big\| \\
&\times\Big\|Q_\ell\frac{1}{1+B_\ell}V_\ell^{1/2}\frac{1}{p^2-k^2}\Big\| \le O(|e_\ell|^{1/2}),
\end{aligned}$$

where we used that the first term is uniformly bounded because of (3.2a), whereas the second term vanishes like $O(|e_\ell|^{1/2})$ thanks to (3.10b). □

4. Proof of Consequences 1 and 2

Proof of Consequence 1. We pick some $\psi\in L^2(\mathbb{R}^3)$ and set

$$\varphi=\frac{1}{1+J_\ell X_\ell}(1-P_\ell)\psi=\frac{1}{J_\ell+X_\ell}J_\ell(1-P_\ell)\psi\,.\tag{4.1}$$

Below, we are going to show that there exists a constant $c>0$ such that for small enough ℓ

$$\langle\varphi|(1-X_\ell^-)\varphi\rangle\ge c\|\varphi\|^2_{L^2}.\tag{4.2}$$

In combination with Lemma 1 this inequality yields

$$\sqrt{2}\|\varphi\|\|(J_\ell+X_\ell)\varphi\|\ge\langle\varphi|(1-X_\ell^-)\varphi\rangle\ge c\|\varphi\|^2,$$

which further implies that

$$\|\psi\|\ge\|J_\ell(1-P_\ell)\psi\|=\|(J_\ell+X_\ell)\varphi\|\ge\frac{c}{\sqrt{2}}\|\varphi\|=\frac{c}{\sqrt{2}}\|(1+B_\ell)^{-1}(1-P_\ell)\psi\|\,,$$

proving the statement.

It remains to show the inequality (4.2). To this aim we denote by ϕ_ℓ^- the eigenvector corresponding to the smallest eigenvalue e_ℓ^- of $1 - X_\ell^-$ and by $P_{\phi_\ell^-}$ the orthogonal projection onto ϕ_ℓ^-. By assumption, the Birman-Schwinger operator X_ℓ^- corresponding to the potential V_ℓ^- has only one eigenvalue close to 1. All other eigenvalues are separated from 1 by a gap of order one. Hence there exists $c_1 > 0$ such that

$$(1 - X_\ell^-)(1 - P_{\phi_\ell^-}) \geq c_1$$

and, therefore,

$$\begin{aligned}\langle\varphi|(1 - X_\ell^-)\varphi\rangle &\geq c_1\langle\varphi|(1 - P_{\phi_\ell^-})\varphi\rangle + e_\ell^-\langle\varphi|P_{\phi_\ell^-}\varphi\rangle \\ &= c_1\|\varphi\|_{L^2}^2 + (e_\ell^- - c_1)\langle\varphi|P_{\phi_\ell^-}\varphi\rangle.\end{aligned}$$

With $P_{J_\ell\phi_\ell} = |J_\ell\phi_\ell\rangle\langle J_\ell\phi_\ell|$ being the orthogonal projection onto $J_\ell\phi_\ell$ we can write

$$\varphi = (1 - P_{J_\ell\phi_\ell})\varphi,$$

simply for the reason that, because of (4.1) and the fact that P_ℓ commutes with B_ℓ,

$$P_{J_\ell\phi_\ell}\varphi = P_{J_\ell\phi_\ell}(1 + B_\ell)^{-1}(1 - P_\ell)\psi = P_{J_\ell\phi_\ell}(1 - P_\ell)(1 + B_\ell)^{-1}\psi = 0\,.$$

Consequently,

$$\begin{aligned}|\langle\varphi|P_{\phi_\ell^-}\varphi\rangle| &= |\langle\varphi|(1 - P_{J_\ell\phi_\ell})P_{\phi_\ell^-}\varphi\rangle| \leq \|\varphi\|_{L^2}^2\|(1 - P_{J_\ell\phi_\ell})P_{\phi_\ell^-}\| \\ &= \|\varphi\|_{L^2}^2\|(1 - P_{J_\ell\phi_\ell})\phi_\ell^-\|^2 = \|\varphi\|_{L^2}^2\|(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\|^2\,.\end{aligned}$$

To estimate $\|(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\|$, we apply Lemma 1 to ϕ_ℓ and obtain

$$\begin{aligned}\sqrt{2}\,e_\ell = \sqrt{2}\,\|(J_\ell + X_\ell)\phi_\ell\| &\geq \langle\phi_\ell|(1 - X_\ell^-)\phi_\ell\rangle = \langle J_\ell\phi_\ell|(1 - X_\ell^-)J_\ell\phi_\ell\rangle \\ &= e_\ell^-|\langle J_\ell\phi_\ell|\phi_\ell^-\rangle|^2 + \langle(1 - P_{\phi_\ell^-})J_\ell\phi_\ell|(1 - X_\ell^-)(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\rangle \\ &\geq e_\ell^-|\langle J_\ell\phi_\ell|\phi_\ell^-\rangle|^2 + c_1\|(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\|^2\,.\end{aligned}$$

This shows that $\|(1 - P_{J_\ell\phi_\ell})P_{\phi_\ell^-}\| = O(|e_\ell|^{1/2})$ and consequently (4.2) holds for small enough ℓ. □

Proof of Consequence 2. (i) Simply bound $|x| \leq \frac{1}{2}(|e_\ell| + |x|^2/|e_\ell|)$ and use Assumptions (A3) and (A4).

(ii) Lemma 1 applied to ϕ_ℓ implies that

$$\begin{aligned}\Big\langle\phi_\ell\Big|(V_\ell^+)^{1/2}\frac{1}{p^2}(V_\ell^+)^{1/2}\phi_\ell\Big\rangle &\leq \sqrt{2}|e_\ell| + |e_\ell^-|, \\ \Big\langle\phi_\ell\Big|\big(1 - (V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2}\big)\phi_\ell\Big\rangle &\leq \sqrt{2}|e_\ell|\,,\end{aligned} \tag{4.3}$$

where we used $1 - (V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2} \geq e_\ell^-$. Note, that by 1 $|e_\ell^-| = O(e_\ell)$. Now (ii) follows from the following argument. Because of (2.8) we know that

$$\begin{aligned}\sqrt{2}|e_\ell| = \sqrt{2}\|(J_\ell + X_\ell)\phi_\ell\|_{L^2} &\geq \langle\phi_\ell^+|(1 + X_\ell^+)\phi_\ell^+\rangle + \langle\phi_\ell^-|(1 - X_\ell^-)\phi_\ell^-\rangle \\ &= \|\phi_\ell^+\|_{L^2}^2 + \langle\phi_\ell^+|X_\ell^+\phi_\ell^+\rangle + \langle\phi_\ell^-|(1 - X_\ell^-)\phi_\ell^-\rangle,\end{aligned}$$

where $\phi_\ell = \phi_\ell^+ + \phi_\ell^-$ with $\mathrm{supp}(\phi_\ell^-) \subseteq \mathrm{supp}(V_\ell^-)$ and $\mathrm{supp}(\phi_\ell^+) \cap \mathrm{supp}(V_\ell^-) = \emptyset$. Using that $1 - X_\ell^-$ has $e_\ell^- = O(e_\ell)$ as lowest eigenvalue, we conclude that

$$\Big\langle\frac{1 + J_\ell}{2}\phi_\ell\Big|\phi_\ell\Big\rangle = \|\phi_\ell^+\|_{L^2}^2 = O(e_\ell). \tag{4.4}$$

(iii), (iv) For $q = 0, 1$ we evaluate

$$\int_{\mathbb{R}^3} |x|^q\,|V_\ell|^{1/2}\,|\phi_\ell|\,\mathrm{d}^3x = \big\langle |V_\ell^+|^{1/2}|\cdot|^q \big| |\phi_\ell| \big\rangle + \big\langle (V_\ell^-)^{1/2}|\cdot|^q \big| |\phi_\ell| \big\rangle$$
$$= \big\langle |V_\ell^+|^{1/2}|\cdot|^q \big| \frac{1}{2}(1+J_\ell)|\phi_\ell| \big\rangle + \big\langle (V_\ell^-)^{1/2}|\cdot|^q \big| |\phi_\ell| \big\rangle$$
$$\leq \| V_\ell^+ |\cdot|^{2q} \|_{L^1}^{1/2} \langle \phi_\ell | \frac{1}{2}(1+J_\ell)\phi_\ell \rangle^{1/2} + \| |\cdot|^{2q} V_\ell^- \|_{L^1}^{1/2},$$

which is $O(|e_\ell|^{1/2})$ for $q = 0$ and $O(|e_\ell|^{3/2})$ for $q = 1$ by Assumption (A4) and (4.4). □

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Received 22/05/2013

A.1.2 On the BCS gap equation for superfluid fermionic gases

On the BCS gap equation for superfluid fermionic gases

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March 12, 2014

Abstract

We present a rigorous derivation of the BCS gap equation for superfluid fermionic gases with point interactions. Our starting point is the BCS energy functional, whose minimizer we investigate in the limit when the range of the interaction potential goes to zero.

1 Introduction

In BCS theory [1, 2, 3] of superfluid fermionic gases the interaction between the spin-1/2 fermions is usually modeled by a contact potential. This approximation is justified for the low density atomic gases usually observed in the lab, since the range of the effective interaction is much smaller than the mean particle distance. In the theoretical physics literature [2, 4, 3] the states of superfluidity are usually characterized via the simplified BCS gap equation

$$-\frac{1}{4\pi a}=\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{\tanh\left(\frac{\sqrt{(p^2-\mu)^2+|\Delta|^2}}{2T}\right)}{\sqrt{(p^2-\mu)^2+|\Delta|^2}}-\frac{1}{p^2}\right)\mathrm{d}^3p\,, \tag{1}$$

where μ is a fixed chemical potential and Δ is the corresponding order parameter of the system. This order parameter does not vanish below the critical temperature T_c, uniquely defined by

$$-\frac{1}{4\pi a}=\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{\tanh\left(\frac{p^2-\mu}{2T_c}\right)}{p^2-\mu}-\frac{1}{p^2}\right)\mathrm{d}^3p$$

for $a < 0$. The parameter a is the scattering length of the corresponding interaction and the usual argument for the derivation of equation (1) involves an ad-hoc renormalization scheme. The main goal of this paper is to give a rigorous derivation of equation (1) starting from the BCS functional of superfluidity [2, 3, 5] for a sequence of interaction potentials V_ℓ with range tending to zero, and scattering length $a(V_\ell)$ converging to a negative a. The present result is a consequence of our previous work [6] where we treated the more general case of BCS-Hartree-Fock theory and where we allowed for potentials with strong repulsive core. Dropping the direct and exchange term, however, as we do here, allows us to give a shorter, more transparent derivation of (1), and also to work with simpler assumptions on the interaction potentials.

2 The Model

We consider a gas of spin 1/2 fermions in the thermodynamic limit at temperature $T \geq 0$ and chemical potential $\mu \in \mathbb{R}$. The particles interact via a local two-body potential which we denote by V. The state of the system is described by two functions $\hat{\gamma} : \mathbb{R}^3 \to \mathbb{R}_+$ and $\hat{\alpha} : \mathbb{R}^3 \to \mathbb{C}$, which are conveniently combined into a 2×2 matrix

$$\Gamma(p) = \begin{pmatrix} \hat{\gamma}(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1 - \hat{\gamma}(-p) \end{pmatrix}, \tag{2}$$

required to satisfy $0 \leq \Gamma \leq \mathbb{1}_{\mathbb{C}^2}$ at every point $p \in \mathbb{R}^3$. The function $\hat{\gamma}$ is interpreted as the momentum distribution of the gas, while α (the inverse Fourier transform of $\hat{\alpha}$) is the Cooper pair wave function. Note that there are no spin variables in Γ; the full, spin dependent Cooper pair wave function is the product of $\alpha(x-y)$ with an antisymmetric spin singlet.

The *BCS functional* $\mathcal{F}_T^V$, whose infimum over all states Γ describes the negative of the pressure of the system, is given as

$$\mathcal{F}_T^V(\Gamma) = \int_{\mathbb{R}^3} (p^2 - \mu)\hat{\gamma}(p)\,\mathrm{d}^3p + \int_{\mathbb{R}^3} |\alpha(x)|^2 V(x)\,\mathrm{d}^3x - TS(\Gamma), \tag{3}$$

where

$$S(\Gamma) = -\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\big(\Gamma(p)\ln\Gamma(p)\big)\,\mathrm{d}^3p$$

is the entropy of the state Γ. The functional (3) can be obtained by restricting the many-body problem on Fock space to translation-invariant and spin-rotation invariant quasi-free states, and dropping the direct and exchange term in the interaction energy, see [5, Appendix A] and [7].

The *normal state* Γ_0 is the minimizer of the functional (3) restricted to states with $\alpha = 0$. It is given by

$$\hat{\gamma}_0(p) = \frac{1}{1 + \mathrm{e}^{\frac{p^2-\mu}{T}}}.$$

The system is said to be in a superfluid phase if and only if the minimum of $\mathcal{F}_T^V$ is not attained at a normal state, and we call a normal state Γ_0 *unstable* in this case.

In a previous work [5] we thoroughly studied the functional (3). It is not difficult to see that this functional has a (not necessarily unique) minimizer (γ, α). More difficult is the question under which circumstances it is possible to guarantee that α does not vanish. Such a non-vanishing α in fact describes a macroscopic coherence of pairs such that the system displays a superfluid behavior. The corresponding Euler-Lagrange equations for γ and α can be equivalently expressed via $\Delta = 2(2\pi)^{-3/2}\hat{V} * \hat{\alpha}$ in the form of the BCS *gap equation*

$$\Delta(p) = -\frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q) \frac{\Delta(q)}{E_\mu^\Delta(q)} \tanh \frac{E_\mu^\Delta(q)}{2T} \, \mathrm{d}^3 q \tag{4}$$

with $E_\mu^\Delta(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$; here, $\hat{V}$ denotes the Fourier transform of V. The function $\Delta(p)$ is the order parameter and is related to the wavefunction of the *Cooper pairs*. The equation (4) is highly non-linear; nonetheless, it is possible to show [5] that the existence of a non-trivial solution to (4) at some temperature T is equivalent to the fact that a certain *linear operator* has a negative eigenvalue. For $T = 0$ this operator is given by the Schrödinger-type operator $|-\Delta - \mu| + V$. This rather astonishing fact that one can reduce a non-linear to a linear problem, allowed for a more thorough mathematical study. Using spectral-theoretic methods, the class of potentials leading to a non-trivial solution for (4) has been precisely characterized. For instance, in [8] it was shown that if $\int V(x)dx < 0$, then there exists a critical temperature $T_c(V) > 0$ such that (4) attains a non-trivial solution for all $T < T_c(V)$, whereas there is no solution for $T \geq T_c(V)$. Additionally, in [8] the precise asymptotic behavior of $T_c(\lambda V)$ in the small coupling limit $\lambda \to 0$ was determined; the resulting expression generalizes well-known formulas in the physics literature [9, 3] valid only at low density. The low density limit $\mu \to 0$ of the critical temperature was studied in [10].

3 Main Results

We study the case of short-range interaction potentials V_ℓ, with range ℓ tending to zero in such a way that V_ℓ converges to a contact interaction. Such contact interactions are thoroughly studied in the literature [11, chap I.1.2-4] and are known to arise as a one parameter family of self-adjoint extensions of the Laplacian on $\mathbb{R}^3 \setminus \{0\}$. The relevant parameter uniquely determining the extension is, in fact, the scattering length, which we assume to be negative, in which case the resulting operator is non-negative, i.e., there are no bound states. In other words, we require that the scattering length $a(V_\ell)$ converges to a negative value as $\ell \to 0$, i.e.,

$$\lim_{\ell \to 0} a(V_\ell) = a < 0.$$

It was pointed out in [10, Equ. (3)] that the scattering length of any potential $V \in L^1 \cap L^{3/2}$ can be written as

$$a(V) = \frac{1}{4\pi} \left\langle |V|^{1/2} \middle| \frac{1}{1+V^{1/2}\frac{1}{p^2}|V|^{1/2}} V^{1/2} \right\rangle \tag{5}$$

where $V^{1/2}$ is defined by $V^{1/2} = V|V|^{-1/2}$. Note that in case of a two-body interaction that does allow bound states the system would display features of a Bose-Einstein condensate of fermion pairs in the low density limit, see [4, 12, 13, 14, 15].

In order to obtain a non-vanishing limit of the sequence of scattering lengths $a(V_\ell)$, we have to adjust the sequence of potentials so that the corresponding Schrödinger operator just barely fails to have a bound state. We shall follow the method of [11, chap I.1.2-4] and first choose a potential V such that $p^2 + V$ is non-negative and has a simple zero-energy resonance. Equivalently this means that the corresponding Birman-Schwinger operator

$$V^{1/2}\tfrac{1}{p^2}|V|^{1/2}$$

has -1 as lowest, simple, eigenvalue. Next we scale this potential and multiply it by a factor $\lambda(\ell) < 1$, such that the corresponding V_ℓ does no longer have a zero resonance, but a negative scattering length. Recall that a potential with zero resonance has an infinite scattering length.

To be precise, we define V_ℓ according to

$$V_\ell(x) = \lambda(\ell)\ell^{-2}V(\tfrac{x}{\ell}), \tag{6}$$

where $\lambda(0) = 1$, $\lambda < 1$ for all $\ell > 0$ and $1 - \lambda(\ell) = O(\ell)$. We are interested in the limit $\ell \to 0$ meaning that the range of the potential converges to zero. This scaling essentially leaves the $L^{3/2}$ norm of V invariant, but the L^1 norm vanishes linearly in ℓ. This is a major difference to the work [6] where we allowed the point interaction to be approximated by a sequence V_ℓ, whose L^1 norm converges to a positive number, with its $L^{3/2}$-norm even diverging. This required a new approach in the proof and led to a more general statement about contact interactions [16]. In the case considered here it suffices to rely on results of [11, chap I.1.2-4].

Our main objective now is to consider the solution Δ_ℓ of the BCS gap-equation (4), coming from a minimizer of the functional $\mathcal{F}_T^{V_\ell}$, and to show that in the limit where the range ℓ goes to zero, i.e., the potentials V_ℓ tend to a contact interaction, the order parameter Δ_ℓ converges to a constant function Δ, which satisfies the simplified equation (1). This equation appears throughout the physics literature as the one describing superfluid systems.

It is obvious that the critical temperature T_c is defined as the temperature where $\Delta = 0$ satisfies the equation (1). More precisely:

Definition 1 (Critical temperature)**.** *Let $\mu > 0$. The* critical temperature T_c *corresponding to the scattering length $a < 0$ is given by the equation*

$$-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{\tanh\left(\frac{p^2-\mu}{2T_c}\right)}{p^2 - \mu} - \frac{1}{p^2} \right) \mathrm{d}^3p. \tag{7}$$

Since the function

$$T \mapsto \int_{\mathbb{R}^3} \left(\frac{\tanh\left(\frac{p^2-\mu}{2T}\right)}{p^2-\mu} - \frac{1}{p^2} \right) \mathrm{d}^3 p$$

is strictly monotone in T the critical temperature T_c is unique.

As our main theorem we reproduce the BCS gap equation for contact interactions, see, e. g., [2, Eq. (10)], [4, Eq. (7)].

Theorem 1 (Effective Gap equation)**.** *Let $T \geq 0$, $\mu \in \mathbb{R}$ and assume $V \in L^{3/2}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ and $|x|V(x) \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Let further $(\hat{\gamma}_\ell, \hat{\alpha}_\ell)$ be a minimizer of $\mathcal{F}_T^{V_\ell}$ with corresponding $\Delta_\ell = 2(2\pi)^{-3/2}\hat{V}_\ell * \hat{\alpha}_\ell$. Then there exist $\Delta \geq 0$ such that $|\Delta_\ell(p)| \to \Delta$ pointwise as $\ell \to 0$. If $\Delta \neq 0$ then it satisfies the equation*

$$\boxed{-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^{\Delta}} - \frac{1}{p^2} \right) \mathrm{d}^3 p\,,} \tag{8}$$

where we use the abbreviations

$$K_{T,\mu}^{\Delta}(p) = \frac{E_\mu^\Delta(p)}{\tanh\left(\frac{E_\mu^\Delta(p)}{2T}\right)}\,, \quad E_\mu^\Delta(p) = \sqrt{(p^2-\mu)^2 + |\Delta|^2}\,.$$

Furthermore, the limiting Δ does not vanish if and only if $T < T_c$.

4 Proofs

Recall that we chose V so that $V^{1/2}\frac{1}{p^2}|V|^{1/2}$ has -1 as lowest simple eigenvalue, i.e., there is a unique ϕ, with

$$\left(V^{1/2}\tfrac{1}{p^2}|V|^{1/2} + 1 \right) \phi = 0.$$

With U_ℓ denoting the unitary operator $(U_\ell \varphi)(x) = \ell^{-3/2}\varphi(\frac{x}{\ell})$, we can rewrite

$$V_\ell(x) = \lambda(\ell)\ell^{-2}V(\tfrac{x}{\ell}) = \lambda(\ell)\ell^{-2}U_\ell V U_\ell^{-1}.$$

Since $U_\ell p^2 U_\ell^{-1} = \ell^2 p^2$, it is easy to see that

$$U_\ell V^{1/2}\frac{1}{p^2}|V|^{1/2}U_\ell^{-1} = \frac{1}{\lambda(\ell)}V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}.$$

Denoting $\phi_\ell = U_\ell \phi$, this implies

$$V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}\phi_\ell = \lambda(\ell)U_\ell V^{1/2}\frac{1}{p^2}|V|^{1/2}\phi = -\lambda(\ell)\phi_\ell. \tag{9}$$

showing that the lowest eigenvalue of $1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ is $1 - \lambda(\ell) = O(\ell)$. Moreover, note that

$$\|V_\ell\|_p = \lambda(\ell)\ell^{3/p-2}\|V\|_p \tag{10}$$

for $p \geq 1$.

Remark 1. *In [6, Appendix A.1], we show that the scattering length corresponding to the potential V_ℓ, indeed, converges to the negative value*

$$\lim_{\ell\to 0} a(V_\ell) = -\frac{1}{\lambda'(0)}\frac{|\langle |V|^{1/2}|\phi\rangle|^2}{\langle \operatorname{sgn}(V)\phi|\phi\rangle} < 0.$$

In the next Lemma, we derive a lower bound for the BCS functional which is uniform in ℓ. This will allow us to obtain limits for the order parameter Δ_ℓ.

Lemma 1. *There exists $C_1 > 0$, independent of ℓ, such that*

$$\mathcal{F}_T^{V_\ell}(\Gamma) \geq -C_1 + \frac{1}{2}\int_{\mathbb{R}^3} (1+p^2)(\hat\gamma - \hat\gamma_0)^2 \,\mathrm{d}^3p + \frac{1}{2}\int_{\mathbb{R}^3} |p|^b |\hat\alpha|^2 \,\mathrm{d}^3 p, \tag{11}$$

for $0 \leq b < 1$, where we denote $\hat\gamma_0(p) = \frac{1}{1+\mathrm{e}^{(p^2-\mu)/T}}$.

Proof. For details of the proof of this Lemma we refer to [6, Lemma 3]. The main observation in the proof is that we may express the difference $\mathcal{F}_T^{V_\ell}(\Gamma) - \mathcal{F}_T^{V_\ell}(\Gamma_0)$ as

$$\mathcal{F}_T^{V_\ell}(\Gamma) - \mathcal{F}_T^{V_\ell}(\Gamma_0) = \frac{T}{2}\mathcal{H}(\Gamma,\Gamma_0) + \int_{\mathbb{R}^3} V_\ell(x)|\alpha(x)|^2 \,\mathrm{d}^3x,$$

where $\mathcal{H}(\Gamma,\Gamma_0)$ is the relative entropy of Γ and Γ_0. By means of [17, Lemma 3], which is an extension of [18, Theorem 1], giving a bound on the relative entropy one obtains

$$\begin{aligned}\mathcal{F}_T^{V_\ell}(\Gamma) - \mathcal{F}_T^{V_\ell}(\Gamma_0) \geq{}& \left\langle \alpha \left| p^2 + V_\ell - \mu \right| \alpha \right\rangle \\ &+ \frac{1}{2}\int_{\mathbb{R}^3} (1+p^2)(\hat\gamma - \hat\gamma_0)^2 \,\mathrm{d}^3p - C\end{aligned}$$

for an appropriate constant C. By means of a Birman-Schwinger type argument one can further show that

$$p^2 + V_\ell \geq |p|^b - C_1\,,$$

uniformly in ℓ for $0 \leq b < 1$ and an appropriate C_1, which, together with the constraint $|\hat\alpha|^2 \leq 1$, then implies the statement.

□

It was shown in [5, Theorem 1] that the functional $\mathcal{F}_T^{V_\ell}$ attains a minimizer $(\gamma_\ell, \alpha_\ell)$ for each V_ℓ. Lemma 1, with $\hat\alpha_\ell(p) \leq 1$, immediately tells us that the terms

$$\int_{\mathbb{R}^3} (1+|p|^b)|\hat\alpha_\ell(p)| \,\mathrm{d}^3p \qquad \text{and} \qquad \int_{\mathbb{R}^3} (1+|p|^2)(\hat\gamma_\ell - \hat\gamma_0)^2 \,\mathrm{d}^3p$$

are uniformly bounded in ℓ. Let us further mention the following useful relations between Δ_ℓ and the minimizer $(\gamma_\ell, \alpha_\ell)$,

$$\hat\gamma_\ell = \frac{1}{2} - \frac{1}{2}\frac{p^2-\mu}{K_{T,\mu}^{\Delta_\ell}}, \qquad \Delta_\ell = 2K_{T,\mu}^{\Delta_\ell}\hat\alpha_\ell, \tag{12}$$

which follow from the corresponding Euler-Lagrange equations. One immediate consequence of these relations and Lemma 1 is the uniform boundedness of $\int_{\mathbb{R}^3} \hat{\gamma}_\ell(p)|p|^b \, \mathrm{d}^3p$, which implies

$$\lim_{R\to\infty} \lim_{\ell\to 0} \int_{|p|^2 \geq R} \hat{\gamma}_\ell(p) \, \mathrm{d}^3p = 0. \tag{13}$$

In the following lemma we show that, as $\ell \to 0$, pointwise limits for the main quantities exist. To this aim we introduce the notation

$$m_\mu^{\Delta_\ell}(T) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^{\Delta_\ell}} - \frac{1}{p^2} \right) \mathrm{d}^3p \, .$$

Lemma 2. *Let $(\gamma_\ell, \alpha_\ell)$ be a sequence of minimizers of $\mathcal{F}_T^{V_\ell}$ and $\Delta_\ell = \frac{2}{(2\pi)^{3/2}} \hat{V}_\ell * \hat{\alpha}_\ell$. Then there is a subsequence of Δ_ℓ, which we continue to denote by Δ_ℓ, and a $\Delta \in \mathbb{R}_+$ such that*

(i) $|\Delta_\ell(p)|$ converges pointwise to the constant function Δ as $\ell \to 0$,

(ii) $\lim_{\ell\to 0} m_\mu^{\Delta_\ell}(T) = m_\mu^{\Delta}(T)$.

We shall see later that it is not necessary to restrict to a subsequence, the result holds in fact for the whole sequence.

Proof. **(i)** Set $c_\ell = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} V_\ell(x)\alpha_\ell(x) \, \mathrm{d}^3x$. Then

$$\begin{aligned} |\Delta_\ell(p) - c_\ell| &\leq \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left| (e^{-ip\cdot x} - 1) V_\ell(x)\alpha_\ell(x) \right| \mathrm{d}^3x \\ &\leq (2\pi)^{-3/2} \|\alpha_\ell\|_2 \left(\int_{\mathbb{R}^3} \left| (e^{-ip\cdot x} - 1) V_\ell(x) \right|^2 \mathrm{d}^3x \right)^{1/2} . \end{aligned}$$

Now $\|\alpha_\ell\|_2$ is uniformly bounded in ℓ and $|\cdot|V \in L^2(\mathbb{R}^3)$ by assumption, so

$$\begin{aligned} \int_{\mathbb{R}^3} \left| (e^{-ip\cdot x} - 1) V_\ell(x) \right|^2 \mathrm{d}^3x &= \ell^{-1}\lambda(\ell)^2 \int_{\mathbb{R}^3} \left| (e^{-i\ell p\cdot x} - 1) V(x) \right|^2 \mathrm{d}^3x \\ &\leq \ell\lambda(\ell)^2 |p|^2 \big\| \, |\cdot| V \big\|_2^2. \end{aligned} \tag{14}$$

Hence, $|\Delta_\ell(p) - c_\ell|$ converges to zero pointwise. Since $\hat{\alpha}_\ell = -2(K_{T,\mu}^{\Delta_\ell})^{-1}\Delta_\ell$ is uniformly bounded in L^2, it is straightforward to see, using $E_\mu^{\Delta_\ell} \geq |\Delta_\ell|$, that the same holds for the sequence $\Delta_\ell / E_\mu^{\Delta_\ell}$. This fact can now be used to show that the sequence $|c_\ell|$ is a uniformly bounded. Assume on the contrary that $\bar{c} = \limsup_{\ell\to 0} |c_\ell| = \infty$. Then by dominated convergence

$$\limsup_{\ell\to 0} \int_{|p|\leq R} \frac{|\Delta_\ell|^2}{(p^2-\mu)^2 + |\Delta_\ell|^2} \, \mathrm{d}^3p = \int_{|p|\leq R} \limsup_{\ell\to 0} \frac{1}{\frac{(p^2-\mu)^2}{|c_\ell|^2} + 1} \, \mathrm{d}^3p = \frac{4}{3}\pi R^3. \tag{15}$$

However, the divergence of right side of Eq. (15) as $R \to \infty$ contradicts the uniform boundedness of $\Delta_\ell / E_\mu^{\Delta_\ell}$ in $L^2(\mathbb{R}^3)$. Hence $\bar{c} < \infty$ and $\lim_{\ell\to 0} |\Delta_\ell(p)| = \bar{c}$ for a suitable subsequence.

(ii) Obviously by (i) the integrand of $m_\mu^{\Delta_\ell}(T)$ converges pointwise to the integrand of $m_\mu^{\Delta}(T)$. By (12) we are able to rewrite the integrand as

$$\frac{1}{K_{T,\mu}^{\Delta_\ell}(p)} - \frac{1}{p^2} = \frac{1}{p^2-\mu} - \frac{1}{p^2} - \frac{2\hat{\gamma}_\ell(p)}{p^2-\mu}. \tag{16}$$

Using (13) we now conclude that

$$\lim_{R\to\infty} \lim_{\ell\to 0} \int_{|p|^2 \geq R} \left(\frac{1}{K_{T,\mu}^{\Delta_\ell}(p)} - \frac{1}{p^2} \right) \mathrm{d}^3 p = 0,$$

which together with the dominated convergence inside $|p|^2 \leq R$, implies the statement of (ii).

□

Proposition 1. *Let* $a = \lim_{\ell\to 0} a(V_\ell)$, *then*

$$\lim_{\ell\to 0} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^{\Delta_\ell}} - \frac{1}{p^2} \right) \mathrm{d}^3 p = -\frac{1}{4\pi a}. \tag{17}$$

Proof. We again follow the proof of [6, Theorem 2]. Observe that with help of the second relation in (12) the BCS gap equation (4) for α_ℓ can be conveniently written in the form

$$(K_{T,\mu}^{\Delta_\ell} + V_\ell)\alpha_\ell = 0, \qquad \text{with } \alpha_\ell \in H^1(\mathbb{R}^3)\,.$$

By means of the Birman–Schwinger principle one concludes that $K_{T,\mu}^{\Delta_\ell} + V_\ell$ having 0 as an eigenvalue is equivalent to $V_\ell^{1/2} \frac{1}{K_{T,\mu}^{\Delta_\ell}} |V_\ell|^{1/2}$ having -1 as eigenvalue.

We now rewrite $V_\ell^{1/2} \frac{1}{K_{T,\mu}^{\Delta_\ell}} |V_\ell|^{1/2}$ as

$$V_\ell^{1/2} \frac{1}{K_{T,\mu}^{\Delta_\ell}} |V_\ell|^{1/2} = V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2} + m_\mu^{\Delta_\ell}(T) |V_\ell^{1/2}\rangle\langle |V_\ell|^{1/2}| + A_{\mu,T,\ell}, \tag{18}$$

where $A_{\mu,T,\ell}$ is given in terms of the integral kernel

$$A_{\mu,T,\ell}(x,y) = \frac{V_\ell(x)^{\frac12} |V_\ell(y)|^{\frac12}}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^{\Delta_\ell}} - \frac{1}{p^2} \right) (\mathrm{e}^{-i(x-y)\cdot p} - 1)\, \mathrm{d}^3 p\,, \tag{19}$$

which can be estimated, e. g., by

$$|A_{\mu,T,\ell}(x,y)| \leq \frac{|V_\ell(x)|^{\frac12} |V_\ell(y)|^{\frac12}}{(2\pi)^3} \int_{\mathbb{R}^3} \left| \frac{1}{K_{T,\mu}^{\Delta_\ell}} - \frac{1}{p^2} \right| (|x-y|\ |p|)^{1/2}\, \mathrm{d}^3 p. \tag{20}$$

Using the relation (16) as well as the uniform boundedness of $\int_{\mathbb{R}^3} \hat{\gamma}_\ell(p)|p|^{1/2}\,\mathrm{d}^3p$ we are able to conclude that the integral

$$\int_{\mathbb{R}^3} \left|\frac{1}{K_{T,\mu}^{\Delta_\ell}} - \frac{1}{p^2}\right| |p|^{1/2}\,\mathrm{d}^3p = \int_{\mathbb{R}^3} \left|\frac{1}{p^2-\mu} - \frac{1}{p^2} - \frac{2\hat{\gamma}_\ell(p)}{p^2-\mu}\right| |p|^{1/2}\,\mathrm{d}^3p$$

is uniformly bounded in ℓ. We can thus bound the Hilbert-Schmidt norm of $A_{\mu,T,\ell}$ by

$$\|A_{\mu,T,\ell}\|_2 \leq \mathrm{const}\,\|V_\ell|\cdot|\|_1^{1/2}\|V_\ell\|_1^{1/2} \leq O(\ell^{3/2})\,. \tag{21}$$

We further proceed with equation (18). By construction, $1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ is invertible and thus can be factored out, i.e.,

$$1 + V_\ell^{1/2}\frac{1}{K_{T,\mu}^{\Delta_\ell}}|V_\ell|^{1/2} = \left(1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}\right)\times$$
$$\times\left[1 + \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}\left(m_\mu^{\Delta_\ell}(T)|V_\ell^{\frac{1}{2}}\rangle\langle|V_\ell|^{\frac{1}{2}}| + A_{T,\mu,\ell}\right)\right],$$

with the second term on the right hand side necessarily having an eigenvalue 0. With $J = V_\ell(x)/|V_\ell(x)|$ and $X = |V_\ell|^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$, we are able to rewrite

$$\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} = \frac{1}{1+JX} = 1 - JX^{1/2}\frac{1}{1+X^{1/2}JX^{1/2}}X^{1/2}\,.$$

This allows us to bound

$$\left\|\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}\right\| \leq 1 + \|X\|\left\|\frac{1}{1+X^{1/2}JX^{1/2}}\right\| \leq O(\ell^{-1}),$$

where we have used that, due to the HLS-inequality, $\|X\| \leq C\|V_\ell\|_{3/2}$, as well as the fact that $1+X^{1/2}JX^{1/2}$ is self-adjoint with its lowest eigenvalue of order $O(\ell)$. Indeed, $X^{1/2}JX^{1/2}$ has the same spectrum as JX. Hence,

$$\left\|\tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}A_{\mu,T,\ell}\right\| \leq \left\|\tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}\right\|\|A_{\mu,T,\ell}\| \leq O(\ell^{1/2}).$$

Since

$$\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}\left(m_\mu^{\Delta_\ell}(T)|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}| + A_{T,\mu,\ell}\right)$$

has an eigenvalue -1 and $1 + (1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2})^{-1}A_{\mu,T,\ell}$ is invertible for small enough ℓ, we can argue by factoring out the term $1+(1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2})^{-1}A_{\mu,T,\ell}$ that the rank one operator

$$m_\mu^{\Delta_\ell}(T)\left(1 + \frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}A_{\mu,T,\ell}\right)^{-1}\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|$$

has an eigenvalue -1, which, by taking the trace, implies

$$-1 = m_\mu^{\Delta_\ell}(T) \left\langle |V_\ell|^{1/2} \middle| \left[1 + \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} A_{\mu,T,\ell}\right]^{-1} \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} \middle| V_\ell^{1/2} \right\rangle . \tag{22}$$

With the aid of Eq. (5) and the resolvent identity, we can rewrite Eq. (22) as

$$\begin{aligned} &4\pi a(V_\ell) + \frac{1}{m_\mu^{\Delta_\ell}(T)} \\ &= \left\langle |V_\ell|^{1/2} \middle| \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} A_{\mu,T,\ell} \left[1 + \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} A_{\mu,T,\ell}\right]^{-1} \times \right. \\ &\quad \left. \times \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} \middle| V_\ell^{1/2} \right\rangle , \end{aligned} \tag{23}$$

where the right hand side is bounded by

$$\begin{aligned} &\|V_\ell\|_1 \left\| \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} \right\| \left\| \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} A_{\mu,T,\ell} \right\| \times \\ &\quad \times \left\| \left[1 + \tfrac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} A_{\mu,T,\ell}\right]^{-1} \right\| \leq O(\ell^{1/2}) . \end{aligned}$$

This implies Eq. (17) and completes the proof.

□

With the aid of Lemma 2 and Proposition 1, we can now finish the proof of Theorem 1.

Proof of Theorem 1. We know from Lemma 2 and Proposition 1 that $|\Delta_\ell(p)|$ has a subsequence that converges to a constant function Δ, which satisfies the equation

$$-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^\Delta} - \frac{1}{p^2} \right) \mathrm{d}^3 p.$$

Since the solution $|\Delta|$ of (8) is unique we obtain that the sequence $|\Delta_\ell(p)|$ converges to the unique solution of (8). Furthermore, this shows that the limit of $|\Delta_\ell|$ does not vanish in the case that $T < T_c$, and that the limit vanishes for $T \geq T_c$. □

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A.1.3 Translation-invariant quasi-free states for fermionic systems and the BCS approximation

Reviews in Mathematical Physics
Vol. 26, No. 7 (2014) 1450012 (37 pages)

DOI: 10.1142/S0129055X14500123

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Translation-invariant quasi-free states for fermionic systems and the BCS approximation*

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Received 24 May 2013
Accepted 6 June 2014
Published 17 July 2014

We study translation-invariant quasi-free states for a system of fermions with two-particle interactions. The associated energy functional is similar to the BCS functional but also includes direct and exchange energies. We show that for suitable short-range interactions, these latter terms only lead to a renormalization of the chemical potential, with the usual properties of the BCS functional left unchanged. Our analysis thus represents a rigorous justification of part of the BCS approximation. We give bounds on the critical temperature below which the system displays superfluidity.

Keywords: Superconductivity; quasi-free states; Birman–Schwinger principle; critical temperature; BCS functional.

Mathematics Subject Classification 2010: 82D50, 46N50

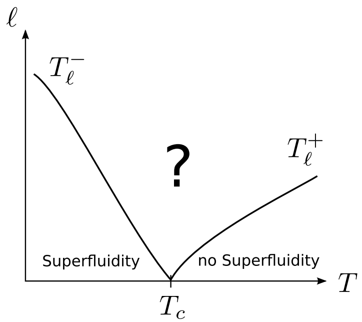
1. Introduction and Main Results

The BCS theory [5] was introduced in 1957 to describe superconductivity, and was later extended to the context of superfluidity [15, 20] as a microscopic description of fermionic gases with local pair interactions at low temperatures. It can be deduced from quantum physics in three steps. One restricts the allowed states of the system to quasi-free states, assumes translation-invariance and $SU(2)$ rotation invariance, and finally dismisses the direct and exchange terms in the energy. With these approximations, the resulting BCS functional depends, besides the temperature T and the chemical potential μ, on the interaction potential V, the momentum distribution γ and the Cooper pair wave function α. A non-vanishing α implies a macroscopic coherence of the particles involved, i.e. the formation of a condensate of Cooper pairs. This motivates the characterization of a superfluid phase by the existence of a minimizer of the BCS functional for which $\alpha \neq 0$.

A rigorous treatment of the BCS functional was presented in [9, 14, 13, 7], where the question was addressed for which interaction potentials V and at which temperatures T a superfluid phase exists. In the present work, we focus on the question to what extent it is justifiable to dismiss the direct and exchange terms in the energy. A heuristic justification was given in [15, 16], where it was argued that as long as the range of the interaction potential is suitably small, the only effect of the direct and exchange terms is to renormalize the chemical potential.

In this paper we derive a gap equation for the extended theory with direct and exchange terms and investigate the existence of non-trivial solutions for general interaction potentials. We give a rigorous justification for dismissing the two terms for potentials whose range ℓ is short compared to the scattering length a and the Fermi wave length $\frac{2\pi}{\sqrt{\mu}}$. The potentials are required to have a suitable repulsive core to assure stability of the system. We show that, for small enough ℓ, the system still can be described by the conventional BCS equation if the chemical potential is renormalized appropriately. In the limit $\ell \to 0$, the spectral gap function $\Delta_\ell(p)$ converges to a constant function and we recover the BCS equation in its form found in the physics literature.

While we do not prove that for fixed, finite ℓ there exists a critical temperature T_c such that superfluidity occurs if and only if $T < T_c$, we find bounds T_ℓ^+ and T_ℓ^- such that $T < T_\ell^-$ implies superfluidity and $T > T_\ell^+$ excludes superfluidity. Moreover, in the limit $\ell \to 0$ the two bounds converge to the same temperature, $\lim_{\ell\to 0} T_\ell^- = \lim_{\ell\to 0} T_\ell^+$, which can be determined by the usual BCS gap equation. The situation is illustrated in the following sketch.



We note that similar models as the one considered in our paper are sometimes referred to as Bogoliubov–Hartree–Fock theory and have been studied previously mainly with Newtonian interactions, modeling stars, and without the restriction to translation-invariant states [3, 17, 10]. The proof of existence of a minimizer in [17] turns out to be surprisingly difficult and even more strikingly, the appearance of pairing is still open. It was confirmed numerically for the Newton model and also for models with short range interaction in [18]. Hence the present work represents the first proof of existence of pairing in a translation-invariant Bogoliubov–Hartree–Fock model in the continuum. For the Hubbard model at half filling this was shown earlier in [4].

1.1. *The model*

We consider a gas of spin 1/2 fermions in the thermodynamic limit at temperature $T \geq 0$ and chemical potential $\mu \in \mathbb{R}$. The particles interact via a local two-body potential which we denote by V. We assume V to be reflection-symmetric, i.e. $V(-x) = V(x)$. The state of the system is described by two functions $\hat{\gamma} : \mathbb{R}^3 \to \mathbb{R}_+$ and $\hat{\alpha} : \mathbb{R}^3 \to \mathbb{C}$, with $\hat{\alpha}(p) = \hat{\alpha}(-p)$, which are conveniently combined into a 2×2 matrix

$$\Gamma(p) = \begin{pmatrix} \hat{\gamma}(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1 - \hat{\gamma}(-p) \end{pmatrix}, \tag{1.1}$$

required to satisfy $0 \leq \Gamma \leq \mathbb{1}_{\mathbb{C}^2}$ at every point $p \in \mathbb{R}^3$. The function $\hat{\gamma}$ is interpreted as the momentum distribution of the gas, while α (the inverse Fourier transform of $\hat{\alpha}$) is the Cooper pair wave function. Note that there are no spin variables in Γ; the full, spin dependent Cooper pair wave function is the product of $\alpha(x - y)$ with an antisymmetric spin singlet.

The *BCS-HF functional* $\mathcal{F}_T^V$, whose infimum over all states Γ describes the negative of the pressure of the system, is given as

$$\begin{aligned} \mathcal{F}_T^V(\Gamma) = &\int_{\mathbb{R}^3} (p^2 - \mu)\hat{\gamma}(p)\mathrm{d}^3p + \int_{\mathbb{R}^3} |\alpha(x)|^2 V(x)\mathrm{d}^3x - TS(\Gamma) \\ &- \int_{\mathbb{R}^3} |\gamma(x)|^2 V(x)\mathrm{d}^3x + 2\gamma(0)^2 \int_{\mathbb{R}^3} V(x)\mathrm{d}^3x, \end{aligned} \tag{1.2}$$

where

$$S(\Gamma) = -\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}(\Gamma(p) \ln \Gamma(p))\mathrm{d}^3p$$

is the entropy of the state Γ. Here, γ and α denote the inverse Fourier transforms of $\hat{\gamma}$ and $\hat{\alpha}$, respectively. The last two terms in (1.2) are referred to as the *exchange term* and *the direct term*, respectively. The functional (1.2) can be obtained by restricting the many-body problem on Fock space to translation-invariant and spin-rotation invariant quasi-free states, see [9, Appendix A] and [4]. The factor 2 in the last term in (1.2) originates from two possible orientations of the particle spin.

A *normal state* Γ_0 is a minimizer of the functional (1.2) restricted to states with $\alpha = 0$. Any such minimizer can easily be shown to be of the form

$$\hat{\gamma}_0(p) = \frac{1}{1 + \mathrm{e}^{\frac{\varepsilon^{\gamma_0}(p) - \tilde{\mu}^{\gamma_0}}{T}}}, \tag{1.3}$$

where we denote, for general γ,

$$\varepsilon^\gamma(p) = p^2 - \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (\hat{V}(p-q) - \hat{V}(0))\hat{\gamma}(q)\mathrm{d}^3q, \tag{1.4}$$

$$\tilde{\mu}^\gamma = \mu - \frac{2}{(2\pi)^{3/2}} \hat{V}(0) \int_{\mathbb{R}^3} \hat{\gamma}(p)\mathrm{d}^3p. \tag{1.5}$$

Notice that Eq. (1.3) is an implicit relation with γ_0 also appearing in the expression on the right-hand side of (1.3) via (1.4) and (1.5). In the absence of the exchange term, the normal state would be unique, but this is not necessarily the case here. The system is said to be in a superfluid phase if and only if the minimum of $\mathcal{F}_T^V$ is not attained at a normal state, and we call a normal state Γ_0 *unstable* in this case.

1.2. *Main results*

Our first goal is to characterize the existence of a superfluid phase for a large class of interaction potentials V. We first find sufficient conditions on V for (1.2) to have a minimizer. These conditions are stated in the following proposition.

Proposition 1 (Existence of Minimizers). *Let $\mu \in \mathbb{R}$, $0 \leq T < \infty$, and let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ be real-valued with $\|\hat{V}\|_\infty \leq 2\hat{V}(0)$. Then $\mathcal{F}_T^V$ is bounded from below and attains a minimizer (γ, α) on*

$$\mathcal{D} = \left\{ \Gamma \text{ of the form (1.1)} \;\middle|\; \begin{matrix} \hat{\gamma} \in L^1(\mathbb{R}^3, (1+p^2)\mathrm{d}^3p), \\ \alpha \in H^1(\mathbb{R}^3, \mathrm{d}^3x), \end{matrix} \; 0 \leq \Gamma \leq \mathbb{1}_{\mathbb{C}^2} \right\}.$$

Moreover, the function

$$\Delta(p) = \frac{2}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q)\hat{\alpha}(q)\mathrm{d}^3q \tag{1.6}$$

satisfies the BCS gap equation

$$\boxed{\frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q) \frac{\Delta(q)}{K_{T,\mu}^{\gamma,\Delta}(q)} \mathrm{d}^3q = -\Delta(p).} \tag{1.7}$$

In (1.7), we have introduced the notation

$$K_{T,\mu}^{\gamma,\Delta}(p) = \frac{E_\mu^{\gamma,\Delta}(p)}{\tanh\left(\dfrac{E_\mu^{\gamma,\Delta}(p)}{2T}\right)}, \tag{1.8}$$

$$E_\mu^{\gamma,\Delta}(p) = \sqrt{(\varepsilon^\gamma(p) - \tilde{\mu}^\gamma)^2 + |\Delta(p)|^2}, \tag{1.9}$$

with ε^γ and $\tilde{\mu}^\gamma$ defined in (1.4) and (1.5), respectively. For $T = 0$, (1.8) is interpreted as $K_{0,\mu}^{\gamma,\Delta}(p) = E_\mu^{\gamma,\Delta}(p)$.

We note that the BCS gap equation (1.7) can equivalently be written as

$$(K_{T,\mu}^{\gamma,\Delta} + V)\hat{\alpha} = 0,$$

where $K_{T,\mu}^{\gamma,\Delta}$ is interpreted as a multiplication operator in Fourier space, and V as multiplication operator in configuration space. This form of the equation will turn out to be useful later on.

Proposition 1 shows that the condition $\|\hat{V}\|_\infty \leq 2\hat{V}(0)$ is sufficient for stability of the system. The simplicity of this criterion is due to the restriction to translation-invariant quasi-free states. Without imposing translation-invariance, the question of stability is much more subtle. Note that $\mathcal{F}_T^V$ is not bounded from below for negative V, in contrast to the BCS model (where the direct and exchange terms are neglected).

Proposition 1 gives no information on whether $\Delta \neq 0$. A sufficient condition for this to happen is given in the following theorem.

Theorem 1 (Existence of a Superfluid Phase). *Let $\mu \in \mathbb{R}$, $0 \leq T < \infty$, and let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ be real-valued with $\|\hat{V}\|_\infty \leq 2\hat{V}(0)$. Let $\Gamma_0 = (\gamma_0, 0)$ be a normal state and recall the definition of $K_{T,\mu}^{\gamma_0,0}(p)$ in* (1.8)–(1.9).

(i) *If* $\inf \operatorname{spec}(K_{T,\mu}^{\gamma_0,0} + V) < 0$, *then Γ_0 is unstable, i.e.* $\inf_{\Gamma \in \mathcal{D}} \mathcal{F}_T^V(\Gamma) < \mathcal{F}_T^V(\Gamma_0)$.
(ii) *If Γ_0 is unstable, then there exist $(\gamma, \alpha) \in \mathcal{D}$, with $\alpha \neq 0$, such that Δ defined in* (1.6) *solves the BCS gap equation* (1.7).

The theorem follows from the following arguments. The operator $K_{T,\mu}^{\gamma_0,0} + V$ naturally appears when looking at the second derivative of $t \mapsto \mathcal{F}_T^V(\Gamma_0 + t\Gamma)$ at $t = 0$. If it has negative eigenvalues, the second derivative is negative for suitable Γ, hence Γ_0 is unstable. On the other hand, an unstable normal state implies the existence of a minimizer with $\alpha \neq 0$, which satisfies the Euler–Lagrange equations for $\mathcal{F}_T^V$, resulting in (1.7) according to Proposition 1. The details are given in Sec. 2.1.

Remark 1. In the usual BCS model, where the direct and exchange terms are neglected, the existence of a non-trivial solution to $(K_{T,\mu}^{0,\Delta} + V)\hat{\alpha} = 0$ implies the existence of a negative eigenvalue of $K_{T,\mu}^{0,0} + V$ [9, Theorem 1]. This follows from the fact that $K_{T,\mu}^{0,\Delta}$ is monotone in Δ, i.e. $K_{T,\mu}^{0,\Delta}(p) > K_{T,\mu}^{0,0}(p)$ for $\Delta \neq 0$. In particular, the system is superfluid if and only if the operator $K_{T,\mu}^{0,0} + V$ has a negative eigenvalue. Since this operator is monotone in T, the equation

$$\inf \operatorname{spec}(K_{T_c,\mu}^{0,0} + V) = 0$$

determines the critical temperature. In the model considered here, where the direct and exchange terms are not neglected, the situation is more complicated. Due to the additional dependence of $K_{T,\mu}^{\gamma,\Delta}$ on γ, we can no longer conclude that $K_{T,\mu}^{\gamma,\Delta}(p) > K_{T,\mu}^{\gamma_0,0}(p)$. But by Theorem 1, the smallest T solving

$$\inf \operatorname{spec}(K_{T,\mu}^{\gamma_0,0} + V) = 0 \tag{1.10}$$

still remains a lower bound for the critical temperature.

Our main result concerns the case of short-range interaction potentials V, where we can recover monotonicity in Δ, and hence conclude that (1.10) indeed defines the correct critical temperature. More precisely, we shall consider a sequence of potentials $\{V_\ell\}_{\ell>0}$ with $\ell \to 0$, which satisfies the following assumptions.

Remark 2. In the following, $\ell \ll 1$ is a small parameter, e.g., it suffices to consider $\ell \leq 1$.

Assumption 1.

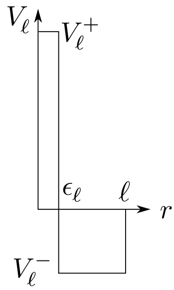
(A1) $V_\ell \in L^1 \cap L^2$.
(A2) The range of V_ℓ is at most ℓ, i.e. $\operatorname{supp} V_\ell \subseteq B_\ell(0)$.
(A3) The scattering length $a(V_\ell)$ is negative and does not vanish as $\ell \to 0$, i.e. $\lim_{\ell\to 0} a(V_\ell) = a < 0$.
(A4) $\limsup_{\ell \to 0} \|V_\ell\|_1 < \infty$.
(A5) $\hat{V}_\ell(0) > 0$ and $\lim_{\ell\to 0} \hat{V}_\ell(0) = \mathcal{V} \geq 0$.
(A6) $\|\hat{V}_\ell\|_\infty \leq 2\hat{V}_\ell(0)$.
(A7) For small ℓ, $\|V_\ell\|_2 \leq C_1 \ell^{-N}$ for some $C_1 > 0$ and $N \in \mathbb{N}$.
(A8) $\exists\, 0 < b < 1$ such that $\inf \operatorname{spec}(p^2 + V_\ell - |p|^b) > C_2 > -\infty$ holds independently of ℓ.
(A9) The operator $1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}$ is invertible, and has an eigenvalue e_ℓ of order ℓ, with corresponding eigenvector ϕ_ℓ. Moreover, $(1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2})^{-1}(1 - P_\ell)$ is uniformly bounded in ℓ, where $P_\ell = \langle J_\ell \phi_\ell | \phi_\ell\rangle^{-1} |\phi_\ell\rangle\langle J_\ell \phi_\ell|$ and $J_\ell = \operatorname{sgn}(V_\ell)$.
(A10) The eigenvector ϕ_ℓ satisfies $|\langle \phi_\ell | \operatorname{sgn}(V_\ell) \phi_\ell\rangle|^{-1} \langle |V_\ell|^{1/2} | |\phi_\ell| \rangle \leq O(\ell^{1/2})$ for small ℓ.

Here we use the notation $\operatorname{sgn}(V) = \left\{\begin{smallmatrix} 1, & V \geq 0 \\ -1, & V < 0 \end{smallmatrix}\right.$ and $V^{1/2}(x) = \operatorname{sgn}(V)|V(x)|^{1/2}$. As discussed in [12], the scattering length of a real-valued potential $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ is given by

$$a(V) = \frac{1}{4\pi} \left\langle |V|^{1/2} \,\middle|\, \frac{1}{1 + V^{1/2} \frac{1}{p^2} |V|^{1/2}} V^{1/2} \right\rangle. \tag{1.11}$$

Assumptions (A6)–(A10) are to some extent technical and are needed, among other things, to guarantee that $\mathcal{F}_T^{V_\ell}$ is bounded from below uniformly in ℓ. Our main results presumably hold for a larger class of potentials with less restrictive assumptions, but to avoid additional complications in the proofs we do not aim here for the greatest possible generality. Assumption 1 implies, in particular, that V_ℓ converges to a point interaction as $\ell \to 0$, and we refer to [6] for a general study of point interactions arising as limits of short-range potentials of the form considered here.

Remark 3. As an example for such a sequence of short-range potentials V_ℓ we have the following picture in mind:



The attractive part allows to adjust the scattering length. The repulsive core is needed to guarantee stability, and can be used to adjust the L^1 norm. If its range is small compared to the range of the attractive part, i.e. $\epsilon_\ell \ll \ell$, the scattering length is essentially unaffected by the repulsive core. In Appendix A, we construct an explicit example of such a sequence, satisfying all the assumptions (A1)–(A10). As $\ell \to 0$, it approximates a contact potential, defined via suitable selfadjoint extensions of $-\Delta$ on $\mathbb{R}^3\backslash\{0\}$. Functions in its domain are known to diverge as $|x|^{-1}$ for small x, hence decay like p^{-2} for large $|p|$. This suggests the validity of (A8) for $b < 1$. Assumption (A9) is easy to show in case V_ℓ is uniformly bounded in $L^{3/2}$ (in which case $\hat{V}_\ell(0) = O(\ell)$) but much harder to prove if $\lim_{\ell\to 0} \hat{V}_\ell(0) > 0$. It is possible to generalize (A9) and allow finitely many eigenvalues of $1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}$ of order ℓ. For simplicity, we restrict to the case of only one eigenvalue of order ℓ, however.

For the remainder of this section, we assume that the sequence V_ℓ satisfies (A1)–(A10). We shall use the notation

$$\tilde{\mu}^{\gamma_\ell} = \mu - \frac{2}{(2\pi)^{3/2}} \hat{V}_\ell(0) \int_{\mathbb{R}^3} \hat{\gamma}_\ell(p) \mathrm{d}^3 p$$

in analogy to (1.5).

Theorem 2 (Effective Gap Equation). *Let* $T \geq 0$, $\mu \in \mathbb{R}$, *and let* $(\hat{\gamma}_\ell, \hat{\alpha}_\ell)$ *be a minimizer of* $\mathcal{F}_T^{V_\ell}$ *with corresponding* $\Delta_\ell = 2(2\pi)^{-3/2} \hat{V}_\ell * \hat{\alpha}_\ell$. *Then there exist* $\Delta \geq 0$ *and* $\hat{\gamma} : \mathbb{R}^3 \to \mathbb{R}_+$ *such that* $|\Delta_\ell(p)| \to \Delta$ *pointwise,* $\hat{\gamma}_\ell(p) \to \hat{\gamma}(p)$ *pointwise and* $\tilde{\mu}^{\gamma_\ell} \to \tilde{\mu}$ *as* $\ell \to 0$, *satisfying*

$$\begin{aligned} \tilde{\mu} &= \mu - \frac{2\mathcal{V}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{\gamma}(p) \mathrm{d}^3 p \\ \hat{\gamma}(p) &= \frac{1}{2} - \frac{p^2 - \tilde{\mu}}{2K_{T,\tilde{\mu}}^{0,\Delta}(p)}. \end{aligned} \tag{1.12}$$

If $\Delta_\ell \neq 0$ for a subsequence of ℓ's going to zero, then, in addition,

$$\boxed{-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{1}{K_{T,\tilde{\mu}}^{0,\Delta}} - \frac{1}{p^2}\right)\mathrm{d}^3p.} \tag{1.13}$$

Recall that, according to our definitions (1.4)–(1.9),

$$K_{T,\tilde{\mu}}^{0,\Delta}(p) = \frac{E_{\tilde{\mu}}^{0,\Delta}(p)}{\tanh\left(\frac{E_{\tilde{\mu}}^{0,\Delta}(p)}{2T}\right)}, \quad E_{\tilde{\mu}}^{0,\Delta}(p) = \sqrt{(p^2-\tilde{\mu})^2 + |\Delta|^2}.$$

Remark 4. If we consider potentials such that $\hat{V}_\ell(0) \to 0$, we obtain at the same time that $\tilde{\mu}^{\gamma_\ell} \to \mu$ and consequently (1.13) becomes

$$-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{1}{K_{T,\mu}^{0,\Delta}} - \frac{1}{p^2}\right)\mathrm{d}^3p. \tag{1.14}$$

Equation (1.14) is the form of the BCS gap equation one finds in the literature, see for instance [15].

The effective gap equation (1.13) suggests to define the critical temperature of the system via the solution of (1.13) for $\Delta = 0$, in which case $\hat{\gamma}$ is given by $(1 + \mathrm{e}^{\frac{p^2-\tilde{\mu}}{T}})^{-1}$.

Definition 1 (Critical Temperature/Renormalized Chemical Potential). Let $\mu > 0$. The *critical temperature* T_c and the *renormalized chemical potential* $\tilde{\mu}$ in the limit of a contact potential with scattering length $a < 0$ and $\lim_{\ell\to 0}\hat{V}_\ell(0) = \mathcal{V} \geq 0$ are implicitly given by the set of equations

$$\begin{aligned} -\frac{1}{4\pi a} &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{\tanh\left(\frac{p^2-\tilde{\mu}}{2T_c}\right)}{p^2-\tilde{\mu}} - \frac{1}{p^2}\right)\mathrm{d}^3p, \\ \tilde{\mu} &= \mu - \frac{2\mathcal{V}}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\frac{1}{1+\mathrm{e}^{\frac{p^2-\tilde{\mu}}{T_c}}}\mathrm{d}^3p. \end{aligned} \tag{1.15}$$

We will show existence and uniqueness of T_c and $\tilde{\mu}$ in Appendix B. Note that it is essential that $\mu > 0$. If $\mu \leq 0$, then $\tilde{\mu} \leq 0$ and hence the right side of the first equation in (1.15) is always non-positive, hence there is no solution for $a < 0$. In other words, $T_c = 0$ for $\mu \leq 0$.

Remark 5. In [13], the behavior of the first integral on the right-hand side of (1.15) as $T_c \to 0$ was examined. This allows one to deduce the asymptotic behavior of T_c as a tends to zero, which equals

$$T_c = \tilde{\mu}\left(\frac{8}{\pi}\mathrm{e}^{\gamma-2} + o(1)\right)\mathrm{e}^{\frac{\pi}{2\sqrt{\tilde{\mu}}a}},$$

with $\gamma \approx 0.577$ denoting Euler's constant. Similarly, one can study the asymptotic behavior as $\mu \to 0$.

Although this definition for T_c is only valid in the limit $\ell \to 0$, it serves to make statements about upper and lower bounds on the critical temperature for small (but non-zero) ℓ, as sketched in the figure on p. 2.

Theorem 3 (Bounds on Critical Temperature). *Let $\mu \in \mathbb{R}$, $T \geq 0$ and let $(\gamma_\ell^0, 0)$ be a normal state for $\mathcal{F}_T^{V_\ell}$.*

(i) *For $T < T_c$, there exists an $\ell_0(T) > 0$ such that for $\ell < \ell_0(T)$, $\inf \operatorname{spec}(K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell) < 0$. Consequently, the system is superfluid.*
(ii) *For $T > T_c$, there exists an $\ell_0(T) > 0$ such that for $\ell < \ell_0(T)$, $\mathcal{F}_T^{V_\ell}$ is minimized by a normal state. I.e. the system is not superfluid.*

Theorem 3 shows that Definition 1 is indeed the correct definition of the critical temperature in the limit $\ell \to 0$. In addition, it also shows that in this limit there is actually equivalence of statements (i) and (ii) in Theorem 1. In particular, one recovers the linear criterion for the existence of a superfluid phase valid in the usual BCS model, as discussed in Remark 1.

2. Proofs

2.1. *General potentials*

In this section we prove Proposition 1 and Theorem 1. As a first step we show that $\mathcal{F}_T^V$ is bounded from below and has a minimizer.

Lemma 1. *Let $V \in L^1 \cap L^{3/2}$, $\hat{V}(0) \geq 0$ and $\hat{V}(p) \leq 2\hat{V}(0)$ for all $p \in \mathbb{R}^3$. Then $\mathcal{F}_T^V$ is bounded from below and there exists a minimizer Γ of $\mathcal{F}_T^V(\Gamma)$.*

Proof. The case without direct and exchange term was treated in [9, Proposition 2]. The Hartree–Fock part of the functional $\mathcal{F}_T^V$ gives the additional contribution

$$-\int_{\mathbb{R}^3} |\gamma(x)|^2 V(x) \mathrm{d}^3x + 2\gamma(0)^2 \int_{\mathbb{R}^3} V(x)\mathrm{d}^3x = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{\gamma}(2\hat{V}(0) - \hat{V}) * \hat{\gamma}\mathrm{d}^3p,$$

which is non-negative because of our assumption $\hat{V}(p) \leq 2\hat{V}(0)$. Hence, the same lower bound as in the case without direct and exchange term applies.

To show the existence of a minimizer, it remains to check the weak lower semi-continuity of $\mathcal{F}_T^V$ in $L^q(\mathbb{R}^3) \times H^1(\mathbb{R}^3, \mathrm{d}^3x)$ (note that $\hat{\gamma} \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$). The exchange term

$$\gamma \mapsto \int_{\mathbb{R}^3} V(x)|\gamma(x)|^2 \mathrm{d}^3x$$

is actually weakly continuous on $H^1(\mathbb{R}^3)$, see, e.g., [19, Theorem 11.4]. Since also for any sequence γ_n converging to γ weakly, we have $\lim_{n\to\infty} \int_{\mathbb{R}^3} \hat{\gamma}_n \mathrm{d}^3p \geq \int_{\mathbb{R}^3} \hat{\gamma}\mathrm{d}^3p$, the direct term is weakly lower semicontinuous. In the proof of [9, Proposition 2] it was shown that all other terms in $\mathcal{F}_T^V$ are weakly lower semicontinuous as well. As a consequence, a minimizing sequence will actually converge to a minimizer. □

Lemma 2. *The Euler–Lagrange equations for a minimizer* (γ, α) *of* $\mathcal{F}_T^V$ *are of the form*

$$\hat{\gamma}(p) = \frac{1}{2} - \frac{\varepsilon^\gamma(p) - \tilde{\mu}^\gamma}{2K_{T,\mu}^{\gamma,\Delta}(p)} \tag{2.1}$$

$$\hat{\alpha}(p) = \frac{1}{2}\Delta(p)\frac{\tanh\left(\frac{E_\mu^{\gamma,\Delta}(p)}{2T}\right)}{E_\mu^{\gamma,\Delta}(p)}, \tag{2.2}$$

where we used the abbreviations introduced in (1.4)–(1.9). *In particular, the BCS gap equation* (1.7) *holds.*

Proof. The proof works similar to [9]. We sketch here an alternative, more concise derivation, restricting our attention to $T > 0$ for simplicity. A minimizer $\Gamma = (\gamma, \alpha)$ of $\mathcal{F}_T^V$ fulfills the inequality

$$0 \le \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathcal{F}_T^V(\Gamma + t(\tilde{\Gamma} - \Gamma)) \tag{2.3}$$

for arbitrary $\tilde{\Gamma} \in \mathcal{D}$. Here we may assume that Γ stays away from 0 and 1 by arguing as in [9, Proof of Lemma 1]. A simple calculation using

$$S(\Gamma) = -\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\, \Gamma \ln \Gamma \mathrm{d}^3p = -\frac{1}{2}\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}(\Gamma \ln(\Gamma) + (1-\Gamma)\ln(1-\Gamma))\mathrm{d}^3p$$

shows that

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \mathcal{F}_T^V(\Gamma + t(\tilde{\Gamma} - \Gamma)) = \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\left[H_\Delta(\tilde{\Gamma} - \Gamma) + T(\tilde{\Gamma} - \Gamma)\ln\left(\frac{\Gamma}{1-\Gamma}\right)\right]\mathrm{d}^3p,$$

with

$$H_\Delta = \begin{pmatrix} \varepsilon^\gamma - \tilde{\mu}^\gamma & \Delta \\ \bar{\Delta} & -(\varepsilon^\gamma - \tilde{\mu}^\gamma) \end{pmatrix},$$

using the definition

$$\Delta = 2(2\pi)^{-3/2}\hat{V} * \hat{\alpha}.$$

Here, $\mathrm{Tr}_{\mathbb{C}^2} G$ denotes the trace of the 2×2 matrix $G(p)$ for fixed p. Separating the terms containing no $\tilde{\Gamma}$ and moving them to the left-hand side in (2.3), we obtain

$$\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\left(H_\Delta\left(\Gamma - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\right) + T\,\Gamma \ln\left(\frac{\Gamma}{1-\Gamma}\right)\right)\mathrm{d}^3p$$
$$\le \int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\left(H_\Delta\left(\tilde{\Gamma} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\right) + T\,\tilde{\Gamma} \ln\left(\frac{\Gamma}{1-\Gamma}\right)\right)\mathrm{d}^3p.$$

Note that $\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}(H_\Delta \Gamma)\mathrm{d}^3p$ is not finite but $\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\left(H_\Delta\left(\tilde{\Gamma} - \left(\begin{smallmatrix}0 & 0\\ 0 & 1\end{smallmatrix}\right)\right)\right)\mathrm{d}^3p$ is. Since $\tilde{\Gamma}$ was arbitrary, Γ also minimizes the linear functional

$$\tilde{\Gamma} \mapsto \int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\left(H_\Delta\left(\tilde{\Gamma} - \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}\right) + T\,\tilde{\Gamma}\ln\left(\frac{\Gamma}{1-\Gamma}\right)\right)\mathrm{d}^3p,$$

whose Euler–Lagrange equation is of the simple form

$$0 = H_\Delta + T\ln\left(\frac{\Gamma}{1-\Gamma}\right), \tag{2.4}$$

which is equivalent to

$$\Gamma = \frac{1}{1+\mathrm{e}^{\frac{1}{T}H_\Delta}}.$$

This in turn implies (2.1) and (2.2). Indeed,

$$\Gamma = \frac{1}{1+\mathrm{e}^{\frac{1}{T}H_\Delta}} = \frac{1}{2} - \frac{1}{2}\tanh\left(\frac{1}{2T}H_\Delta\right).$$

For the simple reason that $\frac{\tanh(x)}{x}$ is an even function and $H_\Delta^2 = [E_\mu^{\gamma,\Delta}]^2\mathbb{1}_{\mathbb{C}^2}$, the expression simplifies to

$$\begin{aligned}\Gamma &= \frac{1}{2} - \frac{1}{2}H_\Delta\frac{\tanh\left(\frac{1}{2T}E_\mu^{\gamma,\Delta}\right)}{E_\mu^{\gamma,\Delta}} = \frac{1}{2} - \frac{1}{2K_{T,\mu}^{\gamma,\Delta}}H_\Delta\\ &= \begin{pmatrix}\frac{1}{2} - \frac{\varepsilon^\gamma - \tilde{\mu}^\gamma}{2K_{T,\mu}^{\gamma,\Delta}} & -\frac{\Delta}{2K_{T,\mu}^{\gamma,\Delta}}\\ -\frac{\bar{\Delta}}{2K_{T,\mu}^{\gamma,\Delta}} & \frac{1}{2} + \frac{\varepsilon^\gamma - \tilde{\mu}^\gamma}{2K_{T,\mu}^{\gamma,\Delta}}\end{pmatrix}.\end{aligned}$$

□

Proof of Proposition 1. This is an immediate consequence of Lemmas 1 and 2. □

Proof of Theorem 1. The proof works exactly as the analog steps in [9, Proof of Theorem 1]. To see (i), note that $\langle\hat{\alpha}, (K_{T,\mu}^{\gamma_0,0} + V)\hat{\alpha}\rangle$ is the second derivative of $\mathcal{F}_T^V$ with respect to α at $\Gamma = \Gamma_0$. For (ii), we use the fact that the gap equation is a combination of the Euler–Lagrange equation (2.2) of the functional and the definition of Δ. □

2.2. *Sequence of short-range potentials*

In the following, we consider a sequence of potentials V_ℓ satisfying the assumptions (A1)–(A10) in Assumption 1. Since V_ℓ converges to a contact potential, Lemma 1 is not sufficient to prove that $\mathcal{F}_T^{V_\ell}$ is uniformly bounded from below. To this aim, we have to use more subtle estimates involving bounds on the relative entropy obtained in [8], and we heavily rely on assumption (A8).

Lemma 3. *There exists $C_1 > 0$, independent of ℓ, such that*

$$\mathcal{F}_T^{V_\ell}(\Gamma) \geq -C_1 + \frac{1}{2}\int_{\mathbb{R}^3}(1+p^2)(\hat\gamma - \hat\gamma_0)^2 \mathrm{d}^3p + \frac{1}{2}\int_{\mathbb{R}^3}|p|^b|\hat\alpha|^2\mathrm{d}^3p, \tag{2.5}$$

where we denote $\hat\gamma_0(p) = \frac{1}{1+\mathrm{e}^{(p^2-\mu)/T}}$.

Proof. We rewrite $\mathcal{F}_T^{V_\ell}(\Gamma)$ as

$$\begin{aligned}\mathcal{F}_T^{V_\ell}(\Gamma) = {} & \frac{1}{2}\int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^2}\left(H_0\left(\Gamma - \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}\right)\right)\mathrm{d}^3p + \int_{\mathbb{R}^3}V_\ell(x)|\alpha(x)|^2\mathrm{d}^3x \\ & - TS(\Gamma) + \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}((2\hat V_\ell(0) - \hat V_\ell) * \hat\gamma)(p)\hat\gamma(p)\mathrm{d}^3p,\end{aligned}$$

where $\Gamma = \Gamma(\gamma,\alpha)$ and

$$H_0 = \begin{pmatrix}p^2-\mu & 0\\ 0 & -(p^2-\mu)\end{pmatrix}.$$

Since $\hat\gamma(p) \geq 0$ and, by assumption (A6), $2\hat V_\ell(0) - \hat V_\ell(p) \geq 0$, the combination of direct plus exchange term is non-negative and it suffices to find a lower bound for

$$\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma) = \frac{1}{2}\int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^2}\left(H_0\left(\Gamma - \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}\right)\right)\mathrm{d}^3p + \int_{\mathbb{R}^3}V_\ell(x)|\alpha(x)|^2\mathrm{d}^3x - TS(\Gamma).$$

We compare $\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma)$ to the value $\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0)$, where $\Gamma_0 = \frac{1}{1+\mathrm{e}^{H_0/T}}$. Their difference equals

$$\begin{aligned}\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma) - \tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0) = {} & \frac{1}{2}\int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^2}(H_0(\Gamma-\Gamma_0))\mathrm{d}^3p - T(S(\Gamma) - S(\Gamma_0)) \\ & + \int_{\mathbb{R}^3}V_\ell(x)|\alpha(x)|^2\mathrm{d}^3x.\end{aligned}$$

Using $H_0 + T\ln(\frac{\Gamma_0}{1-\Gamma_0}) = 0$ in the trace and performing some simple algebraic transformations, we may write

$$\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma) - \tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0) = \frac{T}{2}\mathcal{H}(\Gamma,\Gamma_0) + \int_{\mathbb{R}^3}V_\ell(x)|\alpha(x)|^2\mathrm{d}^3x,$$

where

$$\mathcal{H}(\Gamma,\Gamma_0) = \int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^2}[\Gamma(\ln(\Gamma) - \ln(\Gamma_0)) + (1-\Gamma)(\ln(1-\Gamma) - \ln(1-\Gamma_0))]\mathrm{d}^3p$$

denotes the relative entropy of Γ and Γ_0. Lemma 3 in [8], which is an extension of Theorem 1 in [11], implies the lower bound

$$\frac{T}{2}\mathcal{H}(\Gamma,\Gamma_0) \geq \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{Tr}_{\mathbb{C}^2}\left[\frac{H_0}{\tanh\left(\frac{H_0}{2T}\right)}(\Gamma-\Gamma_0)^2\right]\mathrm{d}^3p$$

$$= \int_{\mathbb{R}^3} K_{T,\mu}^{0,0}(p)((\hat{\gamma}(p)-\hat{\gamma}_0(p))^2+|\hat{\alpha}(p)|^2)\mathrm{d}^3p.$$

Hence we obtain

$$\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma)-\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0) \geq \langle\alpha|K_{T,\mu}^{0,0}+V_\ell|\alpha\rangle + \int_{\mathbb{R}^3} K_{T,\mu}^{0,0}(p)(\hat{\gamma}(p)-\hat{\gamma}_0(p))^2\mathrm{d}^3p.$$

In both terms, we can use $K_{T,\mu}^{0,0} \geq p^2-\mu$, therefore

$$\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma)-\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0) \geq \langle\alpha|p^2+V_\ell-\mu|\alpha\rangle + \frac{1}{2}\int_{\mathbb{R}^3}(1+p^2)(\hat{\gamma}-\hat{\gamma}_0)^2\mathrm{d}^3p$$

$$+\int_{\mathbb{R}^3}\left(\frac{p^2}{2}-\mu-\frac{1}{2}\right)(\hat{\gamma}-\hat{\gamma}_0)^2\mathrm{d}^3p.$$

Using $(\hat{\gamma}-\hat{\gamma}_0)^2 \leq 1$, we can bound

$$\int_{\mathbb{R}^3}\left(\frac{p^2}{2}-\mu-\frac{1}{2}\right)(\hat{\gamma}-\hat{\gamma}_0)^2\mathrm{d}^3p \geq -\int_{\mathbb{R}^3}\left[\frac{p^2}{2}-\mu-\frac{1}{2}\right]_-\mathrm{d}^3p,$$

where $[t]_- = \max\{0,-t\}$ denote the negative part of a real number t. By assumption (A8), $\inf\mathrm{spec}(p^2+V_\ell-|p|^b)$ is bounded by some number C independent of ℓ. Thus

$$\int_{\mathbb{R}^3}(p^2+V_\ell-\mu)|\hat{\alpha}|^2\mathrm{d}^3p \geq \int_{\mathbb{R}^3}(|p|^b+C-\mu)|\hat{\alpha}|^2\mathrm{d}^3p$$

$$= \frac{1}{2}\int_{\mathbb{R}^3}|p|^b|\hat{\alpha}|^2\mathrm{d}^3p + \int_{\mathbb{R}^3}\left(\frac{|p|^b}{2}+C-\mu\right)|\hat{\alpha}|^2\mathrm{d}^3p.$$

With $|\hat{\alpha}|^2 \leq 1$, we conclude

$$\int_{\mathbb{R}^3}\left(\frac{|p|^b}{2}+C-\mu\right)|\hat{\alpha}|^2\mathrm{d}^3p \geq -\int_{\mathbb{R}^3}\left[\frac{|p|^b}{2}-\mu+C\right]_-\mathrm{d}^3p.$$

Our final lower bound is thus

$$\mathcal{F}_T^{V_\ell}(\Gamma) \geq \tilde{\mathcal{F}}_T^{V_\ell}(\Gamma) \geq -C_1 + \frac{1}{2}\int_{\mathbb{R}^3}(1+p^2)(\hat{\gamma}-\hat{\gamma}_0)^2\mathrm{d}^3p + \frac{1}{2}\int_{\mathbb{R}^3}|p|^b|\hat{\alpha}|^2\mathrm{d}^3p,$$

with

$$C_1 = -\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0) + \int_{\mathbb{R}^3}\left[\frac{p^2}{2}-\mu-\frac{1}{2}\right]_-\mathrm{d}^3p + \int_{\mathbb{R}^3}\left[\frac{|p|^b}{2}-\mu+C\right]_-\mathrm{d}^3p.$$

Since $\tilde{\mathcal{F}}_T^{V_\ell}(\Gamma_0)$ does not depend on ℓ (the off-diagonal entries of Γ_0 being 0) this concludes the proof. $\square$

Lemma 4. *If* $(\gamma_\ell, \alpha_\ell)$ *is a minimizer of* $\mathcal{F}_T^{V_\ell}$, *then* $\int_{\mathbb{R}^3} \hat{\gamma}_\ell(p)|p|^b \mathrm{d}^3 p$ *is uniformly bounded in* ℓ.

Proof. To simplify notation, we leave out the index ℓ. A minimizer (γ, α) of $\mathcal{F}_T^V$ satisfies the Euler–Lagrange equation (2.1). Using the abbreviation

$$K_{T,\mu}^{\gamma,\Delta} = \frac{E_\mu^{\gamma,\Delta}(p)}{\tanh\left(\dfrac{E_\mu^{\gamma,\Delta}(p)}{2T}\right)},$$

we may express (2.1) in the form

$$\hat{\gamma} = \frac{1}{2} - \frac{1}{2}\frac{\varepsilon^\gamma - \tilde{\mu}^\gamma}{K_{T,\mu}^{\gamma,\Delta}}.$$

Adding and subtracting $\frac{1}{2}\frac{E_\mu^{\gamma,\Delta}}{K_{T,\mu}^{\gamma,\Delta}} = \frac{1}{2}\tanh(\frac{E_\mu^{\gamma,\Delta}(p)}{2T})$, we may write

$$\begin{aligned}\hat{\gamma} &= \frac{1}{2}\left(1 - \tanh\left(\frac{E_\mu^{\gamma,\Delta}}{2T}\right)\right) + \frac{1}{2}\frac{E_\mu^{\gamma,\Delta} - (\varepsilon^\gamma - \tilde{\mu}^\gamma)}{K_{T,\mu}^{\gamma,\Delta}} \\ &= \frac{1}{1 + \mathrm{e}^{\frac{E_\mu^{\gamma,\Delta}}{T}}} + \frac{1}{2}\frac{|\Delta|^2}{(E_\mu^{\gamma,\Delta} + (\varepsilon^\gamma - \tilde{\mu}^\gamma))K_{T,\mu}^{\gamma,\Delta}}.\end{aligned} \tag{2.6}$$

Using the Euler–Lagrange equation $\Delta = 2K_{T,\mu}^{\gamma,\Delta}\hat{\alpha}$ for α, we obtain

$$\hat{\gamma} = \frac{1}{1 + \mathrm{e}^{\frac{E_\mu^{\gamma,\Delta}}{T}}} + 2\frac{|\hat{\alpha}|^2 K_{T,\mu}^{\gamma,\Delta}}{E_\mu^{\gamma,\Delta} + (\varepsilon^\gamma - \tilde{\mu}^\gamma)}. \tag{2.7}$$

Assumption (A6) implies that $\varepsilon^\gamma - \tilde{\mu}^\gamma \geq p^2 - \mu$. In particular, the contribution of the first term is bounded by

$$\int_{\mathbb{R}^3} \frac{1}{1 + \mathrm{e}^{\frac{E_\mu^{\gamma,\Delta}}{T}}} |p|^b \mathrm{d}^3 p \leq \int_{\mathbb{R}^3} \frac{1}{1 + \mathrm{e}^{\frac{p^2 - \mu}{T}}} |p|^b \mathrm{d}^3 p$$

which is independent of ℓ. To treat the second term, we split the domain of integration $\mathbb{R}^3$ into two disjoint sets and show that the integral is uniformly bounded on each subset. On the set $B = \{p \,|\, \tanh(\frac{p^2 - \mu}{2T}) \geq \frac{2}{3}\}$ we have that $\tanh(\frac{\varepsilon^\gamma - \tilde{\mu}^\gamma}{2T}) \geq \frac{2}{3}$ and $\varepsilon^\gamma - \tilde{\mu}^\gamma \geq 0$. This implies that

$$\frac{|\hat{\alpha}|^2 K_{T,\mu}^{\gamma,\Delta}}{E_\mu^{\gamma,\Delta} + (\varepsilon^\gamma - \tilde{\mu}^\gamma)} \leq \frac{3}{2}|\hat{\alpha}|^2,$$

whose integral over B is bounded uniformly in ℓ by (2.5), even after multiplication by $|p|^b$. The complement $B^c = \{p \,|\, \tanh(\frac{p^2 - \mu}{2T}) \leq \frac{2}{3}\}$ of B is compact and thus also $\int_{B^c} \hat{\gamma}(p)|p|^b \mathrm{d}^3 p$ is trivially bounded, because $0 \leq \hat{\gamma} \leq 1$. $\square$

In the following lemma, we show that, as $\ell \to 0$, pointwise limits for the main quantities exist. In the case of Δ_ℓ, observe that $\check{\Delta}_\ell(x) = 2V_\ell(x)\alpha_\ell(x)$ is supported in $|x| \le \ell$. Heuristically, if the norm $\|\check{\Delta}_\ell\|_1$ stays finite, $\check{\Delta}_\ell$ should converge to a δ distribution and its Fourier transform Δ_ℓ to a constant function. While we do not show that $\|\check{\Delta}_\ell\|_1$ stays finite, we can use assumption (A7) to at least show that it cannot increase too fast as $\ell \to 0$, which will turn out to be sufficient. The pointwise convergence $\gamma_\ell(p) \to \gamma(p)$ then follows from Lemma 4 together with the Euler–Lagrange equation (2.1) for γ_ℓ.

In the following, we use the definition

$$m_\mu^{\gamma_\ell,\Delta_\ell}(T) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}\right)\mathrm{d}^3p.$$

Lemma 5. *Let $(\gamma_\ell, \alpha_\ell)$ be a sequence of minimizers of $\mathcal{F}_T^{V_\ell}$ and $\Delta_\ell = 2(2\pi)^{-3/2}\hat{V}_\ell * \hat{\alpha}_\ell$. Then there are subsequences of γ_ℓ and α_ℓ, which we continue to denote by γ_ℓ and α_ℓ, and $\gamma \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, $\Delta \in \mathbb{R}_+$ such that*

(i) $|\Delta_\ell(p)|$ *converges pointwise to the constant function* Δ *as* $\ell \to 0$,
(ii) $\lim_{\ell\to 0}\int_{\mathbb{R}^3}\hat{\gamma}_\ell \mathrm{d}^3p = \int_{\mathbb{R}^3}\hat{\gamma}\mathrm{d}^3p$,
(iii) $\lim_{\ell\to 0}\tilde{\mu}^{\gamma_\ell} = \tilde{\mu}^\gamma$, *where* $\tilde{\mu}^\gamma = \mu - 2(2\pi)^{-3/2}\mathcal{V}\int_{\mathbb{R}^3}\hat{\gamma}(p)\mathrm{d}^3p$,
(iv) $\varepsilon^{\gamma_\ell}(p) \to p^2$ *pointwise as* $\ell \to 0$,
(v) $\hat{\gamma}_\ell(p) \to \hat{\gamma}(p)$ *pointwise as* $\ell \to 0$, *and Eqs.* (1.12) *are satisfied for* $(\gamma, \tilde{\mu}^\gamma, \Delta)$,
(vi) $\lim_{\ell\to 0} m_\mu^{\gamma_\ell,\Delta_\ell}(T) = m_\mu^{\gamma,\Delta}(T) = m_{\tilde{\mu}^\gamma}^{0,\Delta}(T)$.

We shall see later that it is not necessary to restrict to a subsequence, the result holds in fact for the whole sequence.

Proof. (i) Lemma 3 and assumption (A7) imply that, with $\check{\Delta}_\ell = 2V_\ell\alpha_\ell$,

$$\|\check{\Delta}_\ell\|_1 \le 2\|V_\ell\|_2\|\alpha_\ell\|_2 \le C\ell^{-N}. \tag{2.8}$$

The fact that $\check{\Delta}_\ell$ is compactly supported in $B_\ell(0)$ will allow us to argue that a suitable subsequence of $\Delta_\ell(p)$ converges to a polynomial in p. Furthermore, the fact that $\hat{\alpha}_\ell = -2(K_{T,\mu}^{\gamma_\ell,\Delta_\ell})^{-1}\Delta_\ell$ is uniformly bounded in L^2 forces the polynomial to be a constant.

We denote by

$$P_{\ell,N}(p) = \frac{1}{(2\pi)^{3/2}}\sum_{j=0}^N \frac{(-i)^j}{j!}\sum_{i_1,\ldots,i_j=1}^3 c_{i_1,\ldots,i_j}^{(\ell,j)} p_{i_1}\cdots p_{i_j}$$

the Nth order Taylor approximation of $\Delta_\ell(p) = (2\pi)^{-3/2}\int_{\mathbb{R}^3}\check{\Delta}_\ell(x)\mathrm{e}^{-ip\cdot x}\mathrm{d}^3x$ at $p = 0$, with coefficients given by

$$c_{i_1,\ldots,i_j}^{(\ell,j)} = \int_{\mathbb{R}^3}\check{\Delta}_\ell(x)x_{i_1}\cdots x_{i_j}\mathrm{d}^3x.$$

Using that $\check{\Delta}_\ell$ is supported in $B_\ell(0)$ we may estimate the remainder term as

$$|\Delta_\ell(p) - P_{\ell,N}(p)| = \frac{1}{(2\pi)^{3/2}} \left| \int_{\mathbb{R}^3} \check{\Delta}_\ell(x) \left(e^{-ip\cdot x} - \sum_{j=0}^{N} \frac{(-ip\cdot x)^j}{j!} \right) \mathrm{d}^3 x \right|$$
$$\leq \frac{\ell^{N+1}}{(2\pi)^{3/2}} \|\check{\Delta}_\ell\|_1 |p|^{N+1} \mathrm{e}^{\ell|p|},$$

which goes to zero pointwise for $\ell \to 0$ by (2.8).

Now let $\bar{c}_\ell = \max_{0\leq j\leq N} \max_{1\leq i_1,\ldots,i_j\leq 3}\{|c^{(\ell,j)}_{i_1,\ldots,i_j}|\}$. We want to show that $\bar{c} = \limsup_{\ell\to 0} \bar{c}_\ell < \infty$. If $\bar{c} = 0$, we are done. If not, then there is a subsequence of $P_{\ell,N}(p)/\bar{c}_\ell$ which converges pointwise to some polynomial $P(p)$ of degree $n \leq N$. We now use the uniform boundedness of $2\|\alpha_\ell\|_2 = \|\frac{\Delta_\ell}{K^{\gamma_\ell,\Delta_\ell}_{T,\mu}}\|_2$ to conclude that $P(p)$ cannot be a polynomial of degree $n \geq 1$, and that $\bar{c}$ is finite. We first rewrite $2\hat{\alpha}_\ell$ as

$$\frac{\Delta_\ell}{K^{\gamma_\ell,\Delta_\ell}_{T,\mu}} = \frac{\Delta_\ell}{E^{\gamma_\ell,\Delta_\ell}_\mu} \tanh(E^{\gamma_\ell,\Delta_\ell}_\mu/(2T)) = \frac{\Delta_\ell}{E^{\gamma_\ell,\Delta_\ell}_\mu} - \frac{\Delta_\ell}{E^{\gamma_\ell,\Delta_\ell}_\mu} \frac{2}{1+\exp(E^{\gamma_\ell,\Delta_\ell}_\mu/T)}.$$

Using $E^{\gamma_\ell,\Delta_\ell}_\mu \geq \varepsilon^\gamma - \tilde{\mu}^\gamma \geq p^2 - \mu$ and $|\Delta_\ell| \leq E^{\gamma_\ell,\Delta_\ell}_\mu$, it is easy to see that the L^2 norm of the second summand on the right-hand side is uniformly bounded in ℓ. Furthermore, by assumption (A6) we have $\varepsilon^\gamma - \tilde{\mu}^\gamma \leq p^2 + \nu$ for

$$\nu = -\mu + \frac{6}{(2\pi)^{3/2}} \sup_{\ell>0} \hat{V}_\ell(0)\|\hat{\gamma}_\ell\|_1,$$

which is finite due to assumption (A5) and Lemma 4. In particular,

$$E^{\gamma_\ell,\Delta_\ell}_\mu \leq \sqrt{(p^2+\nu)^2 + |\Delta_\ell|^2}.$$

Recall that $\Delta_\ell(p)/\bar{c}_\ell$ converges pointwise to $P(p)$, and that $\bar{c} = \limsup_{\ell\to 0} \bar{c}_\ell$. Assume, for the moment, that $\bar{c} < \infty$. Then, by dominated convergence,

$$\limsup_{\ell\to 0} \int_{|p|\leq R} \frac{|\Delta_\ell|^2}{(p^2+\nu)^2 + |\Delta_\ell|^2} \mathrm{d}^3 p = \int_{|p|\leq R} \frac{|\bar{c}P(p)|^2}{(p^2+\nu)^2 + |\bar{c}P(p)|^2} \mathrm{d}^3 p \quad (2.9)$$

for any $R > 0$. If $\bar{c} = \infty$, the same holds, with the integrand replaced by 1. In particular, if either $\bar{c} = \infty$ or P is a polynomial of degree $n \geq 1$, the right-hand side of (2.9) diverges as $R \to \infty$, contradicting the uniform boundedness of $\Delta_\ell/E^{\gamma_\ell,\Delta_\ell}_\mu$ in $L^2(\mathbb{R}^3)$. We thus conclude that $n = 0$ and $\bar{c} < \infty$, i.e. $\lim_{\ell\to 0} \Delta_\ell(p) = \bar{c}$ for a suitable subsequence.

(ii) The uniform bound (2.5) for $\mathcal{F}^{V_\ell}_T$ implies that $\hat{\gamma}_\ell$ is uniformly bounded in L^2. Thus, there is a subsequence which converges weakly to some $\hat{\gamma}$ in L^2. For that subsequence, we have for arbitrary $R > 0$

$$\lim_{\ell\to 0} \int_{B_R(0)} \hat{\gamma}_\ell \mathrm{d}^3 p = \int_{B_R(0)} \hat{\gamma} \mathrm{d}^3 p. \quad (2.10)$$

In particular,

$$\lim_{\ell\to 0}\int_{\mathbb{R}^3}\hat{\gamma}_\ell \mathrm{d}^3p \geq \int_{\mathbb{R}^3}\hat{\gamma}\mathrm{d}^3p.$$

Therefore, $\lim_{\ell\to 0}\int_{\mathbb{R}^3}\hat{\gamma}_\ell \mathrm{d}^3p = \int_{\mathbb{R}^3}\hat{\gamma}\mathrm{d}^3p + \delta$ for an appropriate $\delta \geq 0$. Then

$$\begin{aligned}\lim_{\ell\to 0}\int_{|p|\geq R}\hat{\gamma}_\ell(p)|p|^b\mathrm{d}^3p &\geq R^b\lim_{\ell\to 0}\int_{|p|\geq R}\hat{\gamma}_\ell\mathrm{d}^3p\\ &= R^b\lim_{\ell\to 0}\left[\int_{\mathbb{R}^3}\hat{\gamma}_\ell\mathrm{d}^3p - \int_{|p|\leq R}\hat{\gamma}_\ell\mathrm{d}^3p\right]\geq \delta R^b.\end{aligned}$$

Since R can be arbitrarily large and the left-hand side is bounded, δ has to be 0.

(iii) This follows immediately from part (ii) together with assumption (A5).

(iv) Let $D_\ell(p) = \varepsilon^{\gamma_\ell}(p) - p^2$. We compute

$$\begin{aligned}|D_\ell(p)| &= 2(2\pi)^{-3/2}|(\hat{V}_\ell - \hat{V}_\ell(0)) * \hat{\gamma}_\ell|\\ &\leq \frac{2}{(2\pi)^3}\int_{\mathbb{R}^3}\mathrm{d}^3k\int_{\mathbb{R}^3}\mathrm{d}^3x|V_\ell(x)(\mathrm{e}^{-i(p-k)\cdot x}-1)|\hat{\gamma}_\ell(k)\\ &\leq \frac{2\|V_\ell\|_1}{(2\pi)^3}\int_{\mathbb{R}^3}\hat{\gamma}_\ell(k)\sup_{|x|\leq\ell}|\mathrm{e}^{-i(p-k)\cdot x}-1|\mathrm{d}^3k\\ &\leq \frac{2\|V_\ell\|_1}{(2\pi)^3}\ell^b(\|\hat{\gamma}_\ell|\cdot|^b\|_1 + \|\hat{\gamma}_\ell\|_1|p|^b),\end{aligned}\tag{2.11}$$

where we applied the fact that $|e^{it}-1|\leq |t|^b$ for $t\in\mathbb{R}$ and $0\leq b\leq 1$, as well as $|p-k|^b \leq |p|^b + |k|^b$. By Lemma 4, $\|\hat{\gamma}_\ell|\cdot|^b\|_1$ is uniformly bounded in ℓ, hence this concludes the proof.

(v) Recall the Euler–Lagrange equation (2.1) for $\hat{\gamma}_\ell$, which states that

$$\hat{\gamma}_\ell = \frac{1}{2} - \frac{1}{2}\frac{\varepsilon^{\gamma_\ell}(p) - \tilde{\mu}^{\gamma_\ell}}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}(p)}.$$

We have just shown that the right-hand side converges pointwise to

$$\tilde{\gamma}(p) = \frac{1}{2} - \frac{1}{2}\frac{p^2 - \tilde{\mu}^\gamma}{K_{T,\tilde{\mu}^\gamma}^{0,\Delta}(p)}.\tag{2.12}$$

Since $\hat{\gamma}$ is the weak limit of $\hat{\gamma}_\ell$, it has to agree with the pointwise limit $\tilde{\gamma}$, i.e. $\hat{\gamma} = \tilde{\gamma}$ almost everywhere. Therefore γ satisfies Eq. (1.12).

(vi) We have already shown that the integrand converges pointwise. Moreover, assumption (A6) implies $\varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell} \geq p^2 - \mu$ and thus

$$E_\mu^{\gamma_\ell,\Delta_\ell} \geq |\varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell}| \geq \varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell} \geq p^2 - \mu.$$

Together with the fact that

$$\kappa_c(x) = \begin{cases} \dfrac{x}{\tanh(x)}, & x \geq 0 \\ 1, & x \leq 0 \end{cases} \tag{2.13}$$

is monotone increasing, we obtain

$$-\frac{1}{p^2} \leq \frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}(p)} - \frac{1}{p^2} \leq \frac{1}{2T\kappa_c\left(\dfrac{|p^2-\mu|}{2T}\right)} - \frac{1}{p^2}.$$

In particular, by dominated convergence we have, for $R > 0$,

$$\lim_{\ell\to 0} \int_{|p|^2 \leq R} \left(\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2} \right) \mathrm{d}^3 p = \int_{|p|^2 \leq R} \left(\frac{1}{K_{T,\mu}^{\gamma,\Delta}} - \frac{1}{p^2} \right) \mathrm{d}^3 p.$$

For the remaining domain of integration, i.e. $|p|^2 \geq R$, it is useful to rewrite the Euler–Lagrange equation (2.1) to express the integrand in terms of γ,

$$\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2} = \frac{1}{\varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell}} - \frac{1}{p^2} - \frac{2\hat{\gamma}_\ell}{\varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell}}. \tag{2.14}$$

The uniform bound (2.5) from Lemma 3 implies that $\int_{\mathbb{R}^3} \hat{\gamma}_\ell \mathrm{d}^3 p$ is uniformly bounded in ℓ. Therefore

$$\int_{|p|^2 \geq R} \frac{\hat{\gamma}_\ell}{\varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell}} \mathrm{d}^3 p \leq \int_{|p|^2 \geq R} \frac{\hat{\gamma}_\ell}{p^2 - \mu} \mathrm{d}^3 p \leq \frac{1}{R-\mu} \int_{|p|^2 \geq R} \hat{\gamma}_\ell \mathrm{d}^3 p$$

vanishes in the limit $R \to \infty$ (uniformly in ℓ). Together with (2.14) and $\varepsilon^{\gamma_\ell} - \tilde{\mu}^{\gamma_\ell} \geq p^2 - \mu$, this shows

$$\lim_{R\to\infty} \int_{|p|^2 \geq R} \left(\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2} \right) \mathrm{d}^3 p = 0,$$

uniformly in ℓ and finishes the proof. □

With the aid of Lemma 5, we can now give the following proof of Theorem 2.

Proof of Theorem 2. The convergence of $|\Delta_\ell(p)|$, $\tilde{\mu}^{\gamma_\ell}$ and $\hat{\gamma}_\ell(p)$ follows immediately from Lemma 5, at least for a suitable subsequence. To prove the validity of (1.13), we follow a similar strategy as in [12, Lemma 1]. From Theorem 1 we know that

$$(K_{T,\mu}^{\gamma_\ell,\Delta_\ell} + V_\ell)\alpha_\ell = 0, \qquad \text{with } \alpha_\ell \in H^1(\mathbb{R}^3),$$

and we assume that α_ℓ is not identically zero. According to the Birman–Schwinger principle, $K_{T,\mu}^{\gamma_\ell,\Delta_\ell} + V_\ell$ has 0 as eigenvalue if and only if

$$V_\ell^{1/2} \frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} |V_\ell|^{1/2}$$

has -1 as an eigenvalue.

We decompose $V_\ell^{1/2}\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}}|V_\ell|^{1/2}$ as

$$V_\ell^{1/2}\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}}|V_\ell|^{1/2} = V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2} + m_\mu^{\gamma_\ell,\Delta_\ell}(T)|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}| + A_{\mu,T,\ell},$$

where

$$A_{\mu,T,\ell} = V_\ell^{1/2}\left(\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}\right)|V_\ell|^{1/2} - m_\mu^{\gamma_\ell,\Delta_\ell}(T)|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|.$$

By assumption (A9), $1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ is invertible. Hence we can write

$$\begin{aligned}1 &+ V_\ell^{1/2}\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}}|V_\ell|^{1/2}\\ &= \left(1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}\right)\\ &\quad\times\left(1 + \frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}(m_\mu^{\gamma_\ell,\Delta_\ell}(T)|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}| + A_{T,\mu,\ell})\right),\end{aligned}$$

and conclude that the operator

$$\frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}(m_\mu^{\gamma_\ell,\Delta_\ell}(T)|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}| + A_{T,\mu,\ell})$$

has an eigenvalue -1.

We are going to show below that

$$\lim_{\ell\to 0}\left\|\frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}A_{\mu,T,\ell}\right\| = 0. \tag{2.15}$$

As a consequence, $1 + (1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2})^{-1}A_{\mu,T,\ell}$ is invertible for small ℓ, and we can argue as above to conclude that the rank one operator

$$m_\mu^{\gamma_\ell,\Delta_\ell}(T)\left(1 + \frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}A_{\mu,T,\ell}\right)^{-1}\frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}|V_\ell^{1/2}\rangle\langle|V_\ell|^{1/2}|$$

has an eigenvalue -1, i.e.

$$\begin{aligned}-1 &= m_\mu^{\gamma_\ell,\Delta_\ell}(T)\\ &\quad\times\left\langle|V_\ell|^{1/2}\left|\left(1 + \frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}A_{\mu,T,\ell}\right)^{-1}\frac{1}{1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}\right|V_\ell^{1/2}\right\rangle.\end{aligned} \tag{2.16}$$

With the aid of (1.11) and the resolvent identity, we can rewrite (2.16) as

$$4\pi a(V_\ell) + \frac{1}{m_\mu^{\gamma_\ell,\Delta_\ell}(T)}$$
$$= \left\langle |V_\ell|^{1/2} \middle| \frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} A_{\mu,T,\ell} \right.$$
$$\times \left. \left(1+\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}A_{\mu,T,\ell}\right)^{-1} \frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} \middle| V_\ell^{1/2} \right\rangle. \tag{2.17}$$

We are going to show below that the term on the right-hand side of (2.17) goes to zero as $\ell \to 0$ and, as a consequence,

$$\lim_{\ell\to 0} m_\mu^{\gamma_\ell,\Delta_\ell}(T) = -\lim_{\ell\to 0}\frac{1}{4\pi a(V_\ell)} = -\frac{1}{4\pi a}. \tag{2.18}$$

On the other hand, by Lemma 5 there is a subsequence of $(\gamma_\ell, \alpha_\ell)$ such that

$$\lim_{\ell\to 0} m_\mu^{\gamma_\ell,\Delta_\ell}(T) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{1}{K_{T,\tilde\mu}^{0,\Delta}} - \frac{1}{p^2}\right)\mathrm{d}^3p,$$

where Δ is the pointwise limit of $|\Delta_\ell(p)|$ and $\tilde\mu$ is the limit of $\tilde\mu^{\gamma_\ell}$. This shows (1.13), at least for a subsequence.

It remains to show (2.15) and (2.18). We start with the decomposition

$$\frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} = \frac{1}{e_\ell}P_\ell + \frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}}(1-P_\ell), \tag{2.19}$$

where the second summand is uniformly bounded by assumption (A9). The integral kernel of $A_{\mu,T,\ell}$ is given by

$$A_{\mu,T,\ell}(x,y) = \frac{V_\ell(x)^{\frac12}|V_\ell(y)|^{\frac12}}{(2\pi)^3}\int_{\mathbb{R}^3}\left(\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}\right)(\mathrm{e}^{-i(x-y)\cdot p}-1)\mathrm{d}^3p, \tag{2.20}$$

which can be estimated as

$$|A_{\mu,T,\ell}(x,y)| \le \frac{|V_\ell(x)|^{\frac12}|V_\ell(y)|^{\frac12}}{(2\pi)^3}\int_{\mathbb{R}^3}\left|\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}\right|(|x-y|\ |p|)^q\mathrm{d}^3p \tag{2.21}$$

for any $0 \le q \le 1$. As in the proof of Lemma 5(vi), using the decomposition (2.14), one can show that the integral

$$\int_{\mathbb{R}^3}\left|\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}\right||p|^q\mathrm{d}^3p$$

converges as $\ell \to 0$ and thus is uniformly bounded in ℓ for $q < 1$. With the aid of assumption (A1), we can thus bound the Hilbert–Schmidt norm of $A_{\mu,T,\ell}$ as

$$\|A_{\mu,T,\ell}\|_2 \le \mathrm{const}\,\ell^q\|V_\ell\|_1. \tag{2.22}$$

In particular, because of assumption (A4),

$$\left\| \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}} (1 - P_\ell) A_{\mu,T,\ell} \right\| \leq O(\ell^q)$$

for small ℓ. It remains to show that the contribution of the first summand in (2.19) to the norm in question vanishes as well. We have

$$\|P_\ell A_{\mu,T,\ell}\| = \frac{\|A^*_{\mu,T,\ell} J_\ell \phi_\ell\|}{|\langle J_\ell \phi_\ell | \phi_\ell \rangle|}.$$

By (2.21),

$$|(A^*_{\mu,T,\ell} J_\ell \phi_\ell)(x)| \leq C \ell^q |V_\ell(x)|^{1/2} \int_{\mathbb{R}^3} |V_\ell(y)|^{1/2} |\phi_\ell(y)| \mathrm{d}^3 y,$$

and hence

$$\|P_\ell A_{\mu,T,\ell}\| \leq \text{const } \ell^q \frac{1}{|\langle J_\ell \phi_\ell | \phi_\ell \rangle|} \left\langle |V_\ell|^{1/2} \middle| |\phi_\ell| \right\rangle \|V_\ell\|_1^{1/2}. \tag{2.23}$$

By (A10), we know that $\frac{\langle |V_\ell|^{1/2} | |\phi_\ell| \rangle}{|\langle J_\ell \phi_\ell | \phi_\ell \rangle|} \leq O(\ell^{1/2})$. Since $e_\ell = O(\ell)$ by assumption, we arrive at

$$\left\| \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}} A_{\mu,T,\ell} \right\| \leq O(\ell^{q-1/2}),$$

which vanishes by choosing $1/2 < q < 1$.

To show (2.18), i.e. that the term on the right-hand side of (2.17) vanishes as $\ell \to 0$, we can again use the decomposition (2.19) to argue that

$$\left\| \left(1 + \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}} A_{\mu,T,\ell} \right)^{-1} \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}} |V_\ell^{1/2}\rangle \right\| \leq O(\ell^{-1/2}), \tag{2.24}$$

where we used (2.15) as well as assumptions (A4), (A9) and (A10). Moreover,

$$\left\| A^*_{\mu,T,\ell} \frac{1}{1 + |V_\ell|^{1/2} \frac{1}{p^2} V_\ell^{1/2}} ||V_\ell|^{1/2}\rangle \right\|$$
$$\leq O(\ell^q) + \frac{1}{e_\ell} \|P_\ell A_{\mu,T,\ell}\| \, \|P_\ell^* ||V_\ell|^{1/2}\rangle\| \leq O(\ell^q) \tag{2.25}$$

using (2.23). The last term in (2.17) thus is of order $\ell^{q-1/2}$, and vanishes as $\ell \to 0$ for any $1/2 < q < 1$. This proves (2.18).

As a last step, we show that the limit points for $\tilde{\mu}^{\gamma_\ell}$ and $|\Delta_\ell(p)|$, and thus also of $\hat{\gamma}_\ell(p)$, are unique. We use the fact that the limit points solve the two implicit equations (1.12) and (1.13), i.e.

$$F(\tilde{\mu}, \Delta) = 0, \quad G(\tilde{\mu}, \Delta) = 0,$$

where

$$F(\nu, \Delta) = \nu - \mu + \frac{\mathcal{V}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left(1 - \frac{p^2 - \nu}{K_{T,\nu}^{0,\Delta}}\right) \mathrm{d}^3 p,$$

$$G(\nu, \Delta) = \frac{1}{4\pi a} + \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\nu}^{0,\Delta}} - \frac{1}{p^2}\right) \mathrm{d}^3 p.$$

It is straightforward to check that

$$\partial_\nu F > 0 \quad \partial_\nu G > 0$$
$$\partial_\Delta F > 0 \quad \partial_\Delta G < 0$$

(compare with similar computations in Appendix B). Hence the set where F vanishes defines a strictly decreasing curve $\mathbb{R}_+ \to \mathbb{R}$, while the analogous curve for the zero-set of G is strictly increasing. Consequently, they can intersect at most once.

This proves uniqueness under the assumptions that $\Delta_\ell \neq 0$ for a sequence of ℓ's going to zero. In the opposite case, $\Delta_\ell = 0$ for ℓ small enough, hence $\Delta = 0$. The uniqueness in this case follows as above, looking at the equation $F(\tilde{\mu}, 0) = 0$. This completes the proof of Theorem 2. □

Remark 6. In case $K_{T,\mu}^{\gamma_\ell,\Delta_\ell}$ is reflection-symmetric in p, one can show that the bound (2.22) holds also for $q = 1$. Indeed, in this case only the symmetric part of $\mathrm{e}^{-i(x-y)\cdot p} - 1$ contributes to the integral kernel of $A_{\mu,T,\ell}$, and hence

$$A_{\mu,T,\ell}(x, y) = \frac{V_\ell^{\frac{1}{2}}(x)|V_\ell|^{\frac{1}{2}}(y)}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}\right) (\cos((x - y) \cdot p) - 1) \mathrm{d}^3 p.$$

It is easy to see, that

$$\left| \frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2} \right| \leq \mathrm{const} \frac{1}{1 + p^4} + R_\ell(p),$$

such that

$$\int_{\mathbb{R}^3} |p R_\ell(p)| \mathrm{d}^3 p$$

is uniformly bounded in ℓ. Indeed, if $|p|^2 > \mu$ we have

$$\left| \frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2} \right| \leq \frac{1}{p^2 - \mu} - \frac{1}{p^2} = \frac{1}{p^4 + 1} \frac{\mu}{1 - \dfrac{1 + \mu p^2}{p^4 + 1}},$$

where on the compact set $|p|^2 \leq \mu$, we just set $R_\ell(p) = |\frac{1}{K_{T,\mu}^{\gamma_\ell,\Delta_\ell}} - \frac{1}{p^2}|$. Since

$$\int_{\mathbb{R}^3} \frac{1-\cos(p\cdot(x-y))}{1+p^4} \mathrm{d}^3p = \sqrt{2}\pi^2 \left[1 - \mathrm{e}^{-\frac{|x-y|}{\sqrt{2}}} \frac{\sin\left(\frac{|x-y|}{\sqrt{2}}\right)}{|x-y|/\sqrt{2}}\right] \leq \pi^2|x-y|,$$

we get

$$\|A_{\mu,T,\ell}\|_2 \leq \text{const}\left[\int_{\mathbb{R}^3} |V_\ell(x)||V_\ell(y)||x-y|^2 \mathrm{d}^3x\mathrm{d}^3y\right]^{1/2} \leq O(\ell)$$

in this case.

2.3. *Critical temperature*

In this section, we will prove Theorem 3. We start with the following observation.

Lemma 6. *Let $\mu > 0$, $T < T_c$, and let $(\gamma_\ell^0, 0)$ be a family of normal states for $\mathcal{F}_T^{V_\ell}$. Then*

$$\liminf_{\ell\to 0} m_\mu^{\gamma_\ell^0,0}(T) > -\frac{1}{4\pi a}. \tag{2.26}$$

Proof. By mimicking the proof of Lemma 5, we observe that (for a suitable subsequence)

$$\lim_{\ell\to 0} m_\mu^{\gamma_\ell^0,0}(T) = m_{\tilde{\mu}^\gamma}^{0,0}(T)$$

where $\tilde{\mu}^\gamma = \mu - 2(2\pi)^{-3/2}\mathcal{V}\int_{\mathbb{R}^3} \hat{\gamma}(p)\mathrm{d}^3p$ and $\hat{\gamma}(p) = (1+\mathrm{e}^{(p^2-\tilde{\mu}^\gamma)/T})^{-1}$. It is shown in Appendix B that $m_{\tilde{\mu}^\gamma}^{0,0}(T)$ is a strictly decreasing function of T. At $T = T_c$, it equals $-1/(4\pi a)$ according to Definition 1, hence $m_{\tilde{\mu}^\gamma}^{0,0}(T) > -1/(4\pi a)$ for $T < T_c$. □

The first part of Theorem 3 then follows from the following lemma.

Lemma 7. *Let $(\gamma_\ell^0, 0)$ be a normal state of $\mathcal{F}_T^{V_\ell}$. Assume that $\lim_{\ell\to 0} m_\mu^{\gamma_\ell^0,0}(T) > -\frac{1}{4\pi a}$. Then, for small enough ℓ, the linear operator $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$ has at least one negative eigenvalue.*

Proof. With the aid of the Birman–Schwinger principle, we will attribute the existence of an eigenvalue of $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$ below the essential spectrum to a solution of a certain implicit equation. We then show the existence of such a solution, which proves the existence of a negative eigenvalue.

Note that the infimum of the essential spectrum of $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$ is $2T$. Let $e < 2T$. According to the Birman–Schwinger principle, $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$ has an eigenvalue e if and only if

$$V_\ell^{1/2} \frac{1}{K_{T,\mu}^{\gamma_\ell^0,0} - e} |V_\ell|^{1/2} \tag{2.27}$$

has an eigenvalue -1. As in the proof of Theorem 2, we decompose the operator (2.27) as

$$V_\ell^{1/2} \frac{1}{K_{T,\mu}^{\gamma_\ell^0,0} - e} |V_\ell|^{1/2} = V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2} + m_{\mu,e}^{\gamma_\ell^0}(T) |V_\ell^{1/2}\rangle\langle |V_\ell|^{1/2}| + A_{\mu,T,\ell,e}$$

where

$$m_{\mu,e}^{\gamma_\ell^0}(T) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_{T,\mu}^{\gamma_\ell^0,0} - e} - \frac{1}{p^2} \right) \mathrm{d}^3 p. \tag{2.28}$$

We claim that the remainder $A_{\mu,T,\ell,e}$ is bounded above by $O(\ell^q)$ in Hilbert–Schmidt norm, for any $0 \le q < 1$, uniformly in e for $e \le 0$. This will follow from the same estimates as in the proof of Theorem 2 if we can show that

$$\int_{\mathbb{R}^3} |p|^q \left(\frac{1}{K_{T,\mu}^{\gamma_\ell^0,0} - e} - \frac{1}{K_{T,\mu}^{\gamma_\ell^0,0}} \right) \mathrm{d}^3 p$$

is uniformly bounded in ℓ for $0 \le q < 1$. But since

$$\begin{aligned} \frac{1}{K_{T,\mu}^{\gamma_\ell^0,0} - e} - \frac{1}{K_{T,\mu}^{\gamma_\ell^0,0}} &= \frac{e}{K_{T,\mu}^{\gamma_\ell^0,0}(K_{T,\mu}^{\gamma_\ell^0,0} - e)} \\ &\le \frac{e}{(2T)^2} \frac{1}{\kappa_c\left(\frac{p^2-\mu}{2T}\right)\left(\kappa_c\left(\frac{p^2-\mu}{2T}\right) - \frac{e}{2T}\right)}, \end{aligned}$$

with κ_c defined in (2.13), this is indeed the case.

Again, the operator

$$\begin{aligned} &1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2} + A_{\mu,T,\ell,e} \\ &\quad = \left(1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}\right) \left(1 + \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}} A_{\mu,T,\ell,e}\right) \end{aligned}$$

is invertible for small ℓ, by assumption (A9) and the fact that

$$\lim_{\ell \to 0} \left\| \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2}} A_{\mu,T,\ell,e} \right\| = 0, \tag{2.29}$$

with the same argument as in the proof of Theorem 2. We conclude that $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$ has an eigenvalue e if and only if the rank one operator

$$m_{\mu,e}^{\gamma_\ell^0}(T) \left(1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2} + A_{\mu,T,\ell,e}\right)^{-1} |V_\ell^{1/2}\rangle\langle |V_\ell|^{1/2}|$$

has an eigenvalue -1, i.e. if

$$\tilde{a}_{\ell,e} = \left\langle |V_\ell|^{1/2} \left| \frac{1}{1 + V_\ell^{1/2} \frac{1}{p^2} |V_\ell|^{1/2} + A_{\mu,T,\ell,e}} \right| V_\ell^{1/2} \right\rangle = -\frac{1}{m_{\mu,e}^{\gamma_\ell^0}(T)}. \tag{2.30}$$

We claim that, for small enough ℓ, the implicit equation (2.30) has a solution $e < 0$, which implies the existence of a negative eigenvalue of $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$. We first argue that $\lim_{\ell\to 0} \tilde{a}_{\ell,e} = 4\pi a$. This follows from the same arguments as in (2.24)–(2.25), in fact. Recall that, by assumption, $\lim_{\ell\to 0} m_\mu^{\gamma_\ell^0,0}(T) > -\frac{1}{4\pi a}$. Moreover the integral $m_{\mu,e}^{\gamma_\ell^0}(T)$ is monotone increasing in e and $e \mapsto m_{\mu,e}^{\gamma_\ell^0}(T)$ maps $(-\infty, 0]$ onto the interval $(-\infty, m_\mu^{\gamma_\ell^0,0}(T)]$. Since $\tilde{a}_{\ell,e}$ depends continuously on e, there has to be a solution $e < 0$ to (2.30) for small enough ℓ, and thus $K_{T,\mu}^{\gamma_\ell^0,0} + V_\ell$ must have a negative eigenvalue. This completes the proof. □

We now give the proof of Theorem 3.

Proof of Theorem 3. Part (i) follows immediately from Lemmas 6 and 7. To prove part (ii), we argue by contradiction. Suppose that $T > T_c$ and that there does not exist an $\ell_0(T)$ such that for $\ell < \ell_0(T)$ all minimizers of $\mathcal{F}_T^{V_\ell}$ are normal. Then there exists a sequence of ℓ's going to zero and corresponding minimizers $(\gamma_\ell, \alpha_\ell)$ with $\alpha_\ell \neq 0$ and thus, by Theorem 2, Eqs. (1.12) and (1.13) hold in the limit $\ell \to 0$. We claim that these equations do not have a solution for $T > T_c$, thus providing the desired contradiction.

At the end of the proof of Theorem 2, we have already argued that the right-hand side of (1.13) is monotone decreasing in Δ and increasing in $\tilde{\mu}$. Moreover, $\tilde{\mu}$ is decreasing in Δ. In particular, we conclude from Eqs. (1.12) and (1.13) that

$$-\frac{1}{4\pi a} \leq \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{\tanh\left(\frac{p^2 - \tilde{\mu}}{2T}\right)}{p^2 - \tilde{\mu}} - \frac{1}{p^2} \right) \mathrm{d}^3 p$$

with $\tilde{\mu}$ given by

$$\tilde{\mu} = \mu - \frac{2\mathcal{V}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{1}{1 + \mathrm{e}^{\frac{p^2 - \tilde{\mu}}{T}}} \mathrm{d}^3 p.$$

According to our analysis in Appendix B, this implies $T \leq T_c$, however. □

Acknowledgments

We would like to thank Max Lein and Andreas Deuchert for valuable suggestions and remarks. Partial financial support by the NSERC (R.S.) is gratefully acknowledged.

A. Example of a Sequence of Short-Range Potentials

In dimension $d = 3$, contact potentials are realized by a one-parameter family $-\Delta_a$ of self-adjoint extensions of the Laplacian $-\Delta|_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}$, indexed by the scattering length a. Moreover, $-\Delta_a$ can be obtained as a norm resolvent limit of short-range Hamiltonians of the form $-\Delta + V_\ell$. This is presented in [2, 1] in the case of $0 < \lim_{\ell\to 0} \|V_\ell\|_{3/2} < \infty$, and was extended in [6] to cases where $0 < \lim_{\ell\to 0} \|V_\ell\|_1 < \infty$. In this appendix, we use an approach similar to [6] to construct a sequence of potentials V_ℓ converging to a contact potential. In particular, we are interested in the case where the scattering length $a(V_\ell)$ converges to a negative value $a < 0$, and where all the assumptions in Assumption 1 are satisfied.

A.1. *Example* 1

As a first example, we follow [1, Chap. I.1.2-4]. We start with an arbitrary potential $V \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, such that

(1) $p^2 + V(x) \geq 0$, and V has a simple zero-energy resonance, i.e. there is a simple eigenvector $\phi \in L^2(\mathbb{R}^3)$ with $(V^{1/2}\frac{1}{p^2}|V|^{1/2} + 1)\phi = 0$, and $\psi(x) = \frac{1}{p^2}|V|^{1/2}\phi \in L^2_{\text{loc}}(\mathbb{R}^3)$,

(2) $\|\hat{V}\|_\infty \leq 2\hat{V}(0)$.

Define $V_\ell(x) = \lambda(\ell)\ell^{-2}V(\frac{x}{\ell})$, where $\lambda(0) = 1$, $\lambda < 1$ for all $\ell > 0$ and $1-\lambda(\ell) = O(\ell)$. The important point of this scaling is the following. Denote by U_ℓ the unitary scaling operator $(U_\ell\varphi)(x) = \ell^{-3/2}\varphi(\frac{x}{\ell})$. By a simple calculation, one obtains the relation

$$U_\ell V^{1/2}\frac{1}{p^2}|V|^{1/2}U_\ell^{-1} = \frac{1}{\lambda(\ell)}V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2},$$

such that, with $\phi_\ell = U_\ell\phi$,

$$V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}\phi_\ell = \lambda(\ell)U_\ell V^{1/2}\frac{1}{p^2}|V|^{1/2}\phi = -\lambda(\ell)\phi_\ell. \tag{A.1}$$

This shows that the lowest eigenvalue of $1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ is $1 - \lambda(\ell) = O(\ell)$.

Moreover, by construction, $\hat{V}_\ell(p) = \ell\lambda(\ell)\hat{V}(\ell p)$, $\|V_\ell\|_{3/2} = \lambda(\ell)\|V\|_{3/2}$, and the 1-norm can be bounded as $\|V_\ell\|_1 \leq (\frac{4}{3}\pi)^{1/3}\ell\lambda(\ell)\|V\|_{3/2}$, hence (A1), (A2) and (A4)–(A7) hold.

The validity of assumption (A8) is a consequence of the following general fact.

Lemma 8. *If $\|V_\ell\|_{3/2}$ is uniformly bounded, assumptions* (A1) *and* (A9) *imply assumption* (A8).

Proof. We look for $C > 0$ such that $p^2 + V_\ell - |p|^b + C$ is non-negative for all $\ell > 0$. By the Birman–Schwinger principle, this is the case if and only if

$$1 + V_\ell^{1/2}\frac{1}{p^2 - |p|^b + C + E}|V_\ell|^{1/2} = 1 + J_\ell X_\ell^{C+E} + R_\ell^E$$

is invertible for all $E>0$. Here $J_\ell = \begin{cases} 1, & V_\ell \geq 0 \\ -1, & V_\ell < 0 \end{cases}$, $X_\ell^E = |V_\ell|^{1/2}\frac{1}{p^2+E}|V_\ell|^{1/2}$ and

$$R_\ell^E = V_\ell^{1/2}\frac{1}{p^2-|p|^b+C+E}|V_\ell|^{1/2} - V_\ell^{1/2}\frac{1}{p^2+C+E}|V_\ell|^{1/2}.$$

By expanding in a Neumann series, we see that $1+J_\ell X_\ell^{C+E}+R_\ell^E$ has a bounded inverse provided that

$$\|(1+J_\ell X_\ell^{C+E})^{-1}\|\,\|R_\ell^E\| < 1. \tag{A.2}$$

We first examine $\|(1+J_\ell X_\ell^E)^{-1}\|$. We have

$$\frac{1}{1+J_\ell X_\ell^E} = 1 - J_\ell (X_\ell^E)^{1/2}\frac{1}{1+(X_\ell^E)^{1/2}J_\ell (X_\ell^E)^{1/2}}(X_\ell^E)^{1/2},$$

and thus

$$\left\|\frac{1}{1+J_\ell X_\ell^E}\right\| \leq 1 + \|X_\ell^E\|\left\|\frac{1}{1+(X_\ell^E)^{1/2}J_\ell (X_\ell^E)^{1/2}}\right\|.$$

Using the fact that $(4\pi|x-y|)^{-1}\mathrm{e}^{-\sqrt{E}|x-y|}$ is the integral kernel of the operator $\frac{1}{p^2+E}$ for $E\geq 0$, the Hardy–Littlewood–Sobolev inequality [19, Theorem 4.3] implies that $\|X_\ell^E\| \leq \|X_\ell^0\|_2 \leq c_2\|V_\ell\|_{3/2}$. Moreover, $\|(1+(X_\ell^E)^{1/2}J_\ell(X_\ell^E)^{1/2})^{-1}\|$ is the inverse of the eigenvalue of $1+(X_\ell^E)^{1/2}J_\ell(X_\ell^E)^{1/2}$ with smallest modulus, and this latter operator is isospectral to $1+J_\ell X_\ell^E$. We conclude that $\|(1+(X_\ell^E)^{1/2}J_\ell(X_\ell^E)^{1/2})^{-1}\| \leq e_\ell(E)^{-1}$, where $e_\ell(E)$ is the smallest eigenvalue of $1+J_\ell X_\ell^E$. The latter is bigger than $e_\ell(0)$, which is of order $O(\ell)$ by assumption (A9). This shows that there is a constant $c_1>0$ such that

$$\left\|\frac{1}{1+J_\ell X_\ell^{C+E}}\right\| \leq c_1\ell^{-1}$$

for small ℓ.

It remains to bound the operator R_ℓ^E, whose integral kernel is given by

$$R_\ell^E(x,y) = \frac{1}{(2\pi)^3}V_\ell(x)^{1/2}|V_\ell(y)|^{1/2} \times \int_{\mathbb{R}^3}\left(\frac{1}{p^2-|p|^b+C+E} - \frac{1}{p^2+C+E}\right)\mathrm{e}^{-ip\cdot(y-x)}\mathrm{d}^3p.$$

The trace norm $\|R_\ell^E\|_1$ is bounded by

$$\|R_\ell^E\|_1 \leq \frac{4\pi}{(2\pi)^3}\|V_\ell\|_1\int_0^\infty \frac{p^b}{p^2-p^b+C+E}\frac{p^2}{p^2+C+E}\mathrm{d}p.$$

By dominated convergence, the integral tends to 0 as $C\to\infty$. By Hölder's inequality, $\|V_\ell\|_1 \leq O(\ell)$, so there exists a C such that $\|R_\ell^E\| < c_1^{-1}\ell$. This shows (A.2). □

Next we show the validity of (A9). Let $J = \begin{cases} 1, & V \geq 0 \\ -1, & V < 0 \end{cases}$, $X = |V|^{1/2}\frac{1}{p^2}|V|^{1/2}$ and $P = \frac{1}{\langle J\phi|\phi\rangle}|\phi\rangle\langle J\phi|$ the projection onto the eigenfunction ϕ corresponding to the zero eigenvalue of $1+V^{1/2}\frac{1}{p^2}|V|^{1/2} = 1+JX$. Using the unitary scaling operator U_ℓ we also introduce the scaled versions $\phi_\ell = U_\ell\phi$, $J_\ell = U_\ell J U_\ell^{-1}$ and $P_\ell = U_\ell P U_\ell^{-1}$, and let $X_\ell = \lambda(\ell)U_\ell X U_\ell^{-1}$. Then $\langle J_\ell\phi_\ell|\phi_\ell\rangle = \langle J\phi|\phi\rangle = -\langle X\phi|\phi\rangle < 0$ does not vanish, since $X = |V|^{1/2}\frac{1}{p^2}|V|^{1/2}$ is a positive operator whose kernel does not contain ϕ. Note that $[JX, P] = 0$, which follows from

$$(1+JX)P = 0$$

and

$$P(1+JX) = JP^*J(1+JX) = JP^*(1+JX)^*J = J((1+JX)P)^*J = 0.$$

We decompose $1+J_\ell X_\ell$ as

$$1+J_\ell X_\ell = (1+J_\ell X_\ell)P_\ell + (1+J_\ell X_\ell)(1-P_\ell)$$

and examine the two parts separately. For the first summand, note that since $JX\phi = -\phi$,

$$(1+J_\ell X_\ell)P_\ell = (1-\lambda(\ell))P_\ell.$$

Next, we study the operator $J_\ell X_\ell(1-P_\ell)$. The operator

$$T = 1+JX(1-P) = 1+JX+P$$

has no zero eigenvalue. Indeed, if $T\psi = 0$, then

$$0 = (1+JX+P)(P+(1-P))\psi = P\psi + (1-P)(1+JX)\psi,$$

where we used that P commutes with $1+JX$. Projecting onto P and $1-P$, respectively, yields

$$0 = P\psi, \quad 0 = (1-P)(1+JX)\psi = (1+JX)\psi,$$

which constrains ψ to be 0.

Due to the compactness of $P+JX$, eigenvalues of T can only accumulate at 1, and hence T has a bounded inverse T^{-1}. Now $J_\ell X_\ell = \lambda(\ell)U_\ell JXU_\ell^{-1}$, and we have the decomposition

$$U_\ell^{-1}(1+J_\ell X_\ell)U_\ell = 1+\lambda(\ell)JX = (1-\lambda(\ell))P + [1+\lambda(\ell)(T-1)](1-P)$$

with inverse

$$U_\ell^{-1}\frac{1}{1+J_\ell X_\ell}U_\ell = \frac{1}{1-\lambda(\ell)}P + \frac{1}{1-\lambda(\ell)+\lambda(\ell)T}(1-P).$$

This shows that

$$\frac{1}{1+J_\ell X_\ell}(1-P_\ell) = U_\ell\frac{1}{1-\lambda(\ell)+\lambda(\ell)T}(1-P)U_\ell^{-1}.$$

Since 0, and thus also a neighborhood of 0, is not in the spectrum of T, and $\lambda(\ell)\to 1$ as $\ell\to 0$, we conclude that $\frac{1}{1-\lambda(\ell)+\lambda(\ell)T}$ is uniformly bounded for small ℓ. This yields the uniform boundedness of $\frac{1}{1+J_\ell X_\ell}(1-P_\ell)$.

In order to prove (A3) we decompose $\frac{1}{1+J_\ell X_\ell}$ as

$$\frac{1}{1+J_\ell X_\ell} = \frac{1}{1+J_\ell X_\ell}P_\ell + \frac{1}{1+J_\ell X_\ell}(1-P_\ell) = \frac{1}{1-\lambda(\ell)}P_\ell + \frac{1}{1+J_\ell X_\ell}(1-P_\ell).$$

We have just shown that the second summand is uniformly bounded in ℓ. This allows us to calculate the limit $\ell \to 0$ of the scattering length $a(V_\ell)$, which equals

$$\begin{aligned} 4\pi a(V_\ell) &= \left\langle |V_\ell|^{1/2} \middle| \frac{1}{1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}} V_\ell^{1/2} \right\rangle \\ &= \frac{1}{1-\lambda(\ell)}\langle |V_\ell|^{1/2}|P_\ell V_\ell^{1/2}\rangle + \left\langle |V_\ell|^{1/2} \middle| \frac{1}{1+J_\ell X_\ell}(1-P_\ell)V_\ell^{1/2} \right\rangle. \end{aligned}$$

Using the uniform boundedness of the second summand together with the fact that $\|V_\ell\|_1 \to 0$ as $\ell \to 0$, we see that the second summand vanishes in the limit $\ell \to 0$. Therefore

$$\begin{aligned} \lim_{\ell\to 0} 4\pi a(V_\ell) &= \lim_{\ell\to 0} \frac{1}{1-\lambda(\ell)} \frac{|\langle |V_\ell|^{1/2}|\phi_\ell\rangle|^2}{\langle J_\ell \phi_\ell|\phi_\ell\rangle} \\ &= \lim_{\ell\to 0} \lambda(\ell)\frac{\ell}{1-\lambda(\ell)} \frac{|\langle |V|^{1/2}|\phi\rangle|^2}{\langle J\phi|\phi\rangle} \\ &= -\frac{1}{\lambda'(0)} \frac{|\langle |V|^{1/2}|\phi\rangle|^2}{\langle J\phi|\phi\rangle}. \end{aligned}$$

We are left with demonstrating (A10). This is immediate, since

$$\langle |V_\ell|^{1/2}|\phi_\ell\rangle = \sqrt{\lambda(\ell)}\ell^{1/2}\langle |V|^{1/2}||\phi|\rangle$$

and

$$\langle \phi_\ell|\mathrm{sgn}(V_\ell)\phi_\ell\rangle = \langle \phi|\mathrm{sgn}(V)\phi\rangle.$$

A.2. *Example* 2

We consider a sequence of potentials as suggested in [15], of the form

$$V_\ell = V_\ell^+ - V_\ell^-, \quad \begin{aligned} V_\ell^+(x) &= (k_\ell^+)^2\ \chi_{\{|x|<\epsilon_\ell\}}(x), \\ V_\ell^-(x) &= (k_\ell^-)^2\ \chi_{\{\epsilon_\ell<|x|<\ell\}}(x), \end{aligned} \quad \begin{aligned} k_\ell^+ &= k^+\epsilon_\ell^{-3/2} \\ k_\ell^- &= \frac{\frac{\pi}{2}-\ell\omega}{\ell-\epsilon_\ell}, \end{aligned} \tag{A.3}$$

with $\omega > 0$, $k^+ > 0$ and $0 < \epsilon_\ell < c\ell^2$ with $c < 2\omega/\pi$. The function $\chi_A(x)$ denotes the characteristic function of the set A. (See the sketch on p. 7.) We shall show that this sequence of potentials satisfies assumptions (A1)–(A10).

Assumptions (A1), (A2), (A4), (A5) and (A7) are in fact obvious, and $\mathcal{V} = \lim_{\ell\to 0}\hat{V}_\ell(0) = \sqrt{2/\pi}(k^+)^2/3$.

(A3) To calculate the scattering length $a(V_\ell)$, we have to find the solution ψ_ℓ of $-\Delta\psi_\ell + V_\ell\psi_\ell = 0$, with $\lim_{|x|\to\infty}\psi_\ell(x) = 1$. The scattering length then appears in the asymptotics

$$\psi_\ell(x) \approx 1 - \frac{a(V_\ell)}{|x|}$$

for large $|x|$. To solve the zero-energy scattering equation, we write $\psi_\ell(x) = \frac{u_\ell(|x|)}{|x|}$ with $u_\ell(0) = 0$. Then u_ℓ solves the equation

$$-u_\ell'' + V_\ell u_\ell = 0.$$

For $r \geq \ell$ the function u_ℓ is of the form $u_\ell(r) = c_1 r + c_2$. The normalization at infinity requires $c_1 = 1$, and ψ_ℓ automatically has the desired asymptotics with $a(V_\ell) = -c_2$.

In our example, the equation we have to solve is

$$\begin{cases} -u_\ell''(r) + (k_\ell^+)^2 u_\ell(r) = 0, & 0 \leq r \leq \epsilon_\ell \\ -u_\ell''(r) - (k_\ell^-)^2 u_\ell(r) = 0, & \epsilon_\ell \leq r \leq \ell \\ -u_\ell''(r) = 0, & r \geq \ell, \end{cases}$$

with the solution

$$u_\ell(r) = \begin{cases} A\sinh(k_\ell^+ r), & 0 \leq r \leq \epsilon_\ell \\ B_1\cos(k_\ell^- r) + B_2\sin(k_\ell^- r), & \epsilon_\ell \leq r \leq \ell \\ r - a(V_\ell), & r \geq \ell. \end{cases}$$

Continuity of u_ℓ and u_ℓ' then requires

$$A\sinh(k_\ell^+\epsilon_\ell) = B_1\cos(k_\ell^-\epsilon_\ell) + B_2\sin(k_\ell^-\epsilon_\ell)$$
$$Ak_\ell^+\cosh(k_\ell^+\epsilon_\ell) = -B_1k_\ell^-\sin(k_\ell^-\epsilon_\ell) + B_2k_\ell^-\cos(k_\ell^-\epsilon_\ell)$$

and

$$B_1\cos(k_\ell^-\ell) + B_2\sin(k_\ell^-\ell) = \ell - a(V_\ell)$$
$$-B_1k_\ell^-\sin(k_\ell^-\ell) + B_2k_\ell^-\cos(k_\ell^-\ell) = 1.$$

Solving for $a(V_\ell)$ yields

$$a(V_\ell) = \ell - \frac{1}{k_\ell^-}\frac{k_\ell^+\tan(k_\ell^-(\ell-\epsilon_\ell)) + k_\ell^-\tanh(k_\ell^+\epsilon_\ell)}{k_\ell^+ - k_\ell^-\tan(k_\ell^-(\ell-\epsilon_\ell))\tanh(k_\ell^+\epsilon_\ell)}. \tag{A.4}$$

By Eq. (A.3), $(\ell-\epsilon_\ell)k_\ell^- = \frac{\pi}{2} - \ell\omega$ and $k_\ell^+\epsilon_\ell = k^+\epsilon_\ell^{-1/2}$. Since we assume that $\epsilon_\ell = O(\ell^2)$, we thus obtain as expression for the scattering length in the limit $\ell \to 0$

$$\lim_{\ell\to 0} a(V_\ell) = -\lim_{\ell\to 0}\frac{\tan\left(\frac{\pi}{2} - \ell\omega\right)}{k_\ell^-} = -\frac{2}{\pi\omega}.$$

This shows the validity of (A3).

(A6) To verify assumption (A6), we have to compute the Fourier transform of V_ℓ, which equals

$$\hat{V}_\ell(p) = \sqrt{\frac{2}{\pi}}[\epsilon_\ell^3((k_\ell^+)^2 + (k_\ell^-)^2)\varsigma(|p|\epsilon_\ell) - (k_\ell^-)^2\ell^3\ \varsigma(|p|\ell)],$$

with $\varsigma(x) = \frac{1}{x^3}(\sin(x) - x\cos(x))$. Since $|\varsigma(p)| \le \varsigma(0) = 1/3$, one readily checks that $|\hat{V}_\ell(p)| \le 2|\hat{V}_\ell(0)|$ for ℓ small enough.

(A8) Our next goal is to verify assumption (A8). Let $U(x) = \frac{\pi^2}{4}\chi_{|x|\le 1}(x)$ and set $U_\ell(x) = \ell^{-2}U(x/\ell)$. For $\lambda(\ell) = (\frac{1-2\frac{\omega}{\pi}\ell}{1-\epsilon_\ell/\ell})^2$, the potential $W_\ell(x) = \lambda(\ell)U_\ell(x)$ agrees with $V_\ell^-(x)$ on its support, so obviously $-W_\ell(x) \le -V_\ell^-(x) \le V_\ell(x)$ holds. The function $U_\ell(x)$ is chosen such that $p^2 - U_\ell(x)$ has a zero energy resonance. Indeed,

$$\psi(x) = \begin{cases} \sin\left(\frac{\pi}{2}|x|\right)\Big/|x|, & |x| \le 1 \\ 1/|x|, & |x| \ge 1 \end{cases} \in L^2_{\mathrm{loc}}(\mathbb{R}^3)\backslash L^2(\mathbb{R}^3)$$

is a generalized eigenfunction of $p^2 - U$ and $\psi_\ell(x) = \psi(x/\ell)$ is a generalized eigenfunction of $p^2 - U_\ell$. Therefore, $U_\ell^{1/2}\frac{1}{p^2}U_\ell^{1/2}$ has the eigenvector $U_\ell^{1/2}\psi_\ell \in L^2(\mathbb{R}^3)$ to the eigenvalue 1.

Note that our condition on ϵ_ℓ implies that $\lambda(\ell) < 1 - c\ell$ for some constant $c > 0$ and small enough ℓ. Since $V_\ell^- \le W_\ell$, the largest eigenvalue of $(V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2}$ is smaller or equal to $\lambda(\ell)$, i.e.

$$\left\|(V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2}\right\| \le \lambda(\ell) \le 1 - c\ell. \tag{A.5}$$

Now choose $C > 0$ such that $p^2 - |p|^b + C > 0$ and define the operator

$$R_\ell = (V_\ell^-)^{1/2}\frac{1}{p^2 - |p|^b + C}(V_\ell^-)^{1/2} - (V_\ell^-)^{1/2}\frac{1}{p^2 + C}(V_\ell^-)^{1/2}.$$

Its trace norm equals

$$\|R_\ell\|_1 = \frac{1}{2\pi^2}\|V_\ell^-\|_1\int_0^\infty \frac{p^2}{p^2 + C}\frac{p^b}{p^2 - p^b + C}\mathrm{d}p,$$

which tends to zero as $C \to \infty$ by monotone convergence. Since $\|V_\ell^-\|_1 = O(\ell)$, there is a C such that $\|R_\ell\| < c\ell$, proving that

$$\begin{aligned}\left\|(V_\ell^-)^{1/2}\frac{1}{p^2 - |p|^b + C}(V_\ell^-)^{1/2}\right\| &\le \left\|(V_\ell^-)^{1/2}\frac{1}{p^2 + C}(V_\ell^-)^{1/2}\right\| + \|R_\ell\| \\ &< \left\|(V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2}\right\| + c\ell \le 1,\end{aligned}$$

where we have used (A.5) in the last step. By the Birman–Schwinger principle, this shows that $p^2 - V_\ell^- - |p|^b + C \ge 0$, and hence also $p^2 + V_\ell - |p|^b + C \ge 0$.

(A9) Note that $V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ has an eigenvalue $-\lambda^{-1} \neq 0$ if and only if $p^2 + \lambda V_\ell$ has a zero-energy resonance. Equivalently, the scattering length $a(\lambda V_\ell)$ diverges. According to our calculation (A.4), this happens for $\lambda > 0$ either satisfying

$$k_\ell^+ = k_\ell^- \tan(\sqrt{\lambda}k_\ell^-(\ell - \epsilon_\ell))\tanh(\sqrt{\lambda}k_\ell^+\epsilon_\ell)$$

or $\sqrt{\lambda}k_\ell^-(\ell - \epsilon_\ell) = m\pi/2$ for odd integer m. The smallest λ satisfying either of these equations is $\lambda = 1 + 4\ell\omega/\pi + O(\ell^2)$, hence the smallest eigenvalue of $1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ is

$$e_\ell = 4\ell\omega/\pi + O(\ell^2).$$

We are left with showing that

$$\left(1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}\right)^{-1}(1 - P_\ell)$$

is uniformly bounded in ℓ. This follows directly from [6, Consequence 1]. For the sake of completeness we repeat the argument here.

First, recall that ϕ_ℓ denotes the eigenvector of $1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ to its smallest eigenvalue e_ℓ, and $J_\ell = \begin{cases} 1, & V_\ell \geq 0 \\ -1, & V_\ell < 0\end{cases}$. We also introduce the notation $X_\ell = |V_\ell|^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}$ and $X_\ell^\pm = |V_\ell^\pm|^{1/2}\frac{1}{p^2}|V_\ell^\pm|^{1/2}$.

We now pick some $\psi \in L^2(\mathbb{R}^3)$ and set

$$\varphi = \left(1 + V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2}\right)^{-1}(1 - P_\ell)\psi = \frac{1}{1 + J_\ell X_\ell}(1 - P_\ell)\psi$$
$$= \frac{1}{J_\ell + X_\ell}J_\ell(1 - P_\ell)\psi. \tag{A.6}$$

Below we are going to show that there exists a constant $c > 0$ such that for small enough ℓ

$$\langle\varphi|(1 - X_\ell^-)\varphi\rangle \geq c\|\varphi\|_{L^2}^2. \tag{A.7}$$

In order to utilize this inequality we need the following lemma, which already appeared in [6, Lemma 1].

Lemma 9. *Let $V = V_+ - V_-$, where $V_-, V_+ \geq 0$ have disjoint support. Denote $J = \begin{cases} 1, & V \geq 0 \\ -1, & V < 0\end{cases}$, $X = |V|^{1/2}\frac{1}{p^2}|V|^{1/2}$ and $X_\pm = V_\pm^{1/2}\frac{1}{p^2}V_\pm^{1/2}$. Then for any $\phi \in L^2(\mathbb{R}^3)$, we have*

$$\sqrt{2}\,\|\phi\|\|(J + X)\phi\| \geq \langle\phi|(X_+ + 1 - X_-)\phi\rangle. \tag{A.8}$$

Proof. Decompose $\phi = \phi_+ + \phi_-$, such that $\mathrm{supp}(\phi_-) \subseteq \mathrm{supp}(V_-)$ and $\mathrm{supp}(\phi_+) \cap \mathrm{supp}(V_-) = \emptyset$. By applying the Cauchy–Schwarz inequality, we have

$$\|(J + X)\phi\|\|\phi_+\| \geq \Re\langle\phi_+|(J + X)\phi\rangle$$
$$= \langle\phi_+|(1 + X_+)\phi_+\rangle + \Re\langle\phi_+|V_+^{1/2}\tfrac{1}{p^2}V_-^{1/2}\phi_-\rangle,$$

$$\|(J+X)\phi\|\|\phi_-\| \geq \Re\langle (J+X)\phi| - \phi_-\rangle$$
$$= \langle \phi_-|(1-X_-)\phi_-\rangle - \Re\langle \phi_+|V_+^{1/2}\tfrac{1}{p^2}V_-^{1/2}\phi_-\rangle.$$

We add the two inequalities and obtain

$$\|(J+X)\phi\|(\|\phi_+\|+\|\phi_-\|) \geq \langle \phi_+|(1+X_+)\phi_+\rangle + \langle \phi_-|(1-X_-)\phi_-\rangle$$
$$= \langle \phi|(X_+ + 1 - X_-)\phi\rangle.$$

Finally, we use that $\|\phi_+\|+\|\phi_-\| \leq \sqrt{2}\|\phi\|$, which completes the proof. □

In combination with Lemma 9 the inequality (A.7) immediately yields

$$\sqrt{2}\|\varphi\|\|(J_\ell + X_\ell)\varphi\| \geq \langle \varphi|(1-X_\ell^-)\varphi\rangle \geq c\|\varphi\|^2,$$

which further implies that

$$\|\psi\| \geq \|J_\ell(1-P_\ell)\psi\| = \|(J_\ell+X_\ell)\varphi\| \geq \frac{c}{\sqrt{2}}\|\varphi\| = \frac{c}{\sqrt{2}}\|(1+J_\ell X_\ell)^{-1}(1-P_\ell)\psi\|,$$

proving uniform boundedness of $(1+V_\ell^{1/2}\frac{1}{p^2}|V_\ell|^{1/2})^{-1}(1-P_\ell)$.

It remains to show the inequality (A.7). To this aim we denote by ϕ_ℓ^- the eigenvector corresponding to the smallest eigenvalue $e_\ell^- > 0$ of $1-X_\ell^-$ and by $P_{\phi_\ell^-}$ the orthogonal projection onto ϕ_ℓ^-. The Birman–Schwinger operator X_ℓ^- corresponding to the potential V_ℓ^- has only one eigenvalue close to 1. All other eigenvalues are separated from 1 by a gap of order one. Hence there exists $c_1 > 0$ such that

$$(1-X_\ell^-)(1-P_{\phi_\ell^-}) \geq c_1$$

and, therefore,

$$\langle \varphi|(1-X_\ell^-)\varphi\rangle \geq c_1\langle \varphi|(1-P_{\phi_\ell^-})\varphi\rangle + e_\ell^-\langle \varphi|P_{\phi_\ell^-}\varphi\rangle$$
$$= c_1\|\varphi\|_{L^2}^2 + (e_\ell^- - c_1)\langle \varphi|P_{\phi_\ell^-}\varphi\rangle.$$

With $P_{J_\ell\phi_\ell} = |J_\ell\phi_\ell\rangle\langle J_\ell\phi_\ell|$ being the orthogonal projection onto $J_\ell\phi_\ell$ we can write

$$\varphi = (1-P_{J_\ell\phi_\ell})\varphi,$$

simply for the reason that, because of (A.6) and the fact that P_ℓ commutes with B_ℓ,

$$P_{J_\ell\phi_\ell}\varphi = P_{J_\ell\phi_\ell}(1+J_\ell X_\ell)^{-1}(1-P_\ell)\psi = P_{J_\ell\phi_\ell}(1-P_\ell)(1+J_\ell X_\ell)^{-1}\psi = 0.$$

Consequently,

$$|\langle \varphi|P_{\phi_\ell^-}\varphi\rangle| = |\langle \varphi|(1-P_{J_\ell\phi_\ell})P_{\phi_\ell^-}\varphi\rangle| \leq \|\varphi\|_{L^2}^2\|(1-P_{J_\ell\phi_\ell})P_{\phi_\ell^-}\|$$
$$= \|\varphi\|_{L^2}^2\|(1-P_{J_\ell\phi_\ell})\phi_\ell^-\|^2 = \|\varphi\|_{L^2}^2\|(1-P_{\phi_\ell^-})J_\ell\phi_\ell\|^2.$$

To estimate $\|(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\|$, we apply Lemma 9 to ϕ_ℓ and obtain

$$\begin{aligned}\sqrt{2}\, e_\ell = \sqrt{2}\,\|(J_\ell + X_\ell)\phi_\ell\| \geq \langle \phi_\ell|(1 - X_\ell^-)\phi_\ell\rangle \\ = \langle J_\ell\phi_\ell|(1 - X_\ell^-)J_\ell\phi_\ell\rangle = e_\ell^- \,|\langle J_\ell\phi_\ell|\phi_\ell^-\rangle|^2 \\ + \langle (1 - P_{\phi_\ell^-})J_\ell\phi_\ell|(1 - X_\ell^-)(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\rangle \\ \geq c_1\|(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\|^2.\end{aligned}$$

This shows that $\|(1 - P_{\phi_\ell^-})J_\ell\phi_\ell\| = O(\ell^{1/2})$ and consequently (A.7) holds for small enough ℓ.

(A10) By construction, $1 - (V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2}$ has no negative eigenvalues. By applying Lemma 9 to ϕ_ℓ, we obtain

$$\begin{aligned}\left\langle \phi_\ell \,\middle|\, (V_\ell^+)^{1/2}\frac{1}{p^2}(V_\ell^+)^{1/2}\ \phi_\ell\right\rangle \leq \sqrt{2}e_\ell \quad \text{and} \\ \left\langle \phi_\ell \,\middle|\, \left(1 - (V_\ell^-)^{1/2}\frac{1}{p^2}(V_\ell^-)^{1/2}\right)\ \phi_\ell\right\rangle \leq \sqrt{2}e_\ell.\end{aligned} \tag{A.9}$$

We claim that this implies

$$\lim_{\ell\to 0}\langle J_\ell\phi_\ell|\phi_\ell\rangle = -1.$$

Indeed,

$$(J_\ell + X_\ell)\phi_\ell = e_\ell J_\ell\phi_\ell$$

and thus

$$\begin{aligned}(1 - e_\ell)\langle J_\ell\phi_\ell|\phi_\ell\rangle &= -\langle \phi_\ell|X_\ell\phi_\ell\rangle \\ &= -\langle \phi_\ell|X_\ell^+\phi_\ell\rangle - \langle \phi_\ell|X_\ell^-\phi_\ell\rangle \\ &\quad - \langle \phi_\ell|(V_\ell^-)^{1/2}\tfrac{1}{p^2}(V_\ell^+)^{1/2}\phi_\ell\rangle - \langle \phi_\ell|(V_\ell^+)^{1/2}\tfrac{1}{p^2}(V_\ell^-)^{1/2}\phi_\ell\rangle.\end{aligned}$$

Adding 1 on both sides yields

$$\begin{aligned}(1 - e_\ell)\langle (1 + J_\ell)\phi_\ell|\phi_\ell\rangle + e_\ell &= -\langle \phi_\ell|X_\ell^+\phi_\ell\rangle + \langle \phi_\ell|(1 - X_\ell^-)\phi_\ell\rangle \\ &\quad - \langle \phi_\ell|(V_\ell^-)^{1/2}\tfrac{1}{p^2}(V_\ell^+)^{1/2}\phi_\ell\rangle \\ &\quad - \langle \phi_\ell|(V_\ell^+)^{1/2}\tfrac{1}{p^2}(V_\ell^-)^{1/2}\phi_\ell\rangle.\end{aligned}$$

By taking the absolute value, applying the Cauchy–Schwarz inequality and using (A.9), we obtain

$$\begin{aligned}|\langle (1 + J_\ell)\phi_\ell|\phi_\ell\rangle| &\leq \frac{1}{1 - e_\ell}\Big((1 + 2\sqrt{2})e_\ell + 2\sqrt{\langle \phi_\ell|X_\ell^+\phi_\ell\rangle\langle \phi_\ell|X_\ell^-\phi_\ell\rangle}\Big) \\ &= O(e_\ell^{1/2}).\end{aligned} \tag{A.10}$$

Finally, to bound $\langle |V_\ell|^{1/2} | |\phi_\ell| \rangle$, we note that $\langle |V_\ell^-|^{1/2} | |\phi_\ell| \rangle \le \|V_\ell^-\|_1^{1/2} = O(\ell^{1/2})$. For the analogous bound with V_ℓ^- replaced by V_ℓ^+, we can again employ Lemma 9, which implies that $\sqrt{2} e_\ell \ge \langle \phi_\ell^+ | X_\ell^+ + 1 | \phi_\ell^+ \rangle \ge \|\phi_\ell^+\|_2^2$ (where $\phi_\ell^+ = \frac{1}{2}(1 + J_\ell)\phi_\ell$), hence $\langle |V_\ell^+|^{1/2} | |\phi_\ell| \rangle \le \|V_\ell^+\|_1^{1/2} \|\phi_\ell^+\|_2 \le O(\ell^{1/2})$. This completes the proof.

B. The Definition of T_c

In this appendix, we shall show that Eq. (1.15) define T_c and $\tilde{\mu}$ uniquely. To start, let $F : \mathbb{R} \times \mathbb{R}_+ \to \mathbb{R}^2$ be defined by its components

$$F_1(\nu, T) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{\tanh\left(\dfrac{p^2 - \nu}{2T}\right)}{p^2 - \nu} - \frac{1}{p^2} \right) \mathrm{d}^3 p \tag{B.1}$$

and

$$F_2(\nu, T) = \nu + \frac{2\mathcal{V}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{1}{1 + \mathrm{e}^{\frac{p^2 - \nu}{T}}} \mathrm{d}^3 p. \tag{B.2}$$

We clearly have $\partial F_1 / \partial T < 0$ and $\partial F_2 / \partial \nu > 0$ (since $\mathcal{V} \ge 0$ by assumption). By dominated convergence, we may interchange the derivative with the integral and compute

$$\frac{\partial F_1}{\partial \nu} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{\kappa'\left(\dfrac{p^2 - \nu}{2T}\right)}{\kappa\left(\dfrac{p^2 - \nu}{2T}\right)^2} \mathrm{d}^3 p, \tag{B.3}$$

where $\kappa(x) = x / \tanh(x)$. If $\nu \le 0$, this is positive, since $\kappa'(t) \ge 0$ for $t \ge 0$. If $\nu > 0$, on the other hand, we can integrate out the angular coordinates and change variables to $\pm t = p^2 - \nu$, respectively, to obtain

$$\frac{\partial F_1}{\partial \nu} = \frac{1}{4\pi^2} \int_0^\infty \frac{\kappa'\left(\dfrac{t}{2T}\right) \sqrt{\nu + t}}{\kappa^2\left(\dfrac{t}{2T}\right)} \mathrm{d}t - \frac{1}{4\pi^2} \int_0^\nu \frac{\kappa'\left(\dfrac{t}{2T}\right) \sqrt{\nu - t}}{\kappa^2\left(\dfrac{t}{2T}\right)} \mathrm{d}t. \tag{B.4}$$

Since $\sqrt{\nu + t} > \sqrt{\nu - t}$, it is clear that this sum is positive, i.e. $\partial F_1 / \partial \nu > 0$.

We proceed similarly to show that $\partial F_2 / \partial T > 0$. We have

$$\begin{aligned} \frac{\partial F_2}{\partial T} &= \frac{\mathcal{V}}{2T^2} \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \frac{p^2 - \nu}{\cosh\left(\dfrac{p^2 - \nu}{2T}\right)^2} \mathrm{d}^3 p \\ &= \frac{\mathcal{V}}{2T^2} \frac{1}{\sqrt{2\pi}} \left(\int_0^\infty \frac{t\sqrt{t + \nu}}{\cosh\left(\dfrac{t}{2T}\right)^2} \mathrm{d}t - \int_0^\nu \frac{t\sqrt{\nu - t}}{\cosh\left(\dfrac{t}{2T}\right)^2} \mathrm{d}t \right) > 0. \end{aligned} \tag{B.5}$$

In particular, the Jacobian determinant of F is strictly positive.

For fixed T, we have $\lim_{\nu\to-\infty} F_2(\nu, T) = -\infty$ and $\lim_{\nu\to\infty} F_2(\nu, T) = \infty$. Hence there is a unique solution ν_T of the equation $F_2(\nu, T) = \mu$, for any $\mu \in \mathbb{R}$, and ν_T is decreasing in T. Moreover, the function $T \mapsto F_1(\nu_T, T)$ is strictly decreasing, and hence the equation $F_1(\nu_T, T) = \lambda$ has a unique solution for λ in its range. In particular, T_c is a strictly decreasing function of $\lambda = -1/(4\pi a)$, hence a strictly decreasing function of a for $a < 0$.

For $\mu \leq 0$, one checks that $\lim_{T\to0} F_1(\nu_T, T) \leq 0$, hence $T_c = 0$. For $\mu > 0$, however, $\lim_{T\to0} F_1(\nu_T, T) = \infty$, hence $T_c > 0$ for any $a < 0$.

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A.2 Ready for submission manuscripts

A.2.1 The Bogolubov-Hartree-Fock theory for strongly interacting fermions in the low density limit

The Bogolubov-Hartree-Fock theory for strongly interacting fermions in the low density limit

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August 26, 2014

Abstract

1 Introduction

We consider a gas of fermions confined in an external macroscopic potential. The particles interact through a two-body potential V which admits a negative energy bound state. At low temperatures and low particle densities, this leads to the formation of bosonic-like diatomic molecules, which can create a Bose-Einstein condensate (BEC). It was realized in the 80-ies [14, 17] that BCS-theory adequately can be applied to such types of tightly bound fermions. It was pointed out in [20, 5, 18, 19] that in the low density limit the macroscopic variations in the pair density is well captured by the Gross-Pitaevskii (GP) equation. From a mathematical point of view, the emergence of the GP functional in the low density limit was recently proven in [13] for the static case and the dynamical case was subsequently treated in [11]. The assumption, that the two-body interaction potential allows for a bound state plays a crucial role. In the case of weak coupling where the potential is not strong enough to form a bound state, the pairing mechanism may still play a decisive role for a macroscopic coherent behavior, however, the separation of paired particles can be much larger than the average particle

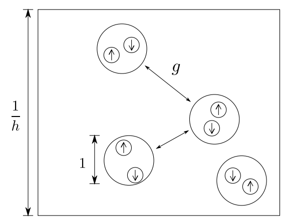


Figure 1: Fermions form bosonic-like diatomic molecules with its repulsive interaction represented by an effective scattering length g.

spacing. In fact this is the case in the usual BCS situation of superconductive materials or superfluid gases. Close to the critical temperature the macroscopic variation of the pairs is captured by the Ginzburg-Landau equation as pointed out by Gorkov [8] soon after the introduction of BCS-theory, see also [4]. The first mathematical proof of the emergence of Ginzburg-Landau theory from BCS theory was recently given in [8, 7], which itself relied on earlier work on the BCS functional [9, 12, 6].

In the current paper, in contrast to the usual BCS-functional approach, our starting point is the full BCS Hartree-Fock (BCS-HF) functional. In other words we include the direct and exchange energy terms. In the literature one also finds this functional under the name Bogolubov-Hartree-Fock (BHF) functional. In particular the inclusion of the density-density interaction adds additional difficulty with respect to the question of stability. To this aim we will restrict to systems with two-body potential V that, on the one hand, allows for a bound state and, on the other hand, does not spoil the stability of the system. This leads to a class of potentials which have a rather high repulsive core and an attractive tail deep enough to trap a particle. This is consistent with the description of typical interaction potentials in the physics literature [14].

We prove that the ground state anergy of such a BHF-functional (for obvious reasons we prefer the name BHF to BCS-HF) is to leading order given by $-E_b N/2h$, which corresponds to the number of fermion pairs times their internal binding energy. And, more important, the next to leading order is given by the condensation energy of a repulsive Bose gas with each boson consisting of a fermionic pair. This energy is given by the Gross-Pitaevskii energy of a BEC. If $E^{\mathrm{BHF}}(N,h)$ denotes the BHF-energy of N/h fermions, and $E^{\mathrm{GP}}(N)$ describes the Gross-Pitaevskii energy of N bosons and parameter g this fact can be expressed as

$$E^{\mathrm{BHF}}(N,h) = -E_b \frac{N}{2h} + hE^{\mathrm{GP}}(g,N) + O(h^{3/2}).$$

The small parameter h represents the relation between the macroscopic and macroscopic scale of the system. Notice the external field varies on the scale of order $1/h$ whereas the fermions via V vary on a scale of order one. Since we can imagine that the external potential convinces the particles in a box of order $1/h^3$ the particle density is Nh^2, such that the parameter h also represents the square root of the particle density. In other words in the low density limit the fermions group together in pairs, such that the leading order in the energy is given by the number of pairs, $N/2h$ times the binding energy of one pair. The next to leading order is given by the energy of a repulsive bose-gas in an external macroscopic trap. In terms of the ground state of the BHF functional the result can be expressed as follows. Its two particle wavefunction α, to leading order, has the form

$$\alpha(x,y) = h^{-2}\alpha_0\left(\frac{x-y}{h}\right)\psi\left(\frac{x+y}{2}\right),$$

where α_0 is the Schrödinger ground state with energy $-E_b$, and $\psi(x)$ solves the GP-equation and captures the density fluctuations of the pairs due to the external trap.

Our work is an extension of [13] in two directions. First, we include exchange and direct term, second we get rid of the periodic boundary terms in [13], whose proof heavily relies on the involved estimates of [7], and third, we improve the error bounds. In fact our proof implies

$$E^{\mathrm{BHF}}(N,h) = -E_b \frac{N}{2h} + hE^{\mathrm{GP}}(g_{\mathrm{bcs}},N) + O(h^{3/2}),$$

where the g_{bcs} denotes the corresponding parameter due to the BCS-functional and with the the current proof using ideas of [11].

Moreover the work presents a first proof of the appearance of pairing in the ground state of a Bogolubov-Hartree-Fock system. The ground state properties of the Bogoliubov-Hartree-Fock functional, in the context of Newtonian interaction was studied in Lenzmann-Lewin [15], see also [1]. Still it could not be shown that the fermions in the ground state exhibit pairing. In fact, until now, the existence of non-vanishing pairs has not yet been established analytically, but only numerically in [16]. In fact in the low density limit, which we are studying here, the ground state predominately consists of pairs. We remark, that the direct and exchange term were already studied before in the context of the BCS functional in a the translation invariant model in [3].

2 Main Results

In BCS theory, the state of a fermionic system is encoded in a self-adjoint operator $\Gamma \in \mathcal{L}\big(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)\big)$, satisfying $0 \leq \Gamma \leq 1$. In decomposed form, Γ is determined by two operators $\gamma, \alpha \in \mathcal{L}\big(L^2(\mathbb{R}^3)\big)$ and reads

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1-\overline{\gamma} \end{pmatrix},$$

where γ is trace class and α is Hilbert-Schmidt and where we denote by $\overline{\gamma}$, $\overline{\alpha}$ the operators with kernels $\overline{\gamma(x,y)}$ and $\overline{\alpha(x,y)}$ respectively.

Given an external potential W and an external vector potential A and a two-particle interaction potential V, the corresponding BCS Hartree-Fock functional, which we denote with BHF functional for Bogolubov-Hartree-Fock, is given by

$$\begin{aligned}\mathcal{E}^{\mathrm{BHF}}(\Gamma) = \operatorname{Tr}\big([-i\nabla + A(x)]^2 + W\big)\gamma + \frac{1}{2}\int_{\mathbb{R}^6} V(x-y)|\alpha(x,y)|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y \\ - \frac{1}{2}\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y + \int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y)V(x-y)\,\mathrm{d}^3x\,\mathrm{d}^3y.\end{aligned} \tag{2.1}$$

A formal derivation of such an energy functional from Quantum mechanics is given in [9, Appendix].

We study a system of fermions interacting by means of a two-body interaction $V = V(x-y)$, confined in an external macroscopic potential $W = W(hx)$. I.e., the potential W lives on a scale of order $1/h$ whereas V varies on a scale of order one. In other words $1/h$ represents the relation between the macroscopic and microscopic length scales. Let us remark that the trap W confines the particles within a volume of order $1/h^3$. We assume now that the number of particles is of the order of $1/h$. Consequently the particle density ρ is of the order of h^2. In that sense the limit of small h corresponds to a low density limit. For simplicity, we neglect the magnetic field A.

Mathematically we are interested in the effect of weak external potentials, i.e., we replace W by h^2W. Further, it is convenient to use macroscopic variables instead of microscopic ones, i.e., we define $x_h = hx$, $y_h = hy$, $\alpha_h(x,y) = h^{-3}\alpha(\frac{x}{h},\frac{y}{h})$, $\gamma_h(x,y) = h^{-3}\gamma(\frac{x}{h},\frac{y}{h})$.

The resulting BHF functional is given by (now denoting the macroscopic quantities by x, y, γ, α in favor of $x_h, y_h, \gamma_h, \alpha_h$)

$$\begin{aligned}\mathcal{E}^{\mathrm{BHF}}(\Gamma) = \operatorname{Tr}(-h^2\Delta + h^2W)\gamma + \frac{1}{2}\int_{\mathbb{R}^6} V\Big(\frac{x-y}{h}\Big)|\alpha(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y \\ - \frac{1}{2}\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y + \int_{\mathbb{R}^6}\gamma(x,x)\gamma(y,y)V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y,\end{aligned} \tag{2.2}$$

with corresponding ground state energy

$$E^{\mathrm{BHF}}(N,h) = \inf\{\mathcal{E}^{\mathrm{BHF}}(\Gamma)\,|\,0 \leq \Gamma \leq 1,\ \operatorname{Tr}\gamma = N/h\} \tag{2.3}$$

On the other hand, given $\psi \in H^1(\mathbb{R}^3)$ the GP functional is defined by

$$\mathcal{E}^{\mathrm{GP}}(\psi) = \int_{\mathbb{R}^3}\Big(\frac{1}{4}|\nabla\psi(x)|^2 + W(x)|\psi(x)|^2 + g|\psi(x)|^4\Big)\,\mathrm{d}^3x, \tag{2.4}$$

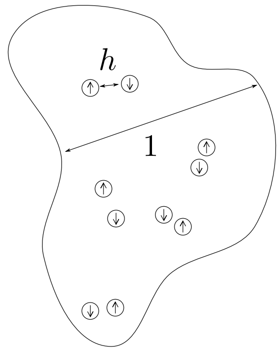


Figure 2: Separation of scales: The interaction between the fermions lives on a scale of order h, while the external potential is of order 1.

where the parameter $g > 0$ will be determined by the BHF functional and represents the interaction strength among different pairs. The function $\psi(x)$ represents the spatial fluctuation of the pairs. This also explains the factor $1/4$ in front of the kinetic energy, which accounts for the total mass of the fermion pair. We denote the ground state energy of the GP functional as

$$E^{\mathrm{GP}}(g, N) = \inf\{\mathcal{E}^{\mathrm{GP}}(\psi) \mid \psi \in H^1(\mathbb{R}^3),\ \|\psi\|_2^2 = N\}. \tag{2.5}$$

We consider a minimizer of the functional (2.2) and show that its value in the limit $h \to 0$ is to leading order given by the binding energy of the fermion pairs, i.e. $E_b \frac{N}{2h}$. Moreover, more important, the macroscopic density fluctuations of the pairs are governed by the GP functional. This result holds in case the two-body interaction potential V has a negative energy bound state, which is expressed via the following assumption.

Assumption 1. Let $V \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, with $V(x) = V(-x)$ and such that $-2\Delta + V$ has a ground state α_0 with norm $\|\alpha_0\| = 1$ with corresponding ground state energy $-E_b < 0$.

Including direct and exchange term into the BCS functional gives rise to a new problem. Apriori it is not clear whether the functional is still bounded from below. In order to guarantee stability we impose the following further assumption on V.

Assumption 2. There is $U \in L^2(\mathbb{R}^3)$, with positive Fourier transform $\widehat{U} \geq 0$, such that $V - \frac{1}{2}V_+ \geq U$. Here $V_+ = \frac{1}{2}(|V| + V)$ denotes the positive part of V.

This means we restrict to potentials which can be bounded from below by functions with a positive Fourier transform after we cut its positive part in half. From a physical point of view this means that we restrict to interaction potentials which have a strong enough repulsive core and a small attractive tail, still, large enough to trap a particle. This is a condition typically fulfilled for a gas of atomic fermions. See also [14]. In Appendix B, we will give a concrete example of a potential in the spirit of [14] satisfying Assumption 2.

Remark 1. The following construction shows that it is easy to find a potential V with the desired properties of Assumption 2: Choose a potential U which is strictly negative on an open set $\Omega \subset \mathbb{R}^3$, such that $\widehat{U} \geq 0$. The latter property, e.g., is satisfied for $U(x) = u * u_-$, the convolution of a function

$u(x)$ with its reflection $u_-(x) = u(-x)$, since $\widehat{U} = |\widehat{u}|^2 \geq 0$. Now set $V = 2U_+ - U_-$. Obviously this V fulfills Assumption 2. Finally, scale V according to $V \mapsto \lambda V$ until the negative part is deep enough to ensure binding.

With these assumptions we are ready to formulate our main theorem.

Theorem 1. *Let $W \in H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Under Assumptions 1 and 2, we have for small h,*

$$E^{\mathrm{BHF}}(N,h) = -\frac{E_b}{2}\frac{N}{h} + hE^{\mathrm{GP}}(g,N) + O(h^{3/2}), \tag{2.6}$$

where g is given by

$$g = \frac{1}{(2\pi)^3}\int |\widehat{\alpha}_0(p)|^4 (2p^2 + E_b)\,\mathrm{d}^3p - \frac{1}{2}\int_{\mathbb{R}^3} |(\overline{\alpha_0} * \alpha_0)(x)|^2\, V(x)\,\mathrm{d}^3x + \int_{\mathbb{R}^3} V(x)\,\mathrm{d}^3x.$$

Moreover, if Γ is an approximate minimizer of $\mathcal{E}^{\mathrm{BHF}}$, in the sense that

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) \leq -\frac{E_b}{2}\frac{N}{h} + h(E^{\mathrm{GP}}(g,N) + \epsilon)$$

for some $\epsilon > 0$, then the corresponding α can be decomposed as

$$\alpha = \alpha_\psi + \xi, \qquad \|\xi\|_2^2 \leq O(h), \tag{2.7}$$

where

$$\alpha_\psi(x,y) = h^{-2}\psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big), \tag{2.8}$$

and ψ is an approximate minimizer of $\mathcal{E}^{\mathrm{GP}}$ in the sense that

$$\mathcal{E}^{\mathrm{GP}}(\psi) \leq E^{\mathrm{GP}}(g,N) + \epsilon + O(h^{1/2}). \tag{2.9}$$

Remark 2. In contrast to the usual BCS functional [11, Eq. (1.2)] and [13], the coupling constant g, where g only consists of the BCS term

$$g_{\mathrm{BCS}} = \frac{1}{(2\pi)^3}\int |\widehat{\alpha}_0(p)|^4 (2p^2 + E_b)\,\mathrm{d}^3p$$

receives the additional contributions from direct and exchange energy

$$g_{\mathrm{dir}} = \int_{\mathbb{R}^3} V(x)\,\mathrm{d}^3x \quad \text{and} \quad g_{\mathrm{ex}} = -\frac{1}{2}\int_{\mathbb{R}^3} |(\overline{\alpha_0} * \alpha_0)(x)|^2\, V(x)\,\mathrm{d}^3x$$

respectively.

Remark 3. In [13] we proved the emergence of the Gross-Pitaevstii functional within the framework of the BCS functional, i.e., without direct and exchange terms. Of course, our current work would apply as well to the BCS-functional. Following the proof, one obtains the asymptotic statement

$$E^{\mathrm{BHF}}(N,h) = -\frac{E_b}{2}\frac{N}{h} + hE^{\mathrm{GP}}(g_{\mathrm{BCS}},N) + O(h^{3/2}).$$

I.e., compared to [13] we improve the error bound, from $O(h^{6/5})$ to $O(h^{3/2})$. Further we get rid of the boundary condition and we significantly simplify the proof of [13], which relied on the involved estimates of [7]. However, we remark that, for simplicity, we neglect the magnetic field A.

Remark 4. The proof of our current work relies on ideas of [11], where within the same setting of our work, the BCS evolution equation was studied showing that the macroscopic fluctuations are governed by the time-dependent Gross-Pitaevskii equation. Starting point is the evolution equation time evolution for the BCS state Γ_t which takes the form

$$ih^2\partial_t\Gamma_t = [H_{\Gamma_t}, \Gamma_t], \tag{2.10}$$

where the BCS Hamiltonian H_{Γ_t} is given by

$$H_{\Gamma_t} = \begin{pmatrix} -h^2\Delta + h^2W & V\alpha_t \\ V\overline{\alpha_t} & h^2\Delta - h^2W \end{pmatrix}$$

and where $V\alpha_t \in \mathcal{L}\big(L^2(\mathbb{R}^3)\big)$ is the operator with kernel $V\big((x-y)/h\big)\alpha_t(x,y)$. If the energy of the initial BCS state Γ_0 is sufficiently close to the minimal energy, i.e., if

$$\mathcal{E}^{\rm BCS}(\Gamma_0) \le -\frac{E_b}{2}\operatorname{Tr}(\gamma_0) + Ch,$$

then, it is shown in [11], that the macroscopic fluctuations in the center-of-mass variable

$$\psi_t(X) = \frac{\mathrm{e}^{-itE_b/h^2}}{h}\int_{\mathbb{R}^3} \alpha_0(r/h)\alpha_t(X + r/2, X - r/2)\,\mathrm{d}^3 r$$

satisfies to leading order the time-dependent Gross-Pitaevskii equation

$$i\partial_t\varphi_t = -\frac{1}{2}\Delta\varphi_t + 2W\varphi_t + 2g_{\rm BCS}|\varphi_t|^2\varphi_t$$

with initial data $\varphi_{t=0} \equiv \psi_{t=0}$. More precisely, it is shown that ψ_t is close to a φ_t, i.e.,

$$\|\psi_t - \varphi_t\|_2 \le Ch^{1/2}\mathrm{e}^{c|t|}$$

for some constants $c, C > 0$, with φ_t satisfying the GP-equation.

A similar result would now hold as well in the case of the time-dependent BHF equation, which in a different context was treated in [10]. By repeating the strategy of [11] and handling the exchange and direct terms one may obtain the emergence of the time-dependent GP equation with parameter g.

3 Note on stability

Before giving a sketch of the proof we show how Assumption 2 gives rise to stability. In fact we show that the assumption guarantees that the direct and exchange terms are non-negative. To this aim we first consider the exchange term and estimate

$$\begin{aligned}
-\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y &\ge -\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V_+\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
&\ge -\int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y) V_+\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y
\end{aligned}$$

replacing first V by its positive part $V_+ = \frac{1}{2}(|V| + V)$ and using $|\gamma(x,y)|^2 \leq \gamma(x,x)\gamma(y,y)$. Hence, we have for the sum of direct and exchange term

$$
\begin{aligned}
2\int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - \int_{\mathbb{R}^6} |\gamma(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
\geq 2\int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y)\,(V - V_+/2)\,\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y, \\
= 2\int_{\mathbb{R}^3} (\rho * \rho_-)\,(x)\,(V - V_+/2)\,(x/h)\,\mathrm{d}^3x,
\end{aligned}
$$

where we denote by $\rho(x) = \gamma(x,x)$ the density and $\rho_-(x) = \rho(-x)$. By assumption, there is a potential U with $\big(V - \frac{1}{2}V_+\big) \geq U$ and $\widehat{U}(p) \geq 0$ for almost every p. Since $\rho \geq 0$, the last term on the right hand side is bounded below by

$$
2\int_{\mathbb{R}^3} (\rho * \rho_-)\,(x) U(x/h)\,\mathrm{d}^3x = 2\int_{\mathbb{R}^3} |\widehat{\rho}|^2(p)\widehat{U}(p)\,\mathrm{d}^3p \geq 0,
$$

showing the non-negativity of the direct and exchange energy terms.

4 Sketch of the proof of Theorem 1

We decompose the proof of Theorem 1 into an upper and a lower bound. The upper bound is done via a trial argument. We define the trial state Γ_ψ via the pair wavefunction

$$
\alpha_\psi(x,y) = \psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big),
$$

with α_0 being the ground-state in the relative coordinates of the two particle system, i. e.,

$$
(-2\Delta + V)\alpha_0 = -E_b\alpha_0,
$$

whereas ψ accounts for the macroscopic fluctuations in the center-of-mass coordinates. Since we expect that the system in its ground state energy consists predominantly of pairs we define the one particle density γ_ψ such that to leading order it is given by $\overline{\alpha_\psi}\alpha_\psi$, i.e., $\gamma_\psi = \overline{\alpha_\psi}\alpha_\psi + O(h)$. Recall that the number of particles $\operatorname{Tr}\gamma_\psi$ is of the order of $1/h$, such that the error term of order $O(h)$ is in fact by a factor of h^2 higher than the leading term. With the trial state Γ_ψ at hand it is mainly a tedious calculation to obtain the bound

$$
\mathcal{E}^{\mathrm{BHF}}(\Gamma) \leq -\frac{E_b}{2}N/h + h\mathcal{E}^{\mathrm{GP}}(\psi) + O(h^2).
$$

For the lower bound the first step consists of using energy estimates, see [7, 13, 11], in order to conclude that an approximate ground state Γ the corresponding two particle state α necessarily has to be of the form $\alpha = \alpha_\psi + \xi$, with ξ being negligible compared to α_ψ, i.e., $\|\xi\|_2^2 \leq h^2\|\alpha_\psi\|_2$. With the apriori bound at hand we then show that ξ at most contributes a term of the order of $o(h)$ to the energy. Using now the estimates from the upper bound completes the proof of the Theorem.

In the following we give a more detailed sketch of the upper, respectively, lower bound.

4.1 Upper bound

We proceed in analogy to [11]. For the upper bound we use the trial state

$$\Gamma_\psi = \begin{pmatrix} \gamma_\psi & \alpha_\psi \\ \overline{\alpha_\psi} & 1-\overline{\gamma_\psi} \end{pmatrix}$$

with the definition

$$\begin{aligned} \alpha_\psi(x,y) &= h^{-2}\psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big), \\ \gamma_\psi &= \alpha_\psi\overline{\alpha_\psi} + (1+C_\psi h)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi} \\ \operatorname{Tr}\gamma_\psi &= N/h, \end{aligned} \tag{4.1}$$

where the constant C_ψ has to be chosen such that

$$C_\psi\, h \geq \|2(1+C_\psi\, h)\alpha_\psi\overline{\alpha_\psi} + (1+C_\psi\, h)^2(\alpha_\psi\overline{\alpha_\psi})^2\|_\infty$$

in order to guarantee $0 \leq \Gamma_\psi \leq 1$. We will see later, that a good choice for small h is

$$C_\psi = C\|\nabla\psi\|_2^2\|\widehat{\alpha_0}\|_6^2$$

for appropriate C.

In the limit of small h the GP energy-functional will emerge at the order of h from the BHF functional $\mathcal{E}_h^{\mathrm{BHF}}(\Gamma_\psi)$. This appears as follows. If we first consider the kinetic energy term plus the pairing term of $\mathcal{E}_h^{\mathrm{BHF}}(\Gamma_\psi)$ and subtract the total binding energy, $-\frac{E_b}{2}\frac{N}{h} = -\frac{E_b}{2}\operatorname{Tr}\gamma_\psi$, we obtain

$$\begin{aligned} &\operatorname{Tr}\left(-h^2\Delta\right)\gamma_\psi + \frac{1}{2}\int_{\mathbb{R}^6} V\Big(\frac{x-y}{h}\Big)|\alpha_\psi(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y + E_b\frac{N}{2h} \\ &\qquad = \operatorname{Tr}\left(-h^2\Delta + E_b/2\right)\gamma_\psi + \frac{1}{2}\int_{\mathbb{R}^6} V\Big(\frac{x-y}{h}\Big)|\alpha_\psi(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y. \end{aligned} \tag{4.2}$$

If we first only consider the $\alpha_\psi\overline{\alpha_\psi}$ contribution from (4.7) we can rewrite the corresponding term as

$$\int_{\mathbb{R}^3}\left\langle \alpha_\psi(\cdot,y), \left[-h^2\Delta_x + \frac{1}{2}V\Big(\frac{\cdot - y}{h}\Big) + \frac{E_b}{2}\right]\alpha_\psi(\cdot,y)\right\rangle \mathrm{d}^3y.$$

Since $\alpha_\psi(x,y)$ is symmetric we can replace Δ_x by $\frac{1}{2}(\Delta_x+\Delta_y)$. In terms of center of mass $X=(x+y)/2$ and relative coordinates $r = x-y$ we can write $\Delta_x+\Delta_y = \frac{1}{2}\Delta_X + 2\Delta_r$, such that in these coordinates the term can be rewritten as

$$\begin{aligned} &h^{-4}\int_{\mathbb{R}^6}\overline{\alpha_0(r/h)\psi(X)}\left[-h^2\frac{1}{4}\Delta_X - h^2\Delta_r + \frac{1}{2}V(r/h) + E_b/2\right]\alpha_0(r/h)\psi(X)\,\mathrm{d}^3X\,\mathrm{d}^3r \\ &\qquad = \frac{h}{4}\int_{\mathbb{R}^3}|\nabla\psi(X)|^2\,\mathrm{d}^3X + h\|\psi\|_2^2\left\langle\alpha_0, \left[-\Delta_r + V/2 + E_b/2\right]\alpha_0\right\rangle = \frac{h}{4}\int_{\mathbb{R}^3}|\nabla\psi(x)|^2\,\mathrm{d}^3x, \end{aligned} \tag{4.3}$$

using the ground-state property in the last equality and the normalization condition

$$h^{-3}\int_{\mathbb{R}^3}|\alpha_0(r/h)|^2\,\mathrm{d}^3r = 1$$

in the first equality.

Second, we remark that the monomial term $\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}$ of γ_ψ in inserted into

$$\mathrm{Tr}[-h^2\Delta + E_b/2]\gamma_\psi$$

contributes to the quartic term $\int_{\mathbb{R}^3} g_{\mathrm{bcs}}|\psi(x)|^4\,\mathrm{d}^3x$ term in the GP functional. The remaining part of the $\int_{\mathbb{R}^3} g|\psi(x)|^4\,\mathrm{d}^3x$ term is due to the contribution of the monomial $\alpha_\psi\overline{\alpha_\psi}$ in the direct and exchange energy. The estimation of these terms is straightforward but tedious and occupies the main part of the proof.

Further, it will be easy to show that

$$h^2\,\mathrm{Tr}\,W\alpha_\psi\overline{\alpha_\psi} = h^{-2}\int_{\mathbb{R}^3} W(X+r/2)|\psi(X)|^2|\alpha_0(r/h)|^2\,\mathrm{d}^3r = h\int_{\mathbb{R}^3} W(X)|\psi(X)|^2\,\mathrm{d}^3X + O(h^2).$$

Consequently we obtain

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma_\psi) + E_b\frac{N}{2h} = h\mathcal{E}^{\mathrm{GP}}(\psi) + O(h^2). \tag{4.4}$$

Finally, we remark that the constraint $\mathrm{Tr}\,\gamma_\psi = N/h$ implies for ψ that

$$\|\psi\|_2^2 = N(1-O(h^2)).$$

Since, however,

$$\left|\mathcal{E}^{\mathrm{GP}}(\psi) - \mathcal{E}^{\mathrm{GP}}\left([1+O(h^2)]\psi\right)\right| \le O(h^2)$$

we obtain the bound

$$\inf_{\substack{0\le\Gamma\le1\\ \mathrm{Tr}(\gamma)=N/h}} \mathcal{E}^{\mathrm{BHF}}(\Gamma) + E_b\frac{N}{2h} \le h \inf_{\substack{\psi\in H^1(\mathbb{R}^3)\\ \|\psi\|_2^2=N}} \mathcal{E}^{\mathrm{GP}}(\psi) + O(h^2), \tag{4.5}$$

which is the content of Section 6.

Remark 5.

- Since the infimum of $\mathcal{E}^{\mathrm{BHF}}$ remains unchanged when restricting Γ to be a projector [2], the natural choice for a trial state Γ_ψ would be a projector, i.e. $\Gamma_\psi = \Gamma_\psi^2$. The operator γ_ψ would then be determined by $\gamma_\psi = \gamma_\psi^2 + \alpha_\psi\overline{\alpha_\psi}$. Following this approach, we would have to deal with additional difficulties. To evaluate $\mathcal{E}^{\mathrm{BHF}}$ at this state, we first had to expand $\gamma_\psi = \frac{1}{2} - \sqrt{\frac{1}{4} - \alpha_\psi\overline{\alpha_\psi}}$ in terms of $\alpha_\psi\overline{\alpha_\psi}$. This would give rise to much more complicated computations.

- Our actual choice for Γ_ψ,

$$\gamma_\psi = \alpha_\psi\overline{\alpha_\psi} + (1+C_\psi\,h)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}$$

  in fact consists of the first two terms of the expansion of $\gamma = \frac{1}{2} - \sqrt{\frac{1}{4} - \alpha_\psi\overline{\alpha_\psi}}$ in terms of $\alpha_\psi\overline{\alpha_\psi}$. It indeed satisfies $0 \le \Gamma_\psi \le 1$ for small enough h. This can be seen as follows. $0 \le \Gamma_\psi \le 1$ is equivalent to $0 \le \Gamma_\psi(1-\Gamma_\psi)$. If γ_ψ is of the special form (4.7) which is a function of $\alpha_\psi\overline{\alpha_\psi}$, the off diagonals of

$$\begin{aligned}\Gamma_\psi(1-\Gamma_\psi) &= \begin{pmatrix} \gamma_\psi - \gamma_\psi^2 - \alpha_\psi\overline{\alpha_\psi} & \alpha_\psi\overline{\gamma_\psi} - \gamma_\psi\alpha_\psi \\ \overline{\gamma_\psi\alpha_\psi} - \overline{\alpha_\psi}\gamma_\psi & \overline{\gamma_\psi} - \overline{\gamma_\psi}^2 - \overline{\alpha_\psi}\alpha_\psi \end{pmatrix} \\ &= \begin{pmatrix} \gamma_\psi - \gamma_\psi^2 - \alpha_\psi\overline{\alpha_\psi} & 0 \\ 0 & \overline{\gamma_\psi} - \overline{\gamma_\psi}^2 - \overline{\alpha_\psi}\alpha_\psi \end{pmatrix}\end{aligned}$$

vanish and thus the statement is equivalent to

$$\gamma_\psi - \gamma_\psi^2 - \alpha_\psi \overline{\alpha_\psi} \geq 0. \tag{4.6}$$

Plugging in the expression for γ_ψ (4.6) is equivalent to

$$\alpha_\psi \overline{\alpha_\psi} \big(C_\psi\, h - 2(1 + C_\psi\, h) \alpha_\psi \overline{\alpha_\psi} - (1 + C_\psi\, h)^2 (\alpha_\psi \overline{\alpha_\psi})^2 \big) \alpha_\psi \overline{\alpha_\psi} \geq 0.$$

Using (see Corollary 1 below) $\|\alpha_\psi\|_\infty \leq \|\alpha_\psi\|_6 = h^{1/2} C \|\nabla \psi\|_2 \, \|\widehat{\alpha_0}\|_6$, this inequality is sure satisfied for small enough h for the choice

$$C_\psi = C \|\nabla \psi\|_2^2 \|\widehat{\alpha_0}\|_6^2$$

4.2 Lower bound

From the upper bound we learn that for an approximate ground state Γ we can assume

$$\mathcal{E}_h^{\mathrm{BHF}}(\Gamma) \leq -E_b \frac{N}{2h} + O(h).$$

We will show in Lemma 4 by energy estimates, that the corresponding α necessarily has to be of the form

$$\alpha(x,y) = \alpha_\psi(x,y) + \xi(x,y) = h^{-2} \psi\Big(\frac{x+y}{2}\Big) \alpha_0\Big(\frac{x-y}{h}\Big) + \xi(x,y)$$

for an appropriate $\psi \in H^1(\mathbb{R}^3)$, and ξ being negligible with respect to α_ψ, e.g.,

$$\|\xi\|_2^2 \leq O(h^2) \|\alpha_\psi\|_2^2 \leq O(h).$$

The function ψ is obtained by projecting α in the direction of α_0 with respect to the relative coordinates, more precisely, with $X = \frac{x+y}{2}$,

$$\psi(X) = \frac{1}{h} \int_{\mathbb{R}^3} \alpha_0(r/h) \alpha(X + r/2, X - r/2) \, \mathrm{d}^3 r.$$

This allows us to define, similar to the upper bound,

$$\Gamma_\psi = \begin{pmatrix} \gamma_\psi & \alpha_\psi \\ \overline{\alpha_\psi} & 1 - \overline{\gamma_\psi} \end{pmatrix}$$

with the definition

$$\begin{aligned} \alpha_\psi(x,y) &= h^{-2} \psi\Big(\frac{x+y}{2}\Big) \alpha_0\Big(\frac{x-y}{h}\Big), \\ \gamma_\psi &= \alpha_\psi \overline{\alpha_\psi} + (1 + C_\psi\, h) \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi}. \end{aligned} \tag{4.7}$$

Next we use the apriori bounds to show in Section 7 that the difference between $\mathcal{E}^{\mathrm{BHF}}(\Gamma)$ and $\mathcal{E}^{\mathrm{BHF}}(\Gamma_\psi)$ is positive or at least of higher order than the contribution from the GP functional, i.e.,

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) \geq \mathcal{E}^{\mathrm{BHF}}(\Gamma_\psi) - O(h^{3/2}). \tag{4.8}$$

Using now our calculation (4.4) from the upper bound immediately implies

$$\inf_{\substack{0 \leq \Gamma \leq 1 \\ \mathrm{Tr}(\gamma) = N/h}} \mathcal{E}^{\mathrm{BHF}}(\Gamma) + E_b \frac{N}{2h} \geq h \inf_{\substack{\psi \in H^1(\mathbb{R}^3) \\ \|\psi\|_2^2 = N}} \mathcal{E}^{\mathrm{GP}}(\psi) + O(h^{3/2}). \tag{4.9}$$

Together with (4.5) this combines to (2.6).

4.3 Properties of approximate minimizers

Let us finally indicate how to prove (2.7), (2.8) and (2.9) under the assumption of the lower and upper bounds. Given an approximate minimizer Γ, for which we have by definition

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) \leq -\frac{E_b}{2}\frac{N}{h} + h\big(E^{\mathrm{GP}}(g,N)+\epsilon\big),$$

the methods from the lower bound immediately apply and we obtain (2.7) and (2.8). To see (2.9), we combine (4.8) with (4.4), implying

$$|E^{\mathrm{GP}}(g,N)+\epsilon-\mathcal{E}^{\mathrm{GP}}(\psi)| \leq O(h^{1/2}).$$

5 Useful properties of the pair-wavefunction

In the following we derive some useful properties for the type of pair-wave function α which we will meet throughout our proof. Recall that α_0 was defined in Assumption 1 to be the normalized ground state of $-2\Delta + V$.

Lemma 1. *Let $\alpha = \alpha_\psi + \xi$, with $\psi \in H^1(\mathbb{R}^3)$, $\|\psi\|_2^2 = N$, and $\|\xi\|_2^2 \leq O(h)$.*

(i) For $n \in 2\mathbb{N}$, there are appropriate constants C, such that

$$\|\alpha_\psi\|_n^n \leq C h^{n-3}\|\psi\|_n^n\,\|\widehat{\alpha_0}\|_n^n, \tag{5.1a}$$

$$\|\nabla_{(x-y)}\alpha_\psi\|_n^n \leq C h^{-3}\|\psi\|_n^n\,\|\widehat{\nabla\alpha_0}\|_n^n, \tag{5.1b}$$

where

$$(\nabla_{(x-y)}\alpha_\psi)(x,y) = h^{-3}\psi\big((x+y)/2\big)(\nabla\alpha_0)\big((x-y)/h\big).$$

(ii) Let $g_{\mathrm{BCS}} = (2\pi)^3\int_{\mathbb{R}^3}|\widehat{\alpha_0}(p)|^4(p^2+E_b/2)\,\mathrm{d}^3p$. Then

$$\operatorname{Tr}\big((-h^2\Delta+E_b/2)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\big) = h\,g_{\mathrm{BCS}}\|\psi\|_4^4 + O(h^2). \tag{5.2}$$

(iii)

$$\|\alpha_\psi\overline{\alpha_\psi}(\cdot,\cdot)\|_\infty = \sup_x|\alpha_\psi\overline{\alpha_\psi}(x,x)| \leq h^{-2}\|\alpha_0\|_3^2\,\|\nabla\psi\|_2^2. \tag{5.3}$$

(iv) Let σ be a Hilbert-Schmidt operator. Then

$$|\sigma\alpha_\psi(x,x)| \leq h^{-1}\|\sigma(\cdot,x)\|_2\|\nabla\psi\|_2\,\|\alpha_0\|_3. \quad \forall x\in\mathbb{R}^3 \tag{5.4}$$

Let us mention that we use the symbol $\|\cdot\|_p$ for the L^p-norm of functions as well as for the operator norm in the corresponding Schatten class, since it is in general clear out of the context, if we talk about a function or an operator. In that sense $\|\sigma(\cdot,x)\|_2$ denotes the L^2-norm of the function, corresponding to the first variable of its kernel. Whereas $\|\sigma\|_2$ denotes its Hilbert-Schmidt operator.

Proof of Lemma 1, Part I. We postpone the proof of (5.1a), (5.1b) and (5.2) to Part II in the Appendix A. In order to see (5.3) we use Hölder

$$\begin{aligned}(\alpha_\psi\overline{\alpha_\psi})(x,x) &= \int_{\mathbb{R}^3}|\alpha_\psi(x,y)|^2\,\mathrm{d}^3y = h^{-4}\int_{\mathbb{R}^3}\big|\alpha_0\big((x-y)/h\big)\big|^2\,\big|\psi\big((x+y)/2\big)\big|^2\,\mathrm{d}^3y\\ &\leq h^{-4}\|\alpha_0(\cdot/h)^2\|_{3/2}\||\psi|^2\|_3 = h^{-2}C\|\alpha_0\|_3^2\|\nabla\psi\|_2^2,\end{aligned}$$

Finally, observe

$$\begin{aligned} |(\sigma\alpha_\psi)(x,x)| &= h^{-2}\left|\int_{\mathbb{R}^6}\overline{\sigma(x,y)}\alpha_0\big((x-y)/h\big)\psi\big((x+y)/2\big)\,\mathrm{d}^3y\right| \\ &\le h^{-2}\|\sigma(\cdot,x)\|_2\|\alpha_0(\cdot/h)\|_3\|\psi\|_6 = h^{-1}\|\sigma(\cdot,x)\|_2\|\psi\|_6\|\alpha_0\|_3, \end{aligned}$$

using Hölder inequality in y, which implies (5.4) □

Since γ_ψ is to leading order equal to $\alpha_\psi\overline{\alpha_\psi}$, we obtain as a corollary that the norm of γ_ψ is at most $O(h)$, meaning that the largest eigenvalue is of order h. However, let us remark, that the idea of Bardeen-Cooper-Schrieffer was that the Quantum mechanical two-particle density matrix is essentially given by

$$\frac{N}{h}|\alpha\rangle\langle\alpha|, \quad |\alpha\rangle = \frac{\alpha_\psi}{N^{1/2}/h^{1/2}},$$

which means that the two particle density matrix has one large eigenvalue N/h.

Corollary 1. *Let the assumptions be as in Lemma 1. Then*

$$\|\alpha_\psi\|_4^4 \le hC(2\pi)^3\|\psi\|_2\|\nabla\psi\|_2^3\,\|\widehat{\alpha_0}\|_4^4, \tag{5.5a}$$
$$\|\alpha_\psi\|_6^6 \le h^3C\|\nabla\psi\|_2^6\,\|\widehat{\alpha_0}\|_6^6, \tag{5.5b}$$
$$\|\nabla_{(x-y)}\alpha_\psi\|_6^6 \le Ch^{-3}\|\nabla\psi\|_6^6\,\|\widehat{\nabla\alpha_0}\|_6^6, \tag{5.5c}$$
$$\|\alpha_\psi\|_\infty \le h^{1/2}C\|\nabla\psi\|_2\,\|\widehat{\alpha_0}\|_6, \tag{5.5d}$$
$$(\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi})(x,x) \le \|\alpha_\psi\|_\infty^2(\alpha_\psi\overline{\alpha_\psi})(x,x) \le O(h^{-1}), \tag{5.5e}$$
$$\|\alpha\|_\infty \le \|\alpha_\psi\|_\infty + \|\xi\|_2 \le O(h^{1/2}). \tag{5.5f}$$

Let γ_ψ *defined as in* (4.7). *Then*

$$\|\gamma_\psi\|_\infty \le \|\alpha_\psi\|_\infty^2 + (1+C_\psi\,h)\|\alpha_\psi\|_\infty^4 \le O(h) \tag{5.6a}$$
$$\gamma_\psi(x,x) \le O(h^{-2}). \tag{5.6b}$$

Proof. The estimates (5.5a), (5.5b) and (5.5c) are a consequence of (5.1a) and (5.1b). In the case of $n=6$, we use the Sobolev inequality to have $\|\psi\|_6 \le \|\nabla\psi\|_2$ and in the case of $n=4$, we use L^p interpolation and the Sobolev inequality to conclude

$$\|\psi\|_4 \le \|\psi\|_2^{1/4}\|\psi\|_6^{3/4} \le C\|\psi\|_2^{1/4}\|\nabla\psi\|_2^{3/4}.$$

Inequality (5.5d) follows immediately from $\|\alpha_\psi\|_\infty \le \|\alpha_\psi\|_6$ together with (5.5b), while inequality (5.5f) is (5.5d) combined with the assumption $\|\xi\|_2 \le O(h^{1/2})$.

Next observe that

$$(\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi})(x,x) \le \|\alpha_\psi\overline{\alpha_\psi}\|_\infty(\alpha_\psi\overline{\alpha_\psi})(x,x).$$

Let us only show it on a more formal level using the physics notation of an integral kernel, i.e.,

$$(\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi})(x,x) = \langle x|\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}|x\rangle \le \|\alpha_\psi\overline{\alpha_\psi}\|_\infty\langle x|\alpha_\psi\overline{\alpha_\psi}|x\rangle \le \|\alpha_\psi\overline{\alpha_\psi}\|_\infty(\alpha_\psi\overline{\alpha_\psi})(x,x).$$

Consequently, using (4.7)

$$\|\gamma_\psi\|_\infty = \|\alpha_\psi\overline{\alpha_\psi} + (1+C_\psi\,h)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\|_\infty \le \|\alpha_\psi\|_\infty^2 + (1+C_\psi\,h)\|\alpha_\psi\|_\infty^4.$$

□

6 Upper bound

As explained above, for any $\psi \in H^1(\mathbb{R}^3)$ we are going to define the trial state

$$\Gamma_\psi = \begin{pmatrix} \gamma_\psi & \alpha_\psi \\ \overline{\alpha_\psi} & 1 - \overline{\gamma_\psi} \end{pmatrix}, \tag{6.1}$$

with

$$\alpha_\psi(x, y) = h^{-2}\psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big), \tag{6.2}$$

$$\gamma_\psi = \alpha_\psi\overline{\alpha_\psi} + (1 + C_\psi\, h)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}, \tag{6.3}$$

and the normalization condition

$$\operatorname{Tr}\gamma_\psi = N/h.$$

Since, by definition,

$$N/h = \operatorname{Tr}\gamma_\psi = \|\psi\|_2^2 + (1+h)\|\alpha_\psi\|_4^4,$$

this implies

$$\big|\|\psi\|_2^2 - N\big| \le Ch\|\psi\|_{H^1}^2.$$

Hence, as an immediate consequence we are able to realize that in order to prove

$$\inf_{\substack{0\le\Gamma\le 1\\ \operatorname{Tr}(\gamma)=N/h}} \mathcal{E}^{\mathrm{BHF}}(\Gamma) + \frac{E_b}{2}\frac{N}{h} \le h \inf_{\substack{\psi\in H^1(\mathbb{R}^3)\\ \|\psi\|_2^2=N}} \mathcal{E}^{\mathrm{GP}}(\psi) + O(h^2). \tag{6.4}$$

it suffices to show the following asymptotic expansion for our trial states.

Lemma 2. *Assume Γ_ψ to be of the form* (6.1)*, then*

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma_\psi) + \frac{E_b}{2}\frac{N}{h} = h\mathcal{E}^{\mathrm{GP}}(\psi) + O(h^2). \tag{6.5}$$

Proof. The remaining part of this section will be dedicated to proving (6.5). Recall the form of the BCS and GP functionals we see that Equation (6.5) can be decomposed in the following estimates

$$\begin{aligned} &\operatorname{Tr}(-h^2\Delta + E_b/2)\gamma_\psi + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha_\psi(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y \\ &\quad = h\int_{\mathbb{R}^3}\Big(\frac{1}{4}|\nabla\psi(x)|^2 + g_{\mathrm{BCS}}|\psi(x)|^4\Big)\,\mathrm{d}^3x + O(h^2) \end{aligned} \tag{6.6a}$$

$$\operatorname{Tr} h^2 W\gamma_\psi = h\int_{\mathbb{R}^3} W(x)|\psi(x)|^2\,\mathrm{d}^3x + O(h^2) \tag{6.6b}$$

$$-\frac{1}{2}\int_{\mathbb{R}^6}|\gamma_\psi(x,y)|^2 V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y = h\,g_{\mathrm{ex}}\int_{\mathbb{R}^3}|\psi(x)|^4\,\mathrm{d}^3x + O(h^2) \tag{6.6c}$$

$$\int_{\mathbb{R}^6}\gamma_\psi(x,x)\gamma_\psi(y,y)V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y = h\,g_{\mathrm{dir}}\int_{\mathbb{R}^3}|\psi(x)|^4\,\mathrm{d}^3x + O(h^2), \tag{6.6d}$$

where the constants g_{BCS}, g_{ex}, and g_{dir} are given in Remark 2. These estimates will be proven in the following subsections. □

6.1 Kinetic and potential energy (Proof of (6.6a))

Using the definition of our trial state (6.3) and (6.2) as well the calculation in (4.3) we obtain

$$
\begin{aligned}
&\operatorname{Tr}(-h^2\Delta + E_b/2)\gamma_\psi + \frac{1}{2}\int_{\mathbb{R}^6} |\alpha_\psi(x,y)|^2 V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
&\quad = \operatorname{Tr}\big(\big(-h^2\Delta + E_b/2\big)\left(\alpha_\psi\overline{\alpha_\psi} + (1+C_\psi\, h)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\right)\big) + \frac{1}{2}\int_{\mathbb{R}^6} |\alpha_\psi(x,y)|^2 V\Big(\frac{x-y}{h}\Big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
&\quad = \frac{h}{4}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2\,\mathrm{d}^3x + h\int_{\mathbb{R}^3} g_{\mathrm{BCS}}|\psi(x)|^4\,\mathrm{d}^3x - O(h^2),
\end{aligned}
$$

where we used (5.2) in order to recover the $|\psi|^4$-term from the contribution involving $\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}$. Hence we obtain (6.6a).

6.2 External potential (Proof of (6.6b))

With our definition (6.3) for γ_ψ we have

$$
\operatorname{Tr} h^2 W\gamma_\psi = h^2\operatorname{Tr}(W\alpha_\psi\overline{\alpha_\psi}) + (1+C_\psi\, h)\operatorname{Tr}(h^2 W\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}). \tag{6.7}
$$

By (5.5a) of Corollary 1, we know that the second term is of higher order, i.e.

$$
\operatorname{Tr}(h^2 W\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}) \le h^2\|W\|_\infty \operatorname{Tr}(\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}) = O(h^3).
$$

In terms of integral kernels and using center-of-mass and relative coordinates for the expression (2.8) for α_ψ we can write

$$
\begin{aligned}
h^2\operatorname{Tr}(W\alpha_\psi\overline{\alpha_\psi}) &= h^2\int_{\mathbb{R}^6} W(x)|\alpha_\psi(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y = h^{-2}\int_{\mathbb{R}^6} W(X+r/2)|\psi(X)|^2|\alpha_0(r/h)|^2\,\mathrm{d}^3X\,\mathrm{d}^3r \\
&= h\int_{\mathbb{R}^6} W(X)|\psi(X-hr/2)|^2|\alpha_0(r)|^2\,\mathrm{d}^3X\,\mathrm{d}^3r,
\end{aligned}
$$

in the last equality we performed a change of variables according to $X + r/2 \to X$ and $r \to hr$.

Next, we apply the fundamental theorem of calculus and obtain

$$
\begin{aligned}
h^2\operatorname{Tr}(W\alpha_\psi\overline{\alpha_\psi}) = h&\int_{\mathbb{R}^6} W(X)|\psi(X)|^2|\alpha_0(r)|^2\,\mathrm{d}^3X\,\mathrm{d}^3r \\
&+ h\int_{\mathbb{R}^6}\int_0^1 W(X)\frac{\partial}{\partial\tau}|\psi(X-\tau hr/2)|^2|\alpha_0(r)|^2\,\mathrm{d}\tau|\alpha_0(r)|^2\,\mathrm{d}^3X\,\mathrm{d}^3r.
\end{aligned}
$$

Using Cauchy-Schwarz in X, the last term is bounded by

$$
\begin{aligned}
&\left|h\int_{\mathbb{R}^6}\int_0^1 W(X)\Re\big(h\,r\cdot\nabla\psi(X-\tau hr/2)\overline{\psi(X-\tau hr/2)}\big)\,\mathrm{d}\tau|\alpha_0(r)|^2\,\mathrm{d}^3X\,\mathrm{d}^3r\right| \\
&\qquad \le h^2\|W\|_\infty\|\nabla\psi\|_2\|\psi\|_2\|\sqrt{|\cdot|}\alpha_0\|_2^2.
\end{aligned}
$$

This shows (6.6a).

6.3 Direct and exchange term (Proof of (6.6c) and (6.6d))

We first argue, that the leading order contribution of the direct and exchange terms stems from replacing γ_ψ by $\alpha_\psi\overline{\alpha_\psi}$ contributes to leading order of the direct and exchange terms. To see this, we simply estimate the differences

$$\int_{\mathbb{R}^6} |\gamma_\psi(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - \int_{\mathbb{R}^6} |(\alpha_\psi\overline{\alpha_\psi})(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \tag{6.8a}$$

and

$$\int_{\mathbb{R}^6} \gamma_\psi(x,x)\gamma_\psi(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - \int_{\mathbb{R}^6} (\alpha_\psi\overline{\alpha_\psi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y. \tag{6.8b}$$

Both expressions are can be reduced to the following form, whose proof is elementary.

Lemma 3. *Let $\sigma(x,y)$ and $\delta(x,y)$ be integral kernels of two positive trace class operators. If $V(r) = V(-r)$, then*

$$\begin{aligned}\left|\int_{\mathbb{R}^6} V(x-y)\,[(\sigma+\delta)(x,x)(\sigma+\delta)(y,y) - \sigma(x,x)\sigma(y,y)]\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \\ \leq 2\int_{\mathbb{R}^6} |V(x-y)|(\sigma+\delta)(x,x)\delta(y,y)\,\mathrm{d}^3x\,\mathrm{d}^3y\end{aligned} \tag{6.9a}$$

and

$$\left|\int_{\mathbb{R}^6} V(x-y)\,\left[|(\sigma+\delta)(x,y)|^2 - |\sigma(x,y)|^2\right]\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \leq 2\int_{\mathbb{R}^6} |V(x-y)|(\sigma+\delta)(x,x)\delta(y,y)\,\mathrm{d}^3x\,\mathrm{d}^3y. \tag{6.9b}$$

Proof. To show (6.9a), we simply use

$$\begin{aligned}&(\sigma+\delta)(x,x)(\sigma+\delta)(y,y) - \sigma(x,x)\sigma(y,y)\\ &\quad= (\sigma+\delta)(x,x)\delta(y,y) + \delta(x,x)\sigma(y,y)\\ &\quad\leq (\sigma+\delta)(x,x)\delta(y,y) + \delta(x,x)(\sigma+\delta)(y,y).\end{aligned}$$

Under the integral on the left hand side of (6.9a), we use the symmetry $V(x-y) = V(y-x)$ to obtain (6.9a).

For (6.9b) we follow a similar strategy and first split

$$\begin{aligned}&V(x-y)\left[|(\sigma+\delta)(x,y)|^2 - |\sigma(x,y)|^2\right]\\ &\quad= V(x-y)\left[\overline{(\sigma+\delta)(x,y)}\delta(x,y) + \overline{\delta(x,y)}\sigma(x,y)\right]\\ &\quad\leq |V(x-y)|\,[|(\sigma+\delta)(x,y)|\,|\delta(x,y)| + |\delta(x,y)|\,|\sigma(x,y)|]\,.\end{aligned}$$

Applying now to σ, δ, and $\sigma+\delta$, that for positive trace class operators a its kernel satisfies

$$|a(x,y)| \leq \sqrt{|a(x,x)|}\sqrt{|a(y,y)|}$$

and using Cauchy-Schwarz inequality we obtain the stated inequality. □

By applying Lemma 3 to $\sigma+\delta=\gamma_\psi$ and $\sigma=\overline{\alpha_\psi}\alpha_\psi$ the differences (6.8a) and (6.8b) can be bounded by

$$\begin{aligned}(1+C_\psi\, h)&\int_{\mathbb{R}^6}\left|V\big((x-y)/h\big)\right|\gamma_\psi(x,x)(\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\alpha_\psi)(y,y)\,\mathrm{d}^3x\,\mathrm{d}^3y\\&\le(1+C_\psi\, h)\|\gamma_\psi(\cdot,\cdot)\|_\infty\int_{\mathbb{R}^6}(\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\alpha_\psi)(x,x)\left|V\big((x-y)/h\big)\right|\,\mathrm{d}^3x\,\mathrm{d}^3y\\&=(1+C_\psi\, h)h^3\|V\|_1\|\gamma_\psi(\cdot,\cdot)\|_\infty\operatorname{Tr}(\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\alpha_\psi)\le O(h^2),\end{aligned}\tag{6.10}$$

where we used (5.6b).

In order to recover the $\|\psi\|_4^4$ contribution we inspect the remaining parts of the direct and the exchange term separately. We begin with the exchange term and write explicitly

$$\begin{aligned}-\frac{1}{2}&\int_{\mathbb{R}^6}|(\alpha_\psi\overline{\alpha_\psi})(x,y)|^2V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\\&=-\frac{1}{2}\int_{\mathbb{R}^{12}}\alpha_\psi(x,z)\overline{\alpha_\psi(z,y)}\alpha_\psi(x,w)\overline{\alpha_\psi(w,y)}V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\,\mathrm{d}^3z\,\mathrm{d}^3w.\end{aligned}$$

Introducing new variables

$$X=\frac{x+y}{2},\ r=x-y,\ s=x-z,\ t=x-w,$$

the last expression becomes

$$\begin{aligned}-\frac{1}{2}&\int_{\mathbb{R}^6}|(\alpha_\psi\overline{\alpha_\psi})(x,y)|^2V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\\&=-\frac{h}{2}\int_{\mathbb{R}^{12}}V(r)\alpha_0(s)\overline{\alpha_0(r-s)}\alpha_0(t)\overline{\alpha_0(r-t)}\\&\quad\times\psi(X+h(r-s)/2)\overline{\psi(X-hs/2)}\psi(X-ht/2)\overline{\psi(X+h(r-t)/2)}\,\mathrm{d}^3X\,\mathrm{d}^3r\,\mathrm{d}^3s\,\mathrm{d}^3t.\end{aligned}$$

The result can be rewritten as

$$\begin{aligned}-\frac{1}{2}\int_{\mathbb{R}^6}|(\alpha_\psi\overline{\alpha_\psi})(x,y)|^2V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y&=-\frac{h}{2}\int_{\mathbb{R}^3}|\psi(X)|^2\,\mathrm{d}^3X\int_{\mathbb{R}^3}V(r)|(\alpha_0*\overline{\alpha_0})(r)|^2\,\mathrm{d}^3r+A_{\mathrm{ex}}\\&=h\,g_{\mathrm{ex}}\int_{\mathbb{R}^3}|\psi(x)|^4\,\mathrm{d}^3x+A_{\mathrm{ex}},\end{aligned}\tag{6.11}$$

where

$$\begin{aligned}A_{\mathrm{ex}}=-\frac{h}{2}&\int_{\mathbb{R}^{12}}V(r)\alpha_0(s)\overline{\alpha_0(r-s)\alpha_0(t)}\alpha_0(r-t)\times\\&\times\int_0^1\frac{\mathrm{d}}{\mathrm{d}\tau}\Big(\psi(X+\tau h(r-s)/2)\overline{\psi(X-\tau hs/2)}\psi(X-\tau ht/2)\overline{\psi(X+\tau h(r-t)/2)}\Big)\,\mathrm{d}\tau\,\mathrm{d}^3X\,\mathrm{d}^3r\,\mathrm{d}^3s\,\mathrm{d}^3t,\end{aligned}$$

which is bounded by

$$|A_{\mathrm{ex}}|\le h^2\|\nabla\psi\|_2\|\psi\|_6^3\|V(\alpha_0*\alpha_0)((|\cdot|\alpha_0)*\alpha_0)\|_1\le Ch^2\|\nabla\psi\|_2^4\|V\|_1\|\alpha_0\|_2^3\big\||\cdot|\alpha_0\big\|_2,$$

using Hölder, Sobolev $\|\psi\|_6 \leq C\|\nabla\psi\|_2$, and Young's inequality. This shows (6.6c). We continue with the direct term. Its remaining part is given by

$$\begin{aligned}
&\int_{\mathbb{R}^6} (\alpha_\psi\overline{\alpha_\psi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \\
&\qquad = \int_{\mathbb{R}^6} |\alpha_\psi(x,z)|^2|\alpha_\psi(y,w)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\,\mathrm{d}^3w\,\mathrm{d}^3z \\
&\qquad = h\int_{\mathbb{R}^{12}} V(r)|\alpha_0(s)|^2|\alpha_0(t)|^2|\psi(X+h(r-s)/2)|^2|\psi(X-h(r+t)/2)|^2\,\mathrm{d}^3X\,\mathrm{d}^3r\,\mathrm{d}^3s\,\mathrm{d}^3t,
\end{aligned}$$

where we changed to the variables

$$X = \frac{x+y}{2},\ r = x-y,\ s = x-z,\ t = y-w.$$

The fundamental theorem of calculus leads to

$$\begin{aligned}
\int_{\mathbb{R}^6} (\alpha_\psi\overline{\alpha_\psi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y &= h\|\alpha_0\|_2^2\int_{\mathbb{R}^3} V(r)\,\mathrm{d}^3r\int_{\mathbb{R}^3}|\psi(X)|^2\,\mathrm{d}^3X + A_{\mathrm{dir}} \\
&= h\,g_{\mathrm{dir}}\int_{\mathbb{R}^3}|\psi(x)|^4\,\mathrm{d}^3x + A_{\mathrm{dir}},
\end{aligned} \tag{6.12}$$

where

$$\begin{aligned}
A_{\mathrm{dir}} = h\int_{\mathbb{R}^{12}} & V(r)|\alpha_0(s)|^2|\alpha_0(t)|^2\times \\
&\times\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\tau}\left(|\psi(X+\tau h(r-s)/2)|^2|\psi(X-\tau h(r+t)/2)|^2\right)\,\mathrm{d}\tau\,\mathrm{d}^3X\,\mathrm{d}^3r\,\mathrm{d}^3s\,\mathrm{d}^3t
\end{aligned}$$

is bounded by

$$|A_{\mathrm{dir}}| \leq 4h^2\|\nabla\psi\|_2\|\psi\|_6^3\,\|\alpha_0\|_2\left(\||\cdot|V\|_1\|\alpha_0\|_2 + \|V\|_1\|\sqrt{|\cdot|}\alpha_0\|_2\right).$$

This shows (6.6d).

7 Lower bound

Our proof of the lower bound on $E^{\mathrm{BHF}}(N,h)$ in Theorem 1 consists of two parts. As first step we obtain apriori bounds on approximate ground states.

Lemma 4 (Apriori bounds)**.** *Let Γ, with $\operatorname{Tr}\gamma = N/h$, be a state satisfying*

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) \leq -E_b\frac{N}{2h} + Ch$$

for some $C > 0$. There exists a function $\psi \in H^1(\mathbb{R}^3)$, with

$$\psi(X) = \frac{1}{h}\int_{\mathbb{R}^3}\alpha_0(r/h)\alpha(X+r/2, X-r/2)\,\mathrm{d}^3r, \tag{7.1}$$

such that

$$\alpha(X+r/2, X-r/2) = \widetilde{\alpha}(X,r) = h^{-2}\psi(X)\alpha_0(r/h) + \widetilde{\xi},$$

with $\widetilde{\xi}(X,r) = \xi(X+r/2, X-r/2)$, satisfy the bounds

$$\operatorname{Tr}\left[(-h^2\Delta + \frac{E_b}{2})(\gamma - \alpha\overline{\alpha})\right] \le O(h), \quad (7.2a)$$

$$\operatorname{Tr}(\gamma^2) \le \operatorname{Tr}(\gamma - \alpha\overline{\alpha}) \le O(h), \quad (7.2b)$$

$$\|\psi\|_2 \le O(1), \quad (7.2c)$$

$$\|\nabla\psi\|_2 \le O(1), \quad (7.2d)$$

$$\|\widetilde{\xi}\|_2^2 \le O(h), \quad (7.2e)$$

$$\|\nabla_X \widetilde{\xi}\|_2 \le O(h^{-1/2}), \quad (7.2f)$$

$$\|\nabla_r \widetilde{\xi}\|_2 \le O(h^{-1/2}), \quad (7.2g)$$

$$\operatorname{Tr}(\alpha\overline{\alpha}\alpha\overline{\alpha}) \le O(h). \quad (7.2h)$$

Proof. According to Section 3 the sum of direct and exchange term is non-negative. Thus, we have that

$$\begin{aligned} Ch &\ge \mathcal{E}^{\mathrm{BHF}}(\Gamma) + E_b \frac{N}{2h} \\ &\ge \operatorname{Tr}(-h^2\Delta + E_b/2)\gamma + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha(x,y)|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y - h^2\|W\|_\infty \operatorname{Tr}(\gamma). \end{aligned}$$

We bring the term $-h^2\|W\|_\infty \operatorname{Tr}(\gamma) = O(h)$ to the left hand side and combine it with Ch. Adding and subtracting an appropriate expression involving $\bar{\alpha}\alpha$, we obtain

$$Ch \ge \operatorname{Tr}(-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha}) + \operatorname{Tr}(-h^2\Delta + E_b/2)\alpha\overline{\alpha} + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha(x,y)|^2 \,\mathrm{d}^3x\,\mathrm{d}^3y.$$

The two terms on the right hand side can be written in the form, and expressed via center-of-mass and relative coordinates as

$$\begin{aligned} &\int_{\mathbb{R}^3} \left\langle \alpha(\cdot,y), \left[-h^2\Delta_x + \frac{1}{2}V\Big(\frac{\cdot - y}{h}\Big) + \frac{E_b}{2}\right]\alpha(\cdot,y)\right\rangle \mathrm{d}^3y \\ &= \left\langle \alpha_0\psi + \tilde{\xi}, \left[-h^2\frac{1}{4}\Delta_X - h^2\Delta_r + \frac{1}{2}V(r/h) + \frac{E_b}{2}\right]\alpha_0\psi + \tilde{\xi}\right\rangle_{L^2(\mathbb{R}^6)} \\ &= \frac{h}{4}\int_{\mathbb{R}^3} |\nabla\psi(X)|^2\,\mathrm{d}^3X + \|\nabla_X\widetilde{\xi}\|_2^2 + \int_{\mathbb{R}^3} \langle \widetilde{\xi}(X,\cdot), (-h^2\Delta + \frac{1}{2}V(\cdot/h) + E_b/2)\widetilde{\xi}(X,\cdot)\rangle\,\mathrm{d}^3X, \end{aligned} \quad (7.3)$$

where we used that the normalized α_0 is the zero eigenvector to the operator $-\Delta + V/2 + E_b/2$ and the fact, that $\widetilde{\xi}(X,\cdot)$ is orthogonal to α_0 for almost every $X \in \mathbb{R}^3$. This implies

$$Ch \ge \operatorname{Tr}(-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha}) + \frac{h}{4}\|\nabla\psi\|_2^2 + h^2\,\|\nabla_X\widetilde{\xi}\|_2^2 + \int_{\mathbb{R}^3} \langle \widetilde{\xi}(X,\cdot), (-h^2\Delta + \frac{1}{2}V(\cdot/h) + E_b/2)\widetilde{\xi}(X,\cdot)\rangle\,\mathrm{d}^3X.$$

Since all terms on the right hand side are positive, and $\gamma - \gamma^2 \ge \alpha\bar{\alpha}$ we read off the estimates (7.2a), (7.2b), (7.2f), and (7.2d). To prove (7.2e) and (7.2g), we use the fact, that the operator $-\Delta + V/2$ has a spectral gap in between the ground state energy $-E_b$ and the next higher eigenvalue. Hence there is a $\kappa > 0$ and an $\varepsilon > 0$ such that

$$(1-\varepsilon)\Delta + V/2 + E_b/2 \ge \kappa$$

on the orthogonal complement of α_0. In other words

$$\int_{\mathbb{R}^3} \langle \widetilde{\xi}(X,\cdot), (-h^2\Delta_r + \frac{1}{2}V(\cdot/h) + E_b/2)\widetilde{\xi}(X,\cdot)\rangle\,\mathrm{d}^3X \ge (1-\varepsilon)\kappa\|\widetilde{\xi}\|_2^2 + \varepsilon h^2\|\nabla_r\widetilde{\xi}\|_2^2,$$

proving (7.2e) and (7.2g). The estimate (7.2c) for the L^2 norm of ψ is obtained using the definition ψ and $\|\alpha\|_2^2 = \operatorname{Tr}(\gamma - \alpha\bar{\alpha}) + \operatorname{Tr}\gamma = O(h)$. Namely

$$\begin{aligned} \|\psi\|_2^2 &= h^{-2}\int_{\mathbb{R}^3} \alpha_0(r_1/h)\widetilde{\alpha}(X,r_2)\alpha_0(r_2/h)\overline{\widetilde{\alpha}(X,r_1)}\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\mathrm{d}^3X \\ &\le h^{-2}\int_{\mathbb{R}^3} |\alpha_0(r_1/h)|^2|\widetilde{\alpha}(X,r_2)|^2\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\mathrm{d}^3X = h\|\alpha\|_2^2 = O(1), \end{aligned} \quad (7.4)$$

where we used Cauchy-Schwarz with respect to the measure $\mathrm{d}^3r_1\,\mathrm{d}^3r_2$. Finally, to see (7.2h), note that in an analogous way

$$\begin{aligned}\mathrm{Tr}(\alpha\overline{\alpha}\alpha\overline{\alpha}) &= \mathrm{Tr}\left(\gamma^2 - \gamma(\gamma-\alpha\overline{\alpha}) - (\gamma-\alpha\overline{\alpha})\gamma + (\gamma-\alpha\overline{\alpha})^2\right)\\ &\leq \mathrm{Tr}(\gamma^2) + \mathrm{Tr}(\gamma-\alpha\overline{\alpha})^2 + 2\sqrt{\mathrm{Tr}(\gamma^2)\,\mathrm{Tr}(\gamma-\alpha\overline{\alpha})^2} = O(h).\end{aligned}$$

□

Observe, that we do not necessarily have $\|\psi\|_2^2 = N$. The norm deviates from N by a correction of order h^2,

$$\left|\|\psi\|_2^2 - N\right| = h\,|\mathrm{Tr}(\alpha_\psi\overline{\alpha_\psi}) - \mathrm{Tr}(\gamma)| \leq h\,|\mathrm{Tr}(\alpha_\psi\overline{\alpha_\psi} - \alpha\overline{\alpha})| + h\,\mathrm{Tr}(\gamma-\alpha\overline{\alpha}). \tag{7.5}$$

By (7.2b) and (7.2e), the right hand side is of order $O(h^2)$.

Now that we have recovered the function $\psi(x)$ starting from an arbitrary approximate ground state Γ, we are able to define a corresponding Γ_ψ via

$$\alpha_\psi(x,y) = h^{-2}\psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big)$$

and the definition (6.1). Observe that we are able to rescale $\psi \mapsto \lambda\psi$, such that we can assume

$$\mathrm{Tr}\,\gamma_\psi = N/h.$$

The second step now consists of proving that for a lower bound we can replace $\mathcal{E}^{\mathrm{BHF}}(\Gamma)$ by $\mathcal{E}^{\mathrm{BHF}}(\Gamma_\psi)$ up to higher order. Together with the calculations from the upper bound this implies the lower bound stated in Theorem 1.

Lemma 5. *With Γ and Γ_ψ defined as above, one has*

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) \geq \mathcal{E}^{\mathrm{BHF}}(\Gamma_\psi) - O(h^{3/2}). \tag{7.6}$$

Proof. Recall the definition of the BHF-functional

$$\mathcal{E}^{\mathrm{BHF}}(\Gamma) = \mathrm{Tr}(-h^2\Delta + h^2W)\gamma + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y \tag{7.7}$$

$$-\frac{1}{2}\int_{\mathbb{R}^6}|\gamma(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y + \int_{\mathbb{R}^6}\gamma(x,x)\gamma(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y. \tag{7.8}$$

Assume for a moment that the following estimates hold.

$$\begin{aligned}&\mathrm{Tr}(-h^2\Delta)\gamma + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y\\ &\qquad \geq \mathrm{Tr}(-h^2\Delta)\gamma_\psi + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha_\psi(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y - O(h^{3/2})\end{aligned} \tag{7.9a}$$

$$\mathrm{Tr}\,h^2W\gamma \geq \mathrm{Tr}\,h^2W\gamma_\psi - O(h^2) \tag{7.9b}$$

$$-\frac{1}{2}\int_{\mathbb{R}^6}|\gamma(x,y)|^2V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \geq -\frac{1}{2}\int_{\mathbb{R}^6}|\gamma_\psi(x,y)|^2V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - O(h^2) \tag{7.9c}$$

$$\int_{\mathbb{R}^6}\gamma(x,x)\gamma(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \geq \int_{\mathbb{R}^6}\gamma_\psi(x,x)\gamma_\psi(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - O(h^{3/2}). \tag{7.9d}$$

Obviously these estimates immediately imply the statement of the Lemma. □

The rest of the section will be dedicated to proving these estimates.

7.1 Kinetic and potential energy (Proof of (7.9a))

First of all, observe that since we chose γ_ψ so that $\operatorname{Tr}\gamma_\psi = N/h$, we have

$$\operatorname{Tr}(-h^2\Delta)\gamma - \operatorname{Tr}(-h^2\Delta)\gamma_\psi = \operatorname{Tr}\big((-h^2\Delta + E_b/2)\gamma\big) - \operatorname{Tr}\big((-h^2\Delta + E_b/2)\gamma_\psi\big).$$

We use the identity

$$\gamma = \alpha\overline{\alpha} + \alpha\overline{\alpha}\alpha\overline{\alpha} + (\gamma - \alpha\overline{\alpha} - \gamma^2) - (\gamma - \alpha\overline{\alpha})^2 + \gamma(\gamma - \alpha\overline{\alpha}) + (\gamma - \alpha\overline{\alpha})\gamma.$$

The strategy is to show, that all terms on the right hand side containing γ are non-negative, or at least of order $O(h^2)$. Since $(\gamma - \alpha\overline{\alpha} - \gamma^2)$ is a positive self-adjoint operator,

$$\operatorname{Tr}\big((-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha} - \gamma^2)\big) \geq 0.$$

The trace of the operator $(-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha})^2$ is bounded by

$$\begin{aligned}\operatorname{Tr}(-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha})^2 &= \operatorname{Tr}(\gamma - \alpha\overline{\alpha})^{1/2}(-h^2\Delta + E_b/2)^{1/2}(-h^2\Delta + E_b/2)^{1/2}(\gamma - \alpha\overline{\alpha})^{1/2}(\gamma - \alpha\overline{\alpha})\\ &\leq \|\gamma - \alpha\overline{\alpha}\|_\infty \operatorname{Tr}(-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha}) \leq O(h^2),\end{aligned}$$

where we used (7.2a) and (7.2b). The traces of the terms $\gamma(\gamma - \alpha\overline{\alpha})$ and $(\gamma - \alpha\overline{\alpha})\gamma$ can be bounded by

$$\begin{aligned}\operatorname{Tr}\big((-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha})\gamma\big) &\leq \|[-h^2\Delta + E_b/2]^{1/2}(\gamma - \alpha\overline{\alpha})\|_2\|[-h^2\Delta + E_b/2]^{1/2}\gamma\|_2\\ &= \operatorname{Tr}\big((-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha})^2\big)^{1/2}\operatorname{Tr}\big((-h^2\Delta + E_b/2)\gamma^2\big)^{1/2}\\ &\leq O(h^{3/2}),\end{aligned}$$

using (7.2a) and

$$\begin{aligned}\operatorname{Tr}\big((-h^2\Delta + E_b/2)\gamma^2\big) &\leq \operatorname{Tr}\big((-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha} - \gamma^2)\big) + \operatorname{Tr}\big((-h^2\Delta + E_b/2)\gamma^2\big)\\ &= \operatorname{Tr}\big((-h^2\Delta + E_b/2)(\gamma - \alpha\overline{\alpha})\gamma\big) \leq O(h).\end{aligned}$$

As a result, we have

$$\operatorname{Tr}\big((-h^2\Delta + E_b/2)\gamma\big) \geq \operatorname{Tr}\big((-h^2\Delta + E_b/2)(\alpha\overline{\alpha} + \alpha\overline{\alpha}\alpha\overline{\alpha})\big) + O(h^{3/2}).$$

Next we redo the calculation in (7.3) in order to conclude

$$\begin{aligned}&\operatorname{Tr}\big((-h^2\Delta + E_b/2)\alpha\overline{\alpha}\big) + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y\\ &\quad\geq \operatorname{Tr}\big((-h^2\Delta + E_b/2)\alpha_\psi\overline{\alpha_\psi}\big) + \frac{1}{2}\int_{\mathbb{R}^6} V\big((x-y)/h\big)|\alpha_\psi(x,y)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y.\end{aligned} \tag{7.10}$$

Finally, we are going to show, that

$$\operatorname{Tr}\big[(-h^2\Delta + E_b/2)\alpha\overline{\alpha}\alpha\overline{\alpha}\big] \geq \operatorname{Tr}\big[(-h^2\Delta + E_b/2)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\big] + O(h^2). \tag{7.11}$$

Recalling the definition of γ_ψ we see that this implies (7.9a). We are left with estimating the difference

$$\begin{aligned}\operatorname{Tr}\big((-h^2\Delta + E_b/2)\big[\alpha\overline{\alpha}\alpha\overline{\alpha} - \alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\big]\big) &= \operatorname{Tr}\big((-h^2\Delta + E_b/2)\big[\alpha\overline{\alpha}\alpha\overline{\alpha} - \alpha_\psi\overline{\alpha}\alpha\overline{\alpha_\psi} + \alpha_\psi(\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi)\overline{\alpha_\psi}\big]\big)\\ &\geq \operatorname{Tr}\big((-h^2\Delta + E_b/2)\big[\alpha_\psi\overline{\alpha}\alpha\overline{\xi} + \xi\overline{\alpha}\alpha\overline{\alpha_\psi} + \alpha_\psi(\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi)\overline{\alpha_\psi}\big]\big),\end{aligned}$$

where we dropped the contribution of the term $\operatorname{Tr}\left((-h^2\Delta + E_b/2)\xi\overline{\alpha}\alpha\overline{\xi}\right) \geq 0$. Applying the Hölder inequality for the term with E_b, we obtain

$$\begin{aligned}\operatorname{Tr}&\left(\alpha_\psi\overline{\alpha}\alpha\overline{\xi} + \xi\overline{\alpha}\alpha\overline{\alpha_\psi} + \alpha_\psi(\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi)\overline{\alpha_\psi}\right)\\ &\leq 2\|\alpha_\psi\|_6\|\alpha\|_6^2\|\xi\|_2 + \|\alpha_\psi\|_6^2\|\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi\|_{3/2} \leq O(h^2),\end{aligned} \tag{7.12}$$

where we used $\|\alpha\|_6 \leq \|\alpha_\psi\|_6 + \|\xi\|_6 \leq \|\alpha_\psi\|_6 + \|\xi\|_2$ together with (7.2e) and (5.5b). The same procedure also holds for the term involving the Laplacian and we obtain

$$\begin{aligned}h^2 \operatorname{Tr}&\left(\nabla\left[\alpha_\psi\overline{\alpha}\alpha\overline{\xi} + \xi\overline{\alpha}\alpha\overline{\alpha_\psi} + \alpha_\psi(\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi)\overline{\alpha_\psi}\right]\nabla\right)\\ &\leq 2h^2\|\nabla\alpha_\psi\|_6\|\alpha\|_6^2\|\nabla\xi\|_2 + h^2\|\nabla\alpha_\psi\|_6^2\|\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi\|_{3/2}.\end{aligned}$$

Note that

$$\|\nabla\alpha_\psi\|_6 \leq \frac{1}{2}\|\nabla_X\alpha_\psi\|_6 + \|\nabla_r\alpha_\psi\|_6.$$

Using $\|\nabla_X\alpha_\psi\|_6 = \|\alpha_{\nabla\psi}\|_6 \leq \|\alpha_{\nabla\psi}\|_2 = \|\nabla\psi\|_2 h^{-1/2}$ and (5.5c), we conclude that

$$\|\nabla\alpha_\psi\|_6 = O(h^{-1/2}).$$

The remaining factor can be bounded as follows.

$$\|\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi\|_{3/2} = \|\overline{\alpha_\psi}\xi + \overline{\xi}\alpha_\psi + \overline{\xi}\xi\|_{3/2} \leq 2\|\alpha_\psi\|_6\|\xi\|_2 + \|\xi\|_6\|\xi\|_2 \leq 2\|\alpha_\psi\|_6\|\xi\|_2 + \|\xi\|_2^2 = O(h),$$

using (5.5b) and (7.2e). This shows that

$$h^2|\operatorname{Tr}\left(-\Delta\left[\alpha_\psi\overline{\alpha}\alpha\overline{\xi} + \xi\overline{\alpha}\alpha\overline{\alpha_\psi} + \alpha_\psi(\overline{\alpha}\alpha - \overline{\alpha_\psi}\alpha_\psi)\overline{\alpha_\psi}\right]\right)| \leq O(h^2)$$

Together with (7.12), this proves (7.11). Moreover, note that $\|\xi\overline{\alpha}\alpha\overline{\xi}\|_1 \leq \|\overline{\alpha}\alpha\|_3\|\xi\|_3^2 \leq \|\alpha\|_6^2\|\xi\|_2^2 \leq O(h^2)$, using (5.5b) and (7.2e). This shows that

$$\|\alpha\overline{\alpha}\alpha\overline{\alpha} - \alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\|_1 \leq O(h^2), \tag{7.13}$$

which we will need later.

7.2 External potential (Proof of (7.9b))

Using the form of γ_ψ we evaluate

$$\begin{aligned}h^2 \operatorname{Tr} W(\gamma - \gamma_\psi) &= h^2 \operatorname{Tr} W(\gamma - \alpha\overline{\alpha}) + h^2 \operatorname{Tr} W(\alpha\overline{\alpha} - \alpha_\psi\overline{\alpha_\psi}) + h^2 \operatorname{Tr} W(\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi})\\ &\geq -h^2\|W\|_\infty\left[\operatorname{Tr}(\gamma - \alpha\overline{\alpha}) + \|\xi\|_2^2 + 2\|\alpha_\psi\xi\|_1 + \operatorname{Tr}\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi})\right] \geq -O(h^2),\end{aligned} \tag{7.14}$$

where we used (7.2b), the explicit form $\alpha = \alpha_\psi + \xi$, and $\|\alpha_\psi\xi\|_1 \leq \|\alpha_\psi\|_2\|\xi\|_2 \leq O(1)$, which shows (7.9b).

7.3 Direct and exchange term (Proof of (7.9c) and (7.9d))

We reduce the direct term and exchange term to expressions in α in favor of γ. We apply Lemma 3 with $\sigma = \alpha\overline{\alpha}$ and $\delta = \gamma - \alpha\overline{\alpha}$ to the differences

$$\int_{\mathbb{R}^6} |\gamma(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - \int_{\mathbb{R}^6} |(\alpha\overline{\alpha})(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y$$

and

$$\int_{\mathbb{R}^6} \gamma(x,x)\gamma(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - \int_{\mathbb{R}^6} (\alpha\overline{\alpha})(x,x)(\alpha\overline{\alpha})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y.$$

They are thus bounded by

$$\begin{aligned} 2\int_{\mathbb{R}^6} &\big|V\big((x-y)/h\big)(\gamma-\alpha\overline{\alpha})(x,x)\gamma(y,y)\big|\,\mathrm{d}^3x\,\mathrm{d}^3y \\ &\le 2\int_{\mathbb{R}^6} \big|V\big((x-y)/h\big)(\gamma-\alpha\overline{\alpha})(x,x)(\gamma-\alpha\overline{\alpha})(y,y)\big|\,\mathrm{d}^3x\,\mathrm{d}^3y \qquad (7.15a) \\ &+ 2\int_{\mathbb{R}^6} \big|V\big((x-y)/h\big)(\gamma-\alpha\overline{\alpha})(x,x)(\alpha\overline{\alpha})(y,y)\big|\,\mathrm{d}^3x\,\mathrm{d}^3y. \qquad (7.15b) \end{aligned}$$

By (7.2b), remainder (7.15a) is bounded by

$$\left|\int_{\mathbb{R}^6} (\gamma-\alpha\overline{\alpha})(x,x)(\gamma-\alpha\overline{\alpha})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \le [\mathrm{Tr}(\gamma-\alpha\overline{\alpha})]^2\|V\|_\infty = O(h^2).$$

For (7.15b), we are going to use the decomposition $\alpha = \alpha_\psi + \xi$ in order to show that

$$\left|\int_{\mathbb{R}^6} (\gamma-\alpha\overline{\alpha})(x,x)(\alpha\overline{\alpha})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \le O(h^{3/2}). \qquad (7.16)$$

Since

$$\alpha\bar{\alpha} = \alpha_\psi\overline{\alpha_\psi} + \xi\overline{\alpha_\psi} + \alpha_\psi\bar{\xi} + \xi\bar{\xi}$$

we have to bound four terms seperately. First, observe

$$\left|\int_{\mathbb{R}^6} (\gamma-\alpha\overline{\alpha})(x,x)(\xi\bar{\xi})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \le \|V\|_\infty \,\mathrm{Tr}(\gamma-\alpha\overline{\alpha})\,\mathrm{Tr}(\xi\bar{\xi}) \le O(h^2).$$

Second,

$$\begin{aligned} &\left|\int_{\mathbb{R}^6} (\gamma-\alpha\overline{\alpha})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \\ &\qquad\qquad \le h^3\,\mathrm{Tr}(\gamma-\alpha\overline{\alpha})\|(\alpha_\psi\overline{\alpha_\psi})(\cdot,\cdot)\|_\infty\|V\|_1 \le O(h^2), \qquad (7.17) \end{aligned}$$

where we used (5.3). For the remaining terms we use (5.4) with $\sigma = \xi$, and Young's inequality to see

$$\begin{aligned} &\left|\int_{\mathbb{R}^6} (\gamma-\alpha\overline{\alpha})(x,x)(\alpha_\psi\bar{\xi})(y,y) V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \\ &\quad \le h^{-1}\|\psi\|_6\|\alpha_0\|_3 \left|\int_{\mathbb{R}^9} (\gamma-\alpha\overline{\alpha})(x,x)\|\xi(\cdot,y)\|_2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y\right| \\ &\quad \le h^{-1}\|\alpha_0\|_3\|\psi\|_6\|\xi\|_2\|V(\cdot/h)\|_2\,\mathrm{Tr}(\gamma-\alpha\overline{\alpha}) = h^{1/2}\|\alpha_0\|_3\|\psi\|_6\|\xi\|_2\|V\|_2\,\mathrm{Tr}(\gamma-\alpha\overline{\alpha}) \le O(h^2). \end{aligned}$$

The only terms from the direct and exchange term contributing to the order h are

$$\int_{\mathbb{R}^6} (\alpha\overline{\alpha})(x,x)(\alpha\overline{\alpha})(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y \qquad \text{and} \qquad \int_{\mathbb{R}^6} |(\alpha\overline{\alpha})(x,y)|^2 V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y$$

respectively. We reduce these integrals to expressions in α_ψ. In the case of the exchange term, the difference is bounded by

$$\frac{1}{2}\|V\|_\infty \operatorname{Tr}(\alpha\overline{\alpha}\alpha\overline{\alpha} - \alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}).$$

Equation (7.13) implies, that this expression is of order $O(h^2)$.

For the direct term we have to estimate the difference

$$\int_{\mathbb{R}^6} (\alpha\overline{\alpha})(x,x)(\alpha\overline{\alpha})(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y - \int_{\mathbb{R}^6} (\alpha_\psi\overline{\alpha_\psi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y)V\big((x-y)/h\big)\,\mathrm{d}^3x\,\mathrm{d}^3y$$

Plugging $\alpha = \alpha_\psi + \xi$ in the difference yields 15 terms. However, due to symmetry, it suffices to estimate the following 5 terms. We begin the term with four ξ's. Obviously

$$\int_{\mathbb{R}^6} (\xi\overline{\xi})(x,x)(\xi\overline{\xi})(y,y)\,\big|V\big((x-y)/h\big)\big|\,\mathrm{d}^3x\,\mathrm{d}^3y \le \|V\|_\infty\big[\operatorname{Tr}(\xi\overline{\xi})\big]^2 \le O(h^2).$$

Second, using (5.3). we obtain

$$\begin{aligned}\int_{\mathbb{R}^6} (\xi\overline{\xi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y)\,\big|V\big((x-y)/h\big)\big|\,\mathrm{d}^3x\,\mathrm{d}^3y&\\ \le \operatorname{Tr}(\xi\overline{\xi})\|(\alpha_\psi\overline{\alpha_\psi})(\cdot,\cdot)\|_\infty h^3\|V\|_1 &\le h\operatorname{Tr}(\xi\overline{\xi})\|V\|_1\|\psi\|_4^2\|\alpha_0\|_4^2 \le O(h^2).\end{aligned}$$

For the last three terms we invoke equation (5.4) from Lemma 1 with $\sigma = \xi$, and Youngs inequality, to evaluate

$$\begin{aligned}&\int_{\mathbb{R}^6} (\xi\overline{\alpha_\psi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y)\,|V\,((x-y)/h)|\,\mathrm{d}^3x\,\mathrm{d}^3y\\ &\quad\le h^{-1}\|\alpha_0\|_3\|\psi\|_6\int_{\mathbb{R}^6}\|\xi(x,\cdot)\|_2(\alpha_\psi\overline{\alpha_\psi})(y,y)\,|V\,((x-y)/h)|\,\mathrm{d}^3x\,\mathrm{d}^3y\\ &\quad\le h^{-1}\|\alpha_0\|_3\|\psi\|_6\|V(\cdot/h)\|_1\|\xi\|_2\|\alpha_\psi\overline{\alpha_\psi}(\cdot,\cdot)\|_2.\end{aligned}$$

The factor $\|\alpha_\psi\overline{\alpha_\psi}(\cdot,\cdot)\|_2$ on the right hand side is of order $O(h^{-1})$,

$$\begin{aligned}\|\alpha_\psi\overline{\alpha_\psi}(\cdot,\cdot)\|_2^2 &= \int_{\mathbb{R}^9}|\alpha_\psi(x,y)|^2|\alpha_\psi(x,z)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y\,\mathrm{d}^3z\\ &= h^{-8}\int_{\mathbb{R}^9}|\alpha_0\big((x-y)/h\big)|^2|\alpha_0\big((x-z)/h\big)|^2|\psi\big((x+y)/2\big)|^2|\psi\big((x+z)/2\big)|^2\,\mathrm{d}^3x\,\mathrm{d}^3y\,\mathrm{d}^3z.\end{aligned}$$

Changing to the variables $r = x-y$, $s = x-z$ and x and using Cauchy-Schwarz in x, we obtain

$$\|\alpha_\psi\overline{\alpha_\psi}(\cdot,\cdot)\|_2^2 = h^{-8}\int_{\mathbb{R}^9}|\alpha_0\big(r/h\big)|^2|\alpha_0\big(s/h\big)|^2|\psi(x-r/2)|^2|\psi(x-s/2)|^2\,\mathrm{d}^3x\,\mathrm{d}^3r\,\mathrm{d}^3s \le h^{-2}\|\alpha_0\|_2^2\|\psi\|_4^4.$$

Therefore

$$\int_{\mathbb{R}^6}(\xi\overline{\alpha_\psi})(x,x)(\alpha_\psi\overline{\alpha_\psi})(y,y)\,|V\,((x-y)/h)|\,\mathrm{d}^3x\,\mathrm{d}^3y \le h\|\alpha_0\|_3\|\psi\|_6\|\psi\|_4^2\|V\|_1\|\xi\|_2 \le O(h^{3/2}).$$

Again using equation (5.4) from Lemma 1 with $\sigma = \xi$, and Youngs inequality, we estimate the remaining terms

$$\begin{aligned}
&\int_{\mathbb{R}^6} (\xi\bar{\xi})(x,x)(\xi\overline{\alpha_\psi})(y,y)\,\big|V\big((x-y)/h\big)\big|\;\mathrm{d}^3x\,\mathrm{d}^3y \\
&\qquad \le h^{-1}\|\alpha_0\|_3\|\psi\|_6 \int_{\mathbb{R}^6} (\xi\bar{\xi})(x,x)\|\xi(y,\cdot)\|_2\,|V\left((x-y)/h\right)|\;\mathrm{d}^3x\,\mathrm{d}^3y \\
&\qquad \le h^{-1}\|\alpha_0\|_3\|\psi\|_6\|V(\cdot/h)\|_2\|\xi\|_2\,\mathrm{Tr}(\xi\bar{\xi}) \le O(h^2)
\end{aligned}$$

and

$$\begin{aligned}
&\int_{\mathbb{R}^6} (\xi\overline{\alpha_\psi})(x,x)(\xi\overline{\alpha_\psi})(y,y)\,\big|V\big((x-y)/h\big)\big|\;\mathrm{d}^3x\,\mathrm{d}^3y \\
&\qquad \le h^{-2}\|\alpha_0\|_3^2\|\psi\|_6^2 \int_{\mathbb{R}^6} \|\xi(x,\cdot)\|_2\|\xi(y,\cdot)\|_2\,|V\left((x-y)/h\right)|\;\mathrm{d}^3x\,\mathrm{d}^3y \\
&\qquad \le h^{-2}\|\alpha_0\|_3^2\|\psi\|_6^2\|\xi\|_2^2\|V(\cdot/h)\|_1 = h\|\alpha_0\|_3^2\|\psi\|_6^2\,\mathrm{Tr}\,\xi\bar{\xi}\|V\|_1 \le O(h^2).
\end{aligned}$$

A Proof of Lemma 1

Proof of Lemma 1, Part II. Recall, that by (4.7) α_ψ is defined by

$$\alpha_\psi(x,y) = h^{-2}\psi\Big(\frac{x+y}{2}\Big)\alpha_0\Big(\frac{x-y}{h}\Big).$$

We first prove (5.1a) and (5.1b). In terms of the integral kernel $\|\alpha_\psi\|_n^n$ is given by

$$\mathrm{Tr}\left((\alpha_\psi\overline{\alpha_\psi})^{n/2}\right) = \int_{\mathbb{R}^{3n}} \alpha_\psi(x_1,x_2)\overline{\alpha_\psi(x_2,x_3)}\cdots\alpha_\psi(x_{n-1},x_n)\overline{\alpha_\psi(x_n,x_1)}\,\mathrm{d}^3x_1\cdots\,\mathrm{d}^3x_n. \tag{A.1}$$

We switch to the following coordinates

$$\begin{aligned}
X &= \frac{1}{n}\sum_{k=1}^n x_k \\
r_k &= x_{k+1} - x_k, \qquad k = 1,\dots,n-1.
\end{aligned} \tag{A.2}$$

It is easy to see, that the corresponding Jacobi determinant is equal to 1. Moreover we can recover the original coordinates via

$$\begin{aligned}
x_1 &= X - \frac{1}{n}\sum_{i=1}^{n-1}(n-i)r_i, \\
x_{k+1} &= x_k + r_k,
\end{aligned}$$

i.e.

$$x_k = X + s_k(r_1,\dots,r_{n-1}),$$

for some linear combinations s_k of r_i, which we do not need to know explicitly. We therefore obtain for the integral in (A.1)

$$\begin{aligned}
\|\alpha_\psi\|_n^n = h^{-2n}\int_{\mathbb{R}^{3n}} &\psi\big(X + s_1(r_1,\dots,r_{n-1})\big)\cdots\overline{\psi\big(X + s_n(r_1,\dots,r_{n-1})\big)}\times \\
&\times \alpha_0(r_1/h)\cdots\overline{\alpha_0(r_n/h)}\,\mathrm{d}^3X\,\mathrm{d}^3r_1\cdots\,\mathrm{d}^3r_{n-1},
\end{aligned}$$

where we introduced $r_n := -\sum_{k=1}^{n-1} r_k$. Scaling $r_k \to hr_k$ and using Hölder in the X variable, we obtain

$$\begin{aligned}\|\alpha_\psi\|_n^n &\le h^{n-3}\|\psi\|_n^n \int_{\mathbb{R}^{3(n-1)}} \left|\alpha_0(r_1/h)\cdots\overline{\alpha_0(r_n/h)}\right| \mathrm{d}^3 r_1 \cdots \mathrm{d}^3 r_{n-1} \\ &= (2\pi)^{3/2(n-2)} h^{n-3}\|\psi\|_n^n \, \|\widehat{\alpha_0}\|_n^n.\end{aligned}$$

Just the same calculation with α_0 replaced by $\nabla\alpha_0$ yields (5.1b).

Due to the symmetry $\alpha_\psi(x,y) = \alpha_\psi(y,x)$, we have

$$\begin{aligned}\mathrm{Tr}\left((\Delta_x\alpha_\psi)\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\right) &= \langle \overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}, \Delta_x\alpha_\psi\rangle_{L^2(\mathbb{R}^6)} = \langle \overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}, \frac{\Delta_x+\Delta_y}{2}\alpha_\psi\rangle_{L^2(\mathbb{R}^6)} \\ &= \langle \overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}, \Delta_X/4 + \Delta_r\alpha_\psi\rangle_{L^2(\mathbb{R}^6)} \\ &= \mathrm{Tr}\left((\Delta_r\alpha_\psi)\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\right) + \frac{1}{4}\,\mathrm{Tr}(\Delta_X\alpha_\psi)\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\big),\end{aligned}$$

where it is meant that r and X are the relative coordinates of the kernel of the α_ψ. Therefore using the coordinates (A.2), for which we have in the case of $n = 4$

$$\begin{aligned}&\frac{x_1+x_2}{2} = X - s \qquad &&\frac{x_3+x_4}{2} = X + s \qquad &&s(r_1,r_2,r_3) = \frac{r_1+2r_2+r_3}{4} \\ &\frac{x_2+x_3}{2} = X - t \qquad &&\frac{x_1+x_4}{2} = X + t \qquad &&t(r_1,r_2,r_3) = \frac{r_3-r_1}{4}\end{aligned}$$

and changing variables according to $r_k \to hr_k$, $k = 1,2,3$, we can write

$$\begin{aligned}\mathrm{Tr}(-h^2\Delta + E_b/2)\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi} &= h\int_{\mathbb{R}^{12}} \psi(X-hs)\overline{\psi(X-ht)}\psi(X+hs)\overline{\psi(X+ht)} \\ &\quad\times\left[(-\Delta + E_b/2)\alpha_0(r_1)\right]\overline{\alpha_0(r_2)}\alpha_0(r_3)\overline{\alpha_0(-r_1-r_2-r_3)}\,\mathrm{d}^3X\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\mathrm{d}^3r_3 \\ &\quad -\frac{h^2}{4}\,\mathrm{Tr}\left((\Delta_X\alpha_\psi)\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\right).\end{aligned}$$

Expanding in h, this term has the form

$$h(2\pi)^3\|\psi\|_4^4\int_{\mathbb{R}^3} |\widehat{\alpha_0}(p)|^4(p^2 + E_b/2)\,\mathrm{d}^3p + A_1\,h^2 + A_2\,h^2,$$

where

$$\begin{aligned}A_1 &= -\frac{1}{4}\,\mathrm{Tr}\left((\Delta_X\alpha_\psi)\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\right), \\ A_2 &= h^{-1}\int_{\mathbb{R}^{12}}\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\psi(X-\tau hs)\overline{\psi(X-\tau ht)}\psi(X+\tau hs)\overline{\psi(X+\tau ht)}\right)\mathrm{d}\tau \\ &\quad\times\left[(-\Delta + E_b/2)\alpha_0(r_1)\right]\overline{\alpha_0(r_2)}\alpha_0(r_3)\overline{\alpha_0(-r_1-r_2-r_3)}\,\mathrm{d}^3X\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\mathrm{d}^3r_3.\end{aligned}$$

Using partial integration, we write A_1 as

$$\begin{aligned}|A_1| &= \frac{1}{4}|\,\mathrm{Tr}\left((\Delta_X\alpha_\psi)\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi}\right)| \\ &= \frac{1}{4}|\,\mathrm{Tr}(\nabla_X\alpha_\psi\nabla_X\overline{\alpha_\psi}\alpha_\psi\overline{\alpha_\psi} + \nabla_X\alpha_\psi\overline{\alpha_\psi}\nabla_X\alpha_\psi\overline{\alpha_\psi} + \nabla_X\alpha_\psi\overline{\alpha_\psi}\alpha_\psi\nabla_X\overline{\alpha_\psi})| \\ &\le \|\nabla_X\alpha_\psi\|_2^2\|\alpha_\psi\overline{\alpha_\psi}\|_\infty + ... \le O(1),\end{aligned}$$

due to (5.5d).

To estimate A_2, we write the τ derivative as gradients and apply the Hölder inequality in the X integral with coefficient 2 for the $\nabla\psi$ factor and coefficient 6 for the remaining ψ factors. Moreover, we replace the Laplacian acting on α_0 by V, using the fact, that $(-\Delta + E_b/2)\alpha_0 = V\alpha_0$.

$$|A_2| \leq \frac{1}{2}\|\nabla\psi\|_2\|\psi\|_6^3 \int_{\mathbb{R}^9} \big(|s| + |t|\big)\big|(V\alpha_0)(r_1)\alpha_0(r_2)\alpha_0(r_3)\alpha_0(-r_1 - r_2 - r_3)\big| \, \mathrm{d}^3r_1 \, \mathrm{d}^3r_2 \, \mathrm{d}^3r_3.$$

We now note that $|s| + |t| \leq |r_1 + r_2 + r_3| + |r_2| + |r_3|$ and apply Cauchy-Schwarz to the r_2 integration in the case of $|r_1 + r_2 + r_3|$ or $|r_2|$ and to the r_3 integration in the case of $|r_3|$ to conclude

$$|A_2| \leq \frac{3}{2}\|\nabla\psi\|_2\|\psi\|_6^3\|V\alpha_0\|_1 \, \|\alpha_0\|_1 \, \|\alpha_0\|_2 \, \big\||\cdot|\alpha_0\big\|_2 \leq O(1).$$

By the Sobolev inequality, we have $\|\psi\|_6^3 \leq C\|\nabla\psi\|_2^3$. □

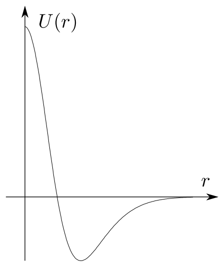
B Explicit example for a potential V for which $\mathcal{E}^{\mathrm{BHF}}$ is bounded from below

To explicitly give an example for a potential V satisfying Assumptions 1 and 2, we will use a more concrete minorant, namely a linear combination of Gaussians with appropriate coefficients. We will consider

$$U(x) = A_+ \, \mathrm{e}^{-\frac{x^2}{\sigma_+^2}} - A_- \, \mathrm{e}^{-\frac{x^2}{\sigma_-^2}}.$$

Then

$$\widehat{U}(p) = A_+\sigma_+^3\mathrm{e}^{-\sigma_+^2 p^2} - A_-\sigma_-^3\mathrm{e}^{-\sigma_-^2 p^2}$$



and $\widehat{U}(p) \geq 0$ whenever

$$\begin{aligned} \sigma_- &\geq \sigma_+ \\ A_+\sigma_+^3 &\geq A_-\sigma_-^3. \end{aligned} \tag{B.1}$$

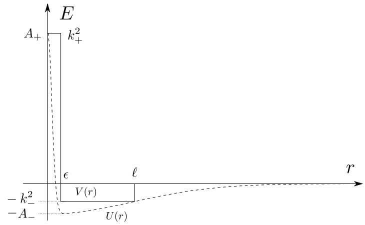
Now consider a potential of the type

$$V = V^+ - V^-, \qquad \begin{aligned} V_+(x) &= k_+^2 \, \chi_{\{|x|<\epsilon\}}(x), \\ V_-(x) &= k_-^2 \, \chi_{\{\epsilon<|x|<\ell\}}(x). \end{aligned} \tag{B.2}$$

with fixed k_- and ℓ, such that the simple potential well $-k_-^2 \, \chi_{\{|x|<\ell\}}(x)$ has a bound state, i.e. $k_-\ell > \frac{\pi}{2}$. We will see, that it is possible to find appropriate k_+ and ϵ such that V has a minorant $\widetilde{V} \geq U$ with $\widehat{U} \geq 0$. The condition for V having a bound state is (see for example [3][Appendix 2, (A9)]

$$k_-(\ell - \epsilon) \geq \arctan\left(\frac{k_+}{k_-}\frac{1}{\tanh(k_+\epsilon)}\right).$$

This is guaranteed by choosing ϵ such that $k_-(\ell - \epsilon) \geq \frac{\pi}{2}$.



We take $-U_-(x) = -A_- \, \mathrm{e}^{-\frac{x^2}{\sigma_-^2}}$ as a minorant of V_-, i.e. $U_- > V_-$ with appropriate constants A_- and σ_-. In a next step, we choose A_+ and σ_+ such that (B.1) holds. Note, that scaling $A_+ \mapsto \lambda^{-3} A_+$ and $\sigma_+ \mapsto \lambda \sigma_+$ leaves (B.1) invariant. That is for every $\lambda > 0$, $U^\lambda = U_+^\lambda - U_-$ has non-negative Fourier transform for $U_+^\lambda(x) = \lambda^{-3} A_+ \, \mathrm{e}^{-\frac{x^2}{\lambda^2 \sigma_+^2}}$. We observe, that for $x \neq 0$ and $\lambda \to 0$, $U_+^\lambda(x)$ converges pointwise to 0. We conclude, that there exists λ such that $U = U^\lambda \leq V_-$.

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