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Various rigorous results on quantum systems with long range magnetic fields

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Publication date:
2012

Document Version
Early version, also known as pre-print

Link to publication from Aalborg University

Citation for published version (APA):
Cornean, H. (2012). *Various rigorous results on quantum systems with long range magnetic fields*.

Doctoral dissertation

Various rigorous results on quantum systems with long range magnetic fields

by

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Denne afhandling er af Akademisk Råd ved Det Teknisk-Naturvidenskabelige Fakultet ved Aalborg Universitet antaget til forsvar for doktorgraden i naturvidenskab. Forsvaret finder sted på Aalborg Universitet, Auditorium B3-104, Frederik Bajers Vej 7B, den 28. marts 2012 kl. 13.00.

Aalborg, den 13. februar 2012

Eskild Holm Nielsen
Dekan

This thesis has been accepted by the Academic Council at the Faculty of Engineering and Science at Aalborg University for public defence in fulfillment of the requirements for the doctoral degree in science. The defence will take place at Aalborg University, Auditorium B3-104, Frederik Bajers Vej 7B, on March 28, 2012, at 1 p.m.

Aalborg, February 13, 2012

Eskild Holm Nielsen
Dean

The following is identical to the dissertation submitted on June 27, 2011, except that the reference [BCS 2] on page 4 and the complete publication list on page 8 have been updated.

Contents

1 Introduction

There are three different topics of mathematical physics which have played a special role in my research activity during the last fifteen years. The first one is the spectral analysis of magnetic Schrödinger operators, including thermodynamic behavior of large magnetic systems and condensed matter theory. The second topic is the rigorous justification of various effective models of low dimensional many-body interacting systems, like excitons, trions and biexcitons in carbon nanotubes. And the third one is the theory of non equilibrium steady states of mesoscopic systems.

This dissertation is based on eight selected papers (see below), which represent the first topic. Since I also passed a French *Habilitation á diriger des recherches* in May 2006, all papers included in the current dissertation have been published after that date and have not been used before. The eight publications are:

- [C] Cornean, H.D.: On the Lipschitz continuity of spectral bands of Harper-like and magnetic Schrödinger operators. Annales Henri Poincaré **11**, 973-990 (2010)
- [CHS] Cornean, H.D., Herbst, I., Skibsted, E.: Spiraling attractors and quantum dynamics for a class of long-range magnetic fields. J. Funct. Anal. **247** (1), 1-94 (2007)
- [BCL 1] Briet, P., Cornean, H.D., Louis, D.: Diamagnetic expansions for perfect quantum gases. J. Math. Phys. **47** 083511 (2006)
- [BCL 2] Briet, P., Cornean, H.D., Louis, D.: Diamagnetic expansions for perfect quantum gases II: uniform bounds. Asymptotic Analysis **59** (1-2), 109-123 (2008)
- [BCS 1] Briet, P., Cornean, H.D., Savoie, B.: Diamagnetism of quantum gases with singular potentials. J. Phys. A: Math. Theor. **43**, 474008 (2010)
- [CN 1] Cornean, H.D., Nenciu, G.: The Faraday effect revisited: Thermodynamic limit. J. Funct. Anal. **257** (7), 2024-2066 (2009)
- [BCS 2] Briet, P., Cornean, H.D., Savoie, B.: A rigorous proof of the Landau-Peierls formula and much more. Annales Henri Poincaré **13**(1), 1-40 (2012)
- [CN 2] Cornean, H.D., Nenciu, G.: The Faraday effect revisited: sum rules and convergence issues. J. Phys. A: Math. Theor. **43**, 474012 (2010)

1.1 The four technical chapters of the dissertation

1. *Spectral theory of Schrödinger and Harper-like operators with constant magnetic fields*. We are interested in magnetic perturbations which are not relatively bounded to the reference operator. In the paper presented here [C], we show for a large class of discrete Harper-like and continuous magnetic Schrödinger

operators that their spectral band edges are Lipschitz continuous with respect to the intensity of the external constant magnetic field.

2. *Scattering theory of 2D particles subjected to long range magnetic fields.* In the paper presented here [CHS] we consider the long time behavior of a classical/quantum particle in a $2D$ magnetic field which is homogeneous of degree -1. If the field never vanishes, above a certain energy the associated classical dynamical system has a globally attracting periodic orbit in a reduced phase space. For that energy regime, we construct a simple approximate evolution based on this attractor, and prove that it completely describes the quantum dynamics of our system.

3. *Thermodynamic behavior of large magnetic quantum systems.* In [BCL 1] and [BCL 2] we consider a perfect quantum gas in the effective mass approximation, and in the grand-canonical ensemble. We prove that the generalized magnetic susceptibilities admit the thermodynamic limit for all admissible fugacities, uniformly on compacts included in the analyticity domain of the grand-canonical pressure. More precisely, in [BCL 1] we prove that the generalized magnetic susceptibilities have a pointwise thermodynamic limit near $z = 0$. [BCL2] contains the proof of the uniform bounds on compacts needed in order to apply Vitali's Convergence Theorem. In a more recent paper [BCS 1] we show how to extend some of the previous results to the case with singular potentials.

   The next paper on thermodynamic limit of magnetic systems is [CN 1], and it deals with the effect of Faraday rotation. We formulate and prove the thermodynamic limit for the transverse electric conductivity of Bloch electrons, as well as for the Verdet constant. Unlike [BCL 1,2] where we considered magnetic semigroups, in [CN 1] we use formulas based on resolvents. The main mathematical tool used here is a regularized magnetic and geometric perturbation theory combined with elliptic regularity and Agmon-Combes-Thomas uniform exponential decay estimates.

4. *A rigorous derivation of the Landau-Peierls formula.* In [BCS 2] we present a mathematical treatment of the zero-field magnetic susceptibility of a non-interacting Bloch electron gas, at fixed temperature and density, for both metals and semiconductors/insulators. In particular, we obtain the Landau-Peierls formula in the low temperature and density limit as conjectured by Kjeldaas and Kohn in 1957. Some technical results about local trace estimates and sum rules are explained in [CN 2].

1.2 The complete publication list

Articles:

1. (with G. Nenciu): On eigenfunction decay of two dimensional magnetic Schrödinger operators. Commun. Math. Phys. **192**, 671-685 (1998)

2. On the essential spectrum of two dimensional periodic magnetic Schroedinger operators. Lett. Math. Phys. **49**, 197-211 (1999)

3. (with G. Nenciu): Two dimensional magnetic Schroedinger operators: width of minibands in the tight-binding approximation. Ann. Henri Poincaré **1**, 203-222 (2000)

4. On the magnetization of a charged Bose gas in the canonical ensemble. Commun. Math. Phys. **212**, 1-27 (2000)

5. (with Ph. Briet): Locating the spectrum for magnetic Dirac and Schrödinger operators. Commun. P.D.E. **27**, 1079-1101 (2002)

6. (with T.M. Bisgaard): Nonexistence in general of a definitizing ideal of the desired codimension. Positivity **7**, 297-302 (2003)

7. Magnetic response in ideal quantum gases: the thermodynamic limit. Markov Process. Related Fields **9**, 547-566 (2003)

8. (with I. Beltita): On a theorem of Arne Persson. CUBO **6** (2), 1-14 (2004)

9. (with P. Duclos and T.G. Pedersen): One dimensional models of excitons in carbon nanotubes. Few-Body Systems **34**, 155-161 (2004)

10. (with Ph. Briet and V.A. Zagrebnov): Do bosons condense in a homogeneous magnetic field? J. Statist. Phys. **116** (5), 1545-1578 (2004)

11. (with P. Duclos, T.G. Pedersen and K. Pedersen): Stability and signatures of biexcitons in carbon nanotubes. Nano Letters **5** (2), 291–294 (2005)

12. (with A. Jensen, A. and V. Moldoveanu): A rigorous proof of the Landauer-Büttiker formula. J. Math. Phys. **46**, 042106 (2005)

13. (with Ph. Briet and D. Louis): Generalized susceptibilities for a perfect quantum gas. Markov Proc. Related Fields **11**, 177–188 (2005)

14. (with K.Knudsen) Reconstruction from one boundary measurement of a potential homogeneous of degree zero. J. Inverse Ill-Posed Probl. **13** (5), 413–435 (2005)

15. (with G. Nenciu and T.G. Pedersen): The Faraday effect revisited: General theory. J. Math. Phys. **47**, 013511 (2006)

16. (with K. Knudsen and S. Siltanen): Towards a d-bar reconstruction method for three-dimensional EIT. J. Inverse Ill-Posed Probl. **14** (2), 111–134 (2006)

17. (with P. Duclos and B. Ricaud): On critical stability of three quantum charges interacting through delta potentials. Few-Body Systems **38** (2-4), 125–131 (2006)

18. (with Ph. Briet and D. Louis): Diamagnetic expansions for perfect quantum gases. J. Math. Phys. **47**, 083511 (2006)
19. (with P. Duclos and B. Ricaud): Effective models for excitons in carbon nanotubes. Ann. Henri Poincaré **8** (1), 135-163 (2007)
20. (with T.G. Pedersen): Optical second harmonic generation from Wannier excitons. Europhysics Letters **78**, 27005 (2007)
21. (with I. Herbst and E. Skibsted): Spiraling attractors and quantum dynamics for a class of long-range magnetic fields. J. Funct. Anal. **247** (1), 1-94 (2007)
22. (with Ph. Briet and D. Louis): Diamagnetic expansions for perfect quantum gases II: uniform bounds. Asymptotic Analysis **59** (1-2), 109-123 (2008)
23. (with A. Nenciu and G. Nenciu): Optimally localized Wannier functions for quasi one-dimensional nonperiodic insulators. J. Phys. A.: Math. Theor. **41**, 125202 (2008)
24. (with K. Hoke, H. Neidhardt, P. Racec and J. Rehberg): A Kohn-Sham system at zero temperature. J. Phys. A.: Math. Theor. **41**, 385304 (2008)
25. (with P. Duclos, G. Nenciu and R. Purice): Adiabatically switched-on electrical bias and the Landauer-Büttiker formula. J. Math. Phys. **49**, 102106 (2008)
26. (with H. Neidhardt and V.A. Zagrebnov): The effect of time-dependent coupling on non-equilibrium steady states. Annales Henri Poincaré **10** (1), 61-93 (2009)
27. (with T. Rønnow and T.G. Pedersen): Stability of singlet and triplet trions in carbon nanotubes . Physics Letters A. **373** (16), 1478-1481 (2009)
28. (with J. Derezinski and P. Zin): On the Infimum of the Energy-Momentum Spectrum of a Homogeneous Bose Gas. J. Math. Phys. **50**, 062103 (2009)
29. (with G. Nenciu): The Faraday effect revisited: Thermodynamic limit. J. Funct. Anal. **257** (7), 2024-2066 (2009)
30. (with T. Rønnow and T.G. Pedersen): Dimensional and correlation effects of charged excitons in low-dimensional semiconductors. J. Phys. A: Math. Theor. **43**, 474031 (2010)
31. (with T. Rønnow and T.G. Pedersen): Correlation and dimensional effects of trions in carbon nanotubes. Phys. Rev. B. **81**, 205446 (2010)
32. (with G. Nenciu): The Faraday effect revisited: sum rules and convergence issues. J. Phys. A: Math. Theor. **43**, 474012 (2010)

33. On the Lipschitz continuity of spectral bands of Harper-like and magnetic Schroedinger operators. Annales Henri Poincaré **11**, 973-990 (2010)

34. (with Ph. Briet and B. Savoie): Diamagnetism of quantum gases with singular potentials. J. Phys. A: Math. Theor. **43**, 474008 (2010)

35. (with C. Gianesello and V.A. Zagrebnov): A partition-free approach to transient and steady-state charge currents. J. Phys. A: Math. Theor. **43**, 474011 (2010)

36. (with F. Bentosela, B. Fleury and N. Marchetti): On the transfer matrix of a MIMO system. Math. Meth. Appl. Sci. **34**(8), 963-976 (2011)

37. (with S. Kumar and N. Marchetti): Power Consumption Optimization Strategy for Wireless Networks. Wireless Personal Communications **59** (3), 487-498 (2011)

38. (with V. Moldoveanu): On the cotunneling regime of interacting quantum dots. J. Phys. A: Math. Theor. **44** 305002 (2011)

39. (with V. Moldoveanu and C.-A. Pillet): Non-equilibrium steady-states for interacting open systems: exact results. Phys. Rev. B. **84** 075464 (2011)

40. (with Ph. Briet and B. Savoie): A rigorous proof of the Landau-Peierls formula and much more. Annales Henri Poincaré **13**(1), 1-40 (2012)

41. (with P. Duclos and R. Purice): Adiabatic Non-Equilibrium Steady States in the Partition Free Approach. Annales Henri Poincaré, Online First. DOI: 10.1007/s00023-011-0144-x (2012)

Refereed proceedings:

1. (with A. Jensen and V. Moldoveanu): The Landauer-Büttiker formula and resonant quantum transport. Selected and Refereed Lectures from QMath9. Lecture Notes in Physics **690** (2006)

2. (with T.G. Pedersen and B. Ricaud): Rigorous perturbation theory versus variational methods in the spectral study of carbon nanotubes. Contemporary Mathematics **447**: "Adventures in Mathematical Physics". Editors: F. Germinet and P. D. Hislop, 2007.

3. (with P. Duclos and B. Ricaud): On the skeleton method and an application to a quantum scissor. Proceedings of Symposia in Pure Mathematics : "Analysis on Graphs and its Applications". Editors: P. Exner, J. Keating, P. Kuchment, T. Sunada, and A. Teplyaev (2008).

2 Spectral theory of Schrödinger and Harper-like operators with constant magnetic fields

2.1 The setting and the main results

Harper-like operators. Let $\Gamma \subset \mathbb{R}^2$ be a (possibly irregular) lattice which has the property that there exists an injective map $F : \Gamma \mapsto \mathbb{Z}^2$ such that $|F(\gamma) - \gamma| < 1/2$. The Hilbert space is $l^2(\Gamma)$.

The elements of the canonical basis in $l^2(\Gamma)$ are denoted by $\{\delta_{\mathbf{x}}\}_{\mathbf{x}\in\Gamma}$, where $\delta_{\mathbf{x}}(\mathbf{y}) = 1$ if $\mathbf{y} = \mathbf{x}$ and zero otherwise. In the discrete case, to any bounded self-adjoint operator $H \in B(l^2(\Gamma))$ it corresponds a bounded and symmetric kernel $H(\mathbf{x}, \mathbf{x}') = \langle H\delta_{\mathbf{x}'}, \delta_{\mathbf{x}}\rangle = \overline{H(\mathbf{x}', \mathbf{x})}$. We will extensively use the Schur-Holmgren upper bound for the norm of a bounded operator:

$$||H|| \leq \max\left\{\sup_{\mathbf{x}'\in\Gamma}\sum_{\mathbf{x}\in\Gamma}|H(\mathbf{x}, \mathbf{x}')|, \sup_{\mathbf{x}\in\Gamma}\sum_{\mathbf{x}'\in\Gamma}|H(\mathbf{x}, \mathbf{x}')|\right\}. \tag{2.1}$$

Denote by $\langle \mathbf{x} - \mathbf{x}_0\rangle^\alpha = [1 + (\mathbf{x} - \mathbf{x}_0)^2]^{\frac{\alpha}{2}}$, $\alpha \geq 0$. We define $\mathcal{C}^\alpha$ to be the set of bounded operators $H \in B(l^2(\Gamma))$ which have the property that their kernels obey a weighted Schur-Holmgren type estimate:

$$||H||_{\mathcal{C}^\alpha} := \max\left\{\sup_{\mathbf{x}'\in\Gamma}\sum_{\mathbf{x}\in\Gamma}\langle \mathbf{x} - \mathbf{x}'\rangle^\alpha|H(\mathbf{x}, \mathbf{x}')|, \sup_{\mathbf{x}\in\Gamma}\sum_{\mathbf{x}'\in\Gamma}\langle \mathbf{x} - \mathbf{x}'\rangle^\alpha|H(\mathbf{x}, \mathbf{x}')|\right\} < \infty. \tag{2.2}$$

We also define the space $\mathcal{H}^\alpha$ which contains bounded operators H which obey:

$$\begin{aligned} &||H||_{\mathcal{H}^\alpha} \\ &:= \max\left\{\sup_{\mathbf{x}'\in\Gamma}\left\{\sum_{\mathbf{x}\in\Gamma}\langle \mathbf{x} - \mathbf{x}'\rangle^{2\alpha}|H(\mathbf{x}, \mathbf{x}')|^2\right\}^{\frac{1}{2}}, \sup_{\mathbf{x}\in\Gamma}\left\{\sum_{\mathbf{x}'\in\Gamma}\langle \mathbf{x} - \mathbf{x}'\rangle^{2\alpha}|H(\mathbf{x}, \mathbf{x}')|^2\right\}^{\frac{1}{2}}\right\} < \infty. \end{aligned} \tag{2.3}$$

The flux of a unit magnetic field orthogonal to the plane through a triangle generated by $\mathbf{x}$, $\mathbf{x}'$ and the origin is given by:

$$\varphi(\mathbf{x}, \mathbf{x}') := -\frac{1}{2}(x_1\, x_2' - x_2\, x_1') = -\varphi(\mathbf{x}', \mathbf{x}). \tag{2.4}$$

Note the important additive identity:

$$\begin{aligned} &\varphi(\mathbf{x}, \mathbf{y}) + \varphi(\mathbf{y}, \mathbf{x}') = \varphi(\mathbf{x}, \mathbf{x}') + \varphi(\mathbf{x} - \mathbf{y}, \mathbf{y} - \mathbf{x}'), \\ &|\varphi(\mathbf{x} - \mathbf{y}, \mathbf{y} - \mathbf{x}')| \leq \frac{1}{2}|\mathbf{x} - \mathbf{y}|\, |\mathbf{y} - \mathbf{x}'|. \end{aligned} \tag{2.5}$$

Let $K \in \mathcal{C}^0$. Let its kernel be $K(\mathbf{x}, \mathbf{x}')$. We are interested in a family of Harper-like operators $\{K_b\}_{b\in\mathbb{R}}$ given by the kernels $e^{ib\varphi(\mathbf{x},\mathbf{x}')}K(\mathbf{x}, \mathbf{x}')$. Clearly, $\{K_b\}_{b\in\mathbb{R}} \subset \mathcal{C}^0$. The usual

Harper operator lives in $l^2(\mathbb{Z}^2)$, and its generating kernel has the form $K(\mathbf{x},\mathbf{x}') = k(\mathbf{x}-\mathbf{x}')$ where $k(\mathbf{x})$ equals 1 if $|\mathbf{x}| = 1$, and 0 otherwise.

One can easily show that $\mathcal{H}^\alpha \subset \mathcal{C}^0$ if $\alpha > 1$, using the following lemma:

Lemma 2.1. *Let $H \in \mathcal{H}^\alpha$ with $\alpha > 1$. Then $H \in \mathcal{C}^\beta$ with $\beta < \alpha - 1$. In particular, if $\alpha > 3$ then the kernel $\langle \mathbf{x}-\mathbf{x}'\rangle^2 |H(\mathbf{x},\mathbf{x}')|$ obeys a Schur-Holmgren estimate and thus defines a bounded operator.*

Another technical estimate interesting in itself claims that if H has a kernel which is localized near the diagonal, then the resolvent's kernel will also have such a localization:

Proposition 2.2. *Let $H \in \mathcal{C}^\alpha$, with $\alpha > 0$. Let $z \in \rho(H)$. Then for every $0 \leq \alpha' < \alpha$ we have $(H-z)^{-1} \in \mathcal{H}^{\alpha'}$, and there exists a constant C independent of z such that*

$$||(H-z)^{-1}||_{\mathcal{H}^{\alpha'}} \leq C\, (1 + ||H||_{\mathcal{C}^\alpha}^{\alpha+1}) \left(\frac{1}{\{\mathrm{dist}(z,\sigma(H))\}^{\alpha+2}} + \frac{1}{\mathrm{dist}(z,\sigma(H))} \right). \tag{2.6}$$

Remark. This proposition is related to what specialists in von Neumann algebras would call dual action, see [100, 101, 102]. Stronger localization results have been earlier obtained by Jaffard [60], later generalized by Gröchenig and Leinert [36].

Now here is the first main result of this chapter:

Theorem 2.3. *Let $\alpha > 3$ and let $K \in \mathcal{H}^\alpha$ be a self-adjoint operator. Construct the corresponding family of Harper-like operators $\{K_b\}_{b\in\mathbb{R}}$. Then we have:*

i. *The resolvent set $\rho(K_b)$ is stable; more precisely, if $\mathrm{dist}(z,\sigma(K_{b_0})) \geq \epsilon > 0$ then there exist $\delta > 0$ and $\eta > 0$ such that $\mathrm{dist}(z,\sigma(K_b)) \geq \eta$ whenever $|b-b_0| < \delta$.*

ii. *Define $E_+(b) := \sup \sigma(K_b)$ and $E_-(b) := \inf \sigma(K_b)$. Then $E_\pm$ are Lipschitz functions of b.*

iii. *Let $\alpha > 4$. Assume that K_{b_0} has a gap in the spectrum of the form $(e_-(b_0), e_+(b_0))$, where $e_\pm(b_0) \in \sigma(K_{b_0})$ are the gap edges. Then as long as the gap is not closing by varying b in a closed interval I containing b_0, the operator K_b will have a gap $(e_-(b), e_+(b))$ whose edges are Lipschitz functions of b on I.*

Remark. Denoting by $\delta b = b - b_0$, then according to our notations we have that $K_b = (K_{b_0})_{\delta b}$. It means that it is enough to prove spectral stability and Lipschitz properties near $b_0 = 0$.

We can complicate the setting by allowing the generating kernel to depend on b.

Corollary 2.4. *Assume that the generating kernel $K(\mathbf{x},\mathbf{x}';b)$ obeys all the spatial localization conditions of Theorem 2.3, uniformly in $b \in \mathbb{R}$. Moreover, assume that it also satisfies an extra condition:*

$$\sup_{\mathbf{x}'\in\Gamma} \sum_{\mathbf{x}\in\Gamma} |K(\mathbf{x},\mathbf{x}';b) - K(\mathbf{x},\mathbf{x}';b_0)| \leq C\, |b-b_0|, \quad |b-b_0| \leq 1. \tag{2.7}$$

Consider the family $\{K_b\}_{b\in\mathbb{R}}$ generated by $e^{ib\varphi(\mathbf{x},\mathbf{x}')}K(\mathbf{x},\mathbf{x}';b)$. Then Theorem 2.3 holds true for K_b.

Continuous Schrödinger operators. Let us consider the operator in $L^2(\mathbb{R}^2)$

$$H(b) := (\mathbf{p} - b\mathbf{a})^2 + V, \quad \mathbf{p} = -i\nabla_{\mathbf{x}}, \quad \mathbf{a}(\mathbf{x}) = (-x_2/2, x_1/2), \quad b \in \mathbb{R}. \tag{2.8}$$

where we assume that the scalar potential V is smooth and bounded together with all its derivatives on $\mathbb{R}^2$. This very strong condition is definitely not necessary for the result given below, but it simplifies the presentation. For the same reason we formulate the result only near $b_0 = 0$.

Theorem 2.5. *Assume that the spectrum of $H(0)$ has a finite and isolated spectral band σ_0, where $\sigma_0 = [s_-(0), s_+(0)]$. Then if $|b|$ is small enough, σ_0 will evolve into a still isolated spectral island $\sigma_b \subset \sigma(H(b))$. Denote by $s_-(b) := \inf \sigma_b$ and $s_+(b) := \sup \sigma_b$. Then these edges are Lipschitz at $b = 0$, i.e. there exists a constant C such that $|s_\pm(b) - s_\pm(0)| \leq C\ |b|$.*

Remark. We do not exclude the appearance of gaps inside σ_b. Moreover, the formulation of this result is slightly different from the one we gave in the discrete case. Here we look at the edges of a finite part of the spectrum, and not at the edges of a gap. In the discrete case both formulations are equivalent. However, our proof does not work in the continuous case if σ_0 is infinite.

2.2 Previous results and open problems

Spectrum stability is a fundamental issue in perturbation theory. It is well known that if W is relatively bounded to H_0, then the spectrum of $H_\lambda = H_0 + \lambda W$ is at a Hausdorff distance of order $|\lambda|$ from the spectrum of H_0. But this is in general not true for perturbations which are not relatively bounded. And the magnetic perturbation coming from a constant field is not relatively bounded, neither in the discrete nor in the continuous case.

With the notable exception of a recent paper by Nenciu [82], all previous results on the discrete case we are aware of deal with the situation in which $\Gamma = \mathbb{Z}^2$ and the generating kernel obeys $K(\mathbf{x}, \mathbf{x}') = k(\mathbf{x} - \mathbf{x}')$, where k is sufficiently fast decaying at infinity. Maybe the first proof of spectral stability of Harper operators is due to Elliott [31]. The result is refined in [17] where it is shown that the gap boundaries are $\frac{1}{3}$-Hölder continuous in b. Later results by Avron, van Mouche and Simon [4], Helffer and Sjöstrand [48, 49], and Haagerup and Rørdam [37] pushed the exponent up to $\frac{1}{2}$. In fact they prove more, they show that the Hausdorff distance between spectra behaves like $|b - b_0|^{\frac{1}{2}}$. These results are optimal in the sense that the Hölder constant is independent of the length of the eventual gaps, and it is known that these gaps can close down precisely like $|b - b_0|^{\frac{1}{2}}$ near rational values of b_0 [49, 46]. Note that Nenciu [82] proves a similar result for a much larger class of Harper-like operators. Many other spectral properties of Harper operators can be found in a paper by Herrmann and Janssen [52].

In the continuous case, the stability of gaps was first shown by Avron and Simon [3], and Nenciu [81]. Nenciu's result implicitly gives a $\frac{1}{2}$-Hölder continuity in b for the Hausdorff distance between spectra. Then in [12] the Hölder exponent of gap edges was pushed up to $\frac{2}{3}$.

The first proof of Lipschitz continuity of gap edges for Harper-like operators was given by Bellissard [5] (later on Kotani [65] extended his method to more general regular lattices and dimensions larger than two). The configuration space is $\Gamma = \mathbb{Z}^2$ and the generating kernel is of the form $K(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}-\mathbf{x}'; b)$, where $k(\mathbf{x}; b)$ decays polynomially in $|\mathbf{x}|$ and is allowed to depend smoothly on b. This extra-dependence is not central for our discussion, so we will consider that k is b independent. Bellissard's innovative idea uses in an essential way that the Harper operators generated by translation invariant and fast decaying kernels $k(\mathbf{x} - \mathbf{x}')$ can be written as linear combinations of magnetic translations:

$$K_b = \sum_{\gamma \in \mathbb{Z}^2} k(\gamma) W_b(\gamma),\ [W_b(\gamma)\psi](\mathbf{x}) = e^{ib\varphi(\mathbf{x},\gamma)}\psi(\mathbf{x} - \gamma), W_b(\gamma)W_b(\gamma') = e^{ib\varphi(\gamma,\gamma')}W_b(\gamma + \gamma').$$

Bellissard's crucial observation was that the C^* algebra $\mathcal{A}_{b_0+\delta}$ generated by $\{W_{b_0+\delta}(\gamma)\}_{\gamma\in\mathbb{Z}^2}$ is isomorphic with a sub-algebra of $\mathcal{A}_{b_0} \otimes \mathcal{A}_\delta$ which is generated by $\{W_{b_0}(\gamma) \otimes W_\delta(\gamma)\}_{\gamma\in\mathbb{Z}^2}$. Thus one can construct an operator $\widetilde{K}_{b_0+\delta}$ which is isospectral with $K_{b_0+\delta}$. The new operator lives in the space $l^2(\mathbb{Z}^2) \otimes L^2(\mathbb{R})$, and $\widetilde{K}_{b_0} = K_{b_0} \otimes \mathrm{Id}$. It turns out that it is more convenient to study the spectral edges of the new operator. The reason is that the singularity induced by the magnetic perturbation is hidden in the extra-dimension. But the proof breaks down in case of irregular lattices or if the generating kernel $K(\mathbf{x}, \mathbf{x}')$ is not just a function of $\mathbf{x} - \mathbf{x}'$.

Coming back to our proof, its crucial ingredient consists in expressing the magnetic phases with the help of the heat kernel of *a continuous Schrödinger operator*. Moreover, the proof in the discrete case also works for continuous kernels living on $\mathbb{R}^2$ and not just on lattices. This is what we use in the last step of the proof of Theorem 2.5 dealing with continuous magnetic Schrödinger operators.

A limitation of our method consists in the fact that the phases $\varphi(\mathbf{x}, \mathbf{x}')$ are generated by a constant magnetic field. A more general discrete problem was formulated by Nenciu in [82] where he proposed to replace the explicit formulas in (2.4) and (2.5) with more general real and antisymmetric phases obeying $\phi(\mathbf{x}, \mathbf{x}') = \overline{\phi(\mathbf{x}, \mathbf{x}')} = -\phi(\mathbf{x}', \mathbf{x})$ and

$$|\phi(\mathbf{x}, \mathbf{y}) + \phi(\mathbf{y}, \mathbf{x}') + \phi(\mathbf{x}', \mathbf{x})| \leq \text{area } \Delta(\mathbf{x}, \mathbf{y}, \mathbf{x}')$$

where $\Delta(\mathbf{x}, \mathbf{y}, \mathbf{x}')$ is the triangle generated by the three points. These phases appear very naturally in the continuous case, see [22, 23, 58, 68, 73, 74, 75, 80], where it is shown that if $\mathbf{a}(\mathbf{x})$ is the transverse gauge generated by a globally bounded magnetic field $|b(\mathbf{x})| \leq 1$, then $\phi(\mathbf{x}, \mathbf{x}')$ can be chosen to be the path integral of $\mathbf{a}(\mathbf{x})$ on the segment linking $\mathbf{x}'$ with $\mathbf{x}$. This is the same as the magnetic flux of b through the triangle generated by $\mathbf{x}$, $\mathbf{x}'$ and the origin.

Using a completely different proof method, Nenciu shows among other things in [82] that the gap edges are Lipschitz up to a logarithmic factor, and he conjectures that they are actually Lipschitz. His method relies on the theory of almost convex functions, and the result provided by this technique is optimal in the sense that it cannot be improved in order to get rid of the logarithm. A new idea would be necessary in order to prove Nenciu's Lipschitz conjecture.

Our current paper supports this conjecture because it provides examples of phases not coming from a constant magnetic field which still generate Lipschitz gap edges. Let us show this here.

Consider an irregular lattice $\Gamma \subset \mathbb{R}^2$ which is a local deformation of $\mathbb{Z}^2$, that is there exists a bijective map $F : \Gamma \to \mathbb{Z}^2$ such that $|F(\gamma) - \gamma| < \frac{1}{2}$. Define the phases $\widetilde{\varphi}(\mathbf{x}, \mathbf{x}') := \varphi(F^{-1}(\mathbf{x}), F^{-1}(\mathbf{x}'))$ where φ is given by (2.4).

Choose any self-adjoint operator $K \in B(l^2(\mathbb{Z}^2))$ given by a kernel $K(\mathbf{x}, \mathbf{x}')$ sufficiently fast decaying outside the diagonal. The same operator can be seen in $B(l^2(\Gamma))$ given by $\widetilde{K}(\gamma, \gamma') := K(F(\gamma), F(\gamma'))$. Thus the operator K_b generated by $K_b(\mathbf{x}, \mathbf{x}') := e^{ib\widetilde{\varphi}(\mathbf{x}, \mathbf{x}')} K(\mathbf{x}, \mathbf{x}')$ is unitary equivalent with an operator in $B(l^2(\Gamma))$ with a kernel

$$\widetilde{K}_b(\gamma, \gamma') := e^{ib\varphi(\gamma, \gamma')} \widetilde{K}(\gamma, \gamma').$$

In this case, we know from Theorem 2.3 that the edges of the spectral gaps of $\widetilde{K}_b$ and thus K_b will have a Lipschitz behavior. But the general case remains open.

3 Scattering theory of $2D$ particles subjected to long range magnetic fields

3.1 Two-dimensional purely magnetic Hamiltonians

A classical particle in a magnetic field is described by the Hamiltonian

$$h(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{2}(\boldsymbol{\xi} - \mathbf{a}(\mathbf{x}))^2, \quad (\mathbf{x}, \boldsymbol{\xi}) \in \mathbb{R}^{2n}. \tag{3.1}$$

The magnetic field $\mathbf{B}(\mathbf{x})$ is obtained from the vector potential $\mathbf{a}$ by exterior differentiation, $\mathbf{B}(\mathbf{x}) = d\mathbf{a}(\mathbf{x})$. Here we study the classical and quantum dynamics of a two dimensional particle in a magnetic field of the form

$$\mathbf{B}(\mathbf{x}) = \frac{b(\theta)}{r} dx_1 \wedge dx_2, \quad \mathbf{x} = (r\cos\theta, r\sin\theta) \in \mathbb{R}^2. \tag{3.2}$$

We are interested in orbits $(\mathbf{x}(t), \boldsymbol{\xi}(t))$ for which

$$\lim_{t\to\infty} r(t) = \infty \tag{3.3}$$

and hence in scattering theory. The decay rate $\langle \mathbf{x} \rangle^{-1}$ in (3.2) seems to be the borderline rate of decay for which we can be assured of (3.3) (at least for some range of energies). For if we take $\mathbf{B}(\mathbf{x}) = (b/r^\gamma) dx_1 \wedge dx_2$ with b a nonzero constant and $0 < \gamma < 1$, a vector potential satisfying $\mathbf{B}(\mathbf{x}) = d\mathbf{a}(\mathbf{x})$ is readily found and leads to the conservation laws

$$l = \frac{\partial h}{\partial \theta} = \text{Const}, \quad E = h = \frac{1}{2}\left(\frac{dr}{dt}\right)^2 + \frac{1}{2}\left(\frac{l}{r} - cr^{1-\gamma}\right)^2 = \text{Const}.$$

Here $c = \frac{b}{2-\gamma}$, l is the angular momentum and E is the energy. It follows that all orbits are confined to a bounded region of phase space. Indeed, Miller and Simon analyzed the corresponding quantum Hamiltonian and showed that its spectrum is pure point, dense in $[0, \infty)$ (for more details, see [27], Theorem 6.2).

On the other hand, much work over the last twenty years has been done in analyzing the quantum problem with $|\mathbf{B}(\mathbf{x})| = \mathcal{O}(\langle \mathbf{x} \rangle^{-1-\epsilon})$ with $\epsilon > 0$ (in any dimension ≥ 2). We briefly review known results in this case. Firstly, the existence part of wave operators for $1 < \gamma < \infty$ is covered by general results of Hörmander (see [54]) which hold in combination with a long-range scalar potential. The comparison dynamics used in [54] to construct a wave operator preserves the momentum (it is a refined Dollard-type dynamics). Asymptotic completeness was proved by Hörmander (using stationary methods) in [55], Chapter 30. In addition we mention here the work of Robert (see [88]) which also includes long-range scalar potentials. The wave operators in [88] are constructed using the stationary modifier of Isozaki-Kitada (see [59] for details). Then Roux and Yafaev revisited this problem in [93], and they also investigated the spectral properties of the corresponding scattering matrix S.

Secondly, the case $\gamma > 3/2$ was further investigated by Loss and Thaller in [69] and [70] for purely magnetic Schrödinger and Dirac operators where they prove existence and completeness for the ordinary Møller operators employing Enss' time-dependent approach. Then Nicoleau and Robert in [84] treat the Schrödinger problem for $\gamma > 3/2$ by using stationary scattering theory; in addition, they allow short-range scalar potentials. Enss (see [32]) extended their Schrödinger result to include long-range scalar potentials, giving a simplified proof of existence and asymptotic completeness of the modified Dollard wave operators. The modification here only uses the scalar and not the vector potentials. We mention that these results for $\gamma > 3/2$ can now be recovered as particular cases of the more general results in [93].

Scattering theory with $\gamma = 1$ (no decay on the vector potential) does not appear to be treated in the literature. Similar problems with homogeneous of degree zero electric potential have been considered by two of the authors in [51], [42]; see also a related work of Hassell, Melrose and Vasy in [41]. In those cases, the Hamiltonian is roughly $H = -\Delta + V(\mathbf{x}/|\mathbf{x}|)$, where V is defined on the unit sphere. The generic behavior for the classical orbits in this situation is that they are eventually trapped in the directions in which V has local extrema (in the quantum case the local maxima and saddle points are excluded), hence very roughly the trajectories are asymptotically straight.

The behavior for the two-dimensional magnetic case with $\gamma = 1$ turns out to be different (at least for the case treated in this paper). Assume that we are given a magnetic field which is homogeneous of degree -1 outside the unit disc, i.e. is given by $r^{-1}b(\theta)$ for $r \geq 1$. For the classical orbits staying outside the unit disc (for all large times) and with energy $E > E_b$ where

$$E_b = \max_{\theta \in [0,2\pi]} b^2(\theta)/2, \tag{3.4}$$

we have an "easy" Mourre estimate implying that their radial velocities eventually become positive, hence these orbits move to infinity. (We remark that when b is constant, E_b equals the mobility edge in the Miller-Simon model, i.e. that particular energy above which the spectrum is purely absolutely continuous while below it the spectrum is dense pure point.) A more detailed analysis under the additional condition that b is strictly negative (a similar analysis may be done for $b > 0$) shows that the asymptotic orbits are logarithmic spirals and not asymptotically straight as in the potential case. Moreover, we can even go below E_b with our considerations if b is not constant.

The main goal of the paper is to demonstrate analogous behavior in quantum mechanics. It is also possible to consider the case in which b has zeros and in particular the zero flux case $\int_0^{2\pi} b(\theta)d\theta = 0$. For the latter case the classical scattering orbits approach a direction in which $b(\theta) = 0$. When b changes sign but the flux is different from zero, both types of behavior may occur: some trajectories are drawn toward the half-lines defined by the zeroes of b while others will spiral.

There are indications of somewhat similar results in dimensions higher than two, although the geometry and analysis are more complicated.

3.2 Classical mechanics: preliminaries and main results

Our system consists here of a classical particle (with charge -1) confined to a plane and subjected to a magnetic field $\mathbf{B}$ which is assumed to be homogeneous of degree -1. As usual, $\mathbf{B}$ is "orthogonal" to the plane in which the particle moves so it has only one nonzero component (the third one) which is of the form $B(\mathbf{x}) = b(\theta)/r$. We assume that b is smooth and negative. The associated transverse magnetic vector potential is $\mathbf{a}(\mathbf{x}) = (-\sin(\theta), \cos(\theta))b(\theta)$.

The corresponding classical Hamiltonian function is (in polar coordinates)

$$h(r, \theta; \rho, l) := \frac{1}{2}\rho^2 + \frac{1}{2}\left(\frac{l}{r} - b(\theta)\right)^2, \tag{3.5}$$

where $\rho = \frac{\mathbf{x}}{|\mathbf{x}|} \cdot (\boldsymbol{\xi} - \mathbf{a})$ is the radial velocity and $l = x_1p_2 - x_2p_1$ is the canonical angular momentum. The Hamilton equations for r and θ are

$$\frac{dr}{dt} = \frac{\partial h}{\partial \rho} = \rho, \quad \frac{d\theta}{dt} = \frac{\partial h}{\partial l} = \frac{1}{r}\left(\frac{l}{r} - b\right). \tag{3.6}$$

The Hamilton equations for ρ and l are

$$\frac{d\rho}{dt} = -\frac{\partial h}{\partial r} = \left(\frac{l}{r} - b(\theta)\right)\frac{l}{r^2} \tag{3.7}$$

and

$$\frac{dl}{dt} = -\frac{\partial h}{\partial \theta} = \left(\frac{l}{r} - b(\theta)\right)b'(\theta). \tag{3.8}$$

Let us introduce the transverse velocity $\xi := \frac{l}{r} - b$, which obeys the equations

$$\frac{d\theta}{dt} = \frac{\xi}{r}, \quad \frac{d\xi}{dt} = -\frac{\xi + b}{r}\rho. \tag{3.9}$$

Since h in (3.5) does not depend on t, the energy is conserved; that is, on a given trajectory one has

$$\rho^2(t) + \xi^2(t) = 2E. \tag{3.10}$$

3.2.1 An attractive Lagrangian manifold

We will now discuss various results obtained in the classical framework. Apart from their own intrinsic interest they serve as motivation for our main result in quantum mechanics (see Theorem 3.1 below).

Define the extended configuration space

$$\mathcal{A} := \{\overline{x} = (t, r, \theta) : \ t > 0, \ r > 0, \ \theta \in \mathbb{T}\},$$

and consider the function

$$\overline{h}(\overline{x}, \overline{\eta}) := \tau + h(r, \theta; \rho, l), \qquad \overline{x} \in \mathcal{A}, \qquad \overline{\eta} = (\tau, \rho, l).$$

We introduce a symplectic form on $T^*\mathcal{A}$ given by

$$d\mathbf{x} \wedge d\boldsymbol{\xi} + dt \wedge d\tau = d\theta \wedge dl + dr \wedge d\rho + dt \wedge d\tau.$$

We construct a solution S (defined on $\mathcal{A}$) to the equation $\overline{h}(\overline{x}, \nabla S) = 0$, which is nothing but the Hamilton-Jacobi equation

$$\partial_t S + h(r, \theta; \partial_r S, \partial_\theta S) = 0.$$

Consider the associated Lagrangian manifold

$$\mathcal{L} := \{\overline{z} = (\overline{x}, \overline{\eta}) : \ \overline{x} \in \mathcal{A}, \ \overline{\eta} = \nabla S\} \subseteq T^*\mathcal{A}.$$

Then $\mathcal{L}$ is invariant under the flow corresponding to $\overline{h}$, which when restricted to $\mathcal{L}$ can be written

$$\frac{d\tilde{r}}{dt} = \partial_r S(t, \tilde{r}, \tilde{\theta}), \quad \frac{d\tilde{\theta}}{dt} = \tilde{r}^{-1}[\tilde{r}^{-1}\partial_\theta S(t, \tilde{r}, \tilde{\theta}) - b(\tilde{\theta})] \tag{3.11}$$

(with the momenta satisfying $\overline{\eta} = \nabla S$). It is natural to ask how closely an orbit originating off $\mathcal{L}$ is approximated by solutions of the equations (3.11). One can indeed show that $\mathcal{L}$ is attractive for all energies above a certain threshold $E_d \leq E_b$. More precisely, assume that $(r, \theta; \rho, l)$ is a solution for the symbol h with energy $E > E_d$ which exists for all $t > 0$. Then for any $\delta > 0$, the quantities $E + \partial_t S$, $\rho - \partial_r S$, $(l - \partial_\theta S)/r$ are all $\mathcal{O}(t^{-1+\delta})$ as $t \to \infty$. Here and henceforth $t \to \infty$ means $t \to +\infty$.

Even though (3.11) may seem somewhat complicated at first glance, we obtain that $\tilde{\theta}(t)$ is strictly increasing and grows logarithmically in time. This allows us to consider the radius as a function of the angle $r(\tilde{\theta}) = \tilde{r}(t(\tilde{\theta}))$ and eventually prove that

$$\ln r = C(E)\tilde{\theta} + R(E, \tilde{\theta}) \tag{3.12}$$

where $C(E)$ is a positive increasing function and R is 2π-periodic in $\tilde{\theta}$. Moreover, $C(E) \searrow 0$ when $E \searrow E_d$, and one can prove that $C(E)/\sqrt{2E}$ approaches a positive constant when E increases to infinity. With $R(E, \tilde{\theta}) = R(E)$ independent of $\tilde{\theta}$, (3.12) is the equation for the so-called logarithmic spiral. On the other hand, if the energy equals E_d, we can construct closed classical orbits which can be put arbitrarily far away from the origin. This indicates that even if there still exist scattering states below E_d, the mechanism through which they go to infinity is different. What we know is that in the constant b case, according to the Miller-Simon model, the spectrum below $E_d = E_b = b^2/2$ is pure point, thus no scattering is possible.

3.2.2 Classical comparison dynamics and asymptotic completeness

Motivated by the above considerations, we introduce

$$\gamma_1 = \rho - \partial_r S, \ \gamma_2 = \frac{l - \partial_\theta S}{r}, \ h_a = h - \frac{1}{2}\left(\gamma_1^2 + \gamma_2^2\right), \ \overline{h}_a(\overline{x}, \overline{\eta}) = \tau + h_a. \tag{3.13}$$

The Hamilton equations for (r, θ) obtained from h_a coincide with the system in (3.11). Moreover, the dynamics of $\overline{h}$ and $\overline{h}_a$ coincide on $\mathcal{L}$, hence the dynamics generated by $\overline{h}_a$ should approximate the real one.

To fix notation, denote by $\mathbf{q}_{a,t} = (\rho_a(t), l_a(t))$ the "momenta" generated by h_a; the flow generated by h_a is denoted with $\mathbf{V}_{a,t}$ and acts as $\mathbf{V}_{a,t}(r_1, \theta_1; \mathbf{q}_{a,1}) = (\mathbf{v}_t; \mathbf{q}_{a,t})$. The flow generated by h is denoted by $\mathbf{V}_t$ and $\mathbf{V}_t(r(1), \theta(1); \rho(1), l(1)) = (r(t), \theta(t); \rho(t), l(t))$ gives the classical solutions of the true dynamics.

Let $\mathbf{W}_{a,t} = \mathbf{V}_{a,t}^{-1}$ denote the inverse flow (explicitly, writing the equations for $\mathbf{V}_{a,t}$ as $d\mathbf{x}/dt = \mathbf{F}(t, \mathbf{x})$, the equations for $\mathbf{W}_{a,t}$ are $d\mathbf{z}/ds = -\mathbf{F}(t+1-s, \mathbf{z})$ where $\mathbf{z}(1) = \mathbf{V}_{a,t}(\mathbf{x})$ and $\mathbf{W}_{a,t}(\mathbf{z}(1)) = \mathbf{z}(t) = \mathbf{x}$). The obvious interpretation of $\mathbf{W}_{a,t}$ is that it gives back the initial conditions used in computing $\mathbf{V}_{a,t}$.

Classical asymptotic completeness would be the existence of

$$\Omega_+ := \lim_{t\to\infty} \mathbf{W}_{a,t} \circ \mathbf{V}_t, \tag{3.14}$$

and the limit represents the initial data one should put into the dynamics $\mathbf{V}_{a,t}$ generated by h_a in order to get a good approximation to any true orbit $\mathbf{V}_t$.

Although we do not prove the existence of the above limit, we do prove for energies larger than E_d the existence of

$$\Pi\Omega_+ := \lim_{t\to\infty} \Pi\mathbf{W}_{a,t} \circ \mathbf{V}_t, \tag{3.15}$$

where Π projects on the configuration space of (r, θ)'s. Note for the flow $\mathbf{V}_{a,t}$ that the equations for the configuration space part $\mathbf{v}_t$ in (3.11) are completely decoupled from the momenta $\mathbf{q}_{a,t}$, and that $\mathbf{W}_{a,t}$ consequently enjoys the same property. In fact denoting the inverse of $\mathbf{v}_t$ by $\mathbf{w}_t$, we obtain $\mathbf{w}_t = \Pi\mathbf{W}_{a,t}$ simplifying the right hand side of (3.15). We denote by (r_+, θ_+) the limit in (3.15) and call the entries the asymptotic radius and angle, respectively. Intuitively, when put into the direct flow $\mathbf{v}_t$ this limit provides us with a good approximation of the configuration space component of the true orbit at time t.

3.3 Quantum mechanics: preliminaries and main results

Motivated by its classical counterpart, we choose a magnetic vector potential (we denote $\mathbf{x} = (r, \theta)$)

$$\mathbf{a}(\mathbf{x}) = (-\sin\theta, \cos\theta) b(\theta) m_+(r) \in C^\infty(\mathbb{R}^2), \tag{3.16}$$

where $0 \le m_+ \le 1$ is a smooth cut-off function equal to zero if $r \le \frac{1}{4}$ and equal to one if $r \ge \frac{1}{2}$. Notice that $\mathbf{a}$ is homogeneous of degree zero outside the unit disc while the corresponding magnetic field is homogeneous of degree -1.

The classical Hamiltonian from (3.5) now becomes an operator

$$\begin{aligned} H = \frac{1}{2}(\mathbf{p} - \mathbf{a})^2 &= \frac{1}{2}\mathbf{p}^2 - \frac{1}{2}(\mathbf{p}\cdot\mathbf{a} + \mathbf{a}\cdot\mathbf{p}) + \frac{1}{2} m_+^2 b^2 \\ &= -\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{1}{2r}\frac{\partial}{\partial r} + \frac{1}{2}\left(\frac{L}{r} - m_+(r) b(\theta)\right)^2, \end{aligned} \tag{3.17}$$

which is essentially self-adjoint on $C_0^\infty(\mathbb{R}^2)$ with the domain $H^2(\mathbb{R}^2)$ (we denoted the angular momentum $L = -i\partial_\theta$).

We will often identify $L^2(\mathbb{R}^2)$ with $L^2(\mathbb{R}_+ \times \mathbb{T})$ through the unitary transformation

$$L^2(\mathbb{R}^2) \ni f(r,\theta) \to r^{1/2} f(r,\theta) \in L^2(\mathbb{R}_+ \times \mathbb{T}). \tag{3.18}$$

As an operator on $L^2(\mathbb{R}_+ \times \mathbb{T})$ the Hamiltonian H takes the form

$$H = -\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{1}{8r^2} + \frac{1}{2}\left(-\frac{i}{r}\frac{\partial}{\partial\theta} - m_+(r)b(\theta)\right)^2. \tag{3.19}$$

We will see that there is an "easy" Mourre estimate with the generator of dilations $A = 1/2(\mathbf{p}\cdot\mathbf{x} + \mathbf{x}\cdot\mathbf{p})$ as conjugate operator,

$$i[H,A] \geq H - b^2(\theta)/2 + K, \tag{3.20}$$

with K being relatively compact to H. Indeed, after easy computations employing polar coordinates one obtains

$$i[\mathbf{p}\cdot\mathbf{a}, \mathbf{p}\cdot\mathbf{x}] = i[\mathbf{p}\cdot\mathbf{a}, \mathbf{x}\cdot\mathbf{p}] = \mathbf{p}\cdot(\mathbf{a}+\mathbf{a}_c),$$

where $\mathbf{a}_c(\mathbf{x}) = (\sin(\theta), -\cos(\theta))b(\theta)rm'_+(r)$ is smooth and compactly supported. Then

$$\begin{aligned} i[H,A] &= \mathbf{p}^2 - (1/2)\mathbf{p}\cdot(\mathbf{a}+\mathbf{a}_c) - (1/2)(\mathbf{a}+\mathbf{a}_c)\cdot\mathbf{p} + \mathbf{a}\cdot\mathbf{a}_c \\ &= H - \frac{(\mathbf{a}-\mathbf{a}_c)^2}{2} + \frac{1}{2}(\mathbf{p}-\mathbf{a}_c)^2 \\ &\geq H - \frac{(\mathbf{a}-\mathbf{a}_c)^2}{2}. \end{aligned} \tag{3.21}$$

Thus we obtain (3.20).

This computation indicates that above $E_b = \max|b|^2/2$ things are somewhat "easier", just as they are in the classical case. If $b < 0$ is not constant, we can go below E_b down to the critical energy E_d by using a more involved conjugate operator; notice though that $E_d = E_b$ when b is constant.

Hence, according to Mourre (see [78]), the interval (E_d, ∞) is a subset of the absolutely continuous spectrum and does not contain singular continuous spectrum. Possible embedded eigenvalues in this interval are discrete and may at most accumulate at E_d.

We introduce a comparison dynamics roughly generated by the quantization of the symbol h_a of (3.13). A similar approximate dynamics was used in [42]. This type of dynamics is motivated by a related one introduced by Yafaev ([104]); see also [28] and [93]. We can define a family of isometries

$$L^2((E_d,\infty)\times\mathbb{T}) \ni f \mapsto U_0(t)f \in L^2(\mathbb{R}_+\times\mathbb{T}),\ t \geq 1,$$

by

$$[U_0(t)f](r,\theta) = e^{iS(t,r,\theta)} J_t^{1/2}(r,\theta) f\left(-(\partial_t S)(1,\mathbf{w}_t(r,\theta)), \theta_1(t,r,\theta)\right), \tag{3.22}$$

where J_t is the Jacobian determinant arising from the various changes of variables which makes $U_0(t)$ an isometry.

With this comparison dynamics we have existence of the direct wave operator (denoted by Ω_+^d) and completeness (this result can be extended in order to include short-range perturbations):

Theorem 3.1. *Denote by* $\mathcal{H}_{E_d} := \mathbf{1}_{(E_d,\infty)\setminus\sigma_{pp}(H)}(H)L^2(\mathbb{R}_+ \times \mathbb{T})$. *Then the following limits exist and define unitary operators which are mutually inverse*

$$\begin{aligned} \Omega_+^d &= s - \lim_{t\to\infty} e^{itH}U_0(t) : L^2((E_d,\infty)\times\mathbb{T}) \mapsto \mathcal{H}_{E_d}, \\ \Omega_+ &= s - \lim_{t\to\infty} U_0^*(t)e^{-itH} : \mathcal{H}_{E_d} \mapsto L^2((E_d,\infty)\times\mathbb{T}). \end{aligned} \tag{3.23}$$

We have the existence of the asymptotic observables defined on $\mathcal{H}_{E_d}$:

$$\begin{aligned} r_+ &:= s.r. - \lim_{t\to\infty} e^{itH} M\left(r_1(t,\cdot,\cdot)\right) e^{-itH}, \\ e^{i\theta_+} &:= s.r. - \lim_{t\to\infty} e^{itH} M\left(e^{i\theta_1(t,\cdot,\cdot)}\right) e^{-itH}, \end{aligned} \tag{3.24}$$

where the notation $M(\cdot)$ signifies multiplication operator and $s.r. - \lim$ means strong resolvent limit. These operators can be expressed in terms of the wave operators of Theorem 3.1; they represent quantum analogs of the classical asymptotic radius and angle, r_+ and θ_+, discussed previously.

In the case where $b < 0$ does not depend on θ we have the result $E_d = E_b = b^2/2$ in (3.23) and (3.24), cf. the Miller-Simon result, and the formula for $U_0(t)$ reads

$$[U_0(t)f](r,\theta) = \exp\left\{ i\frac{r^2}{2t} - i\frac{b^2 t}{2} \right\} \sqrt{\frac{r}{t^2}} f\left(\frac{r^2}{2t^2} + \frac{b^2}{2}, \theta + b\frac{t}{r}\ln(t) \right). \tag{3.25}$$

Moreover in this case the term $R(E,\tilde{\theta})$ in (3.12) is indeed constant in $\tilde{\theta}$.

Heuristically, our comparison dynamics moves the support of an initial state of sufficiently high energy along the integral curves of (3.11) which are spirals moving counterclockwise to infinity with the radius proportional to t and the angle proportional to $\ln t$, cf. (3.12). (Clearly this picture is confirmed by (3.25) in the constant b case.) Asymptotic completeness means that any state with high enough energy can be thought of (asymptotically in time) as a superposition of translates along these logarithmic spirals.

3.4 Gauge covariance of the wave operators and unitarity of the S-matrix

Using an argument similar to the one which led to our "outgoing" wave operators (see (3.23)), we can also give an approximate dynamics at negative times (see Section 9 for details), and consequently define some "incoming" wave operators (denoted by Ω_-^d and Ω_-). It can be shown that Ω_-^d maps unitarily $L^2((E_d,\infty)\times\mathbb{T})$ onto $\mathcal{H}_{E_d}$ and Ω_- is its inverse.

The non-trivial fact that needs to be shown is that the E_d for negative times is the same as that for positive times. One might feel that this follows from time reversal invariance. But it does not seem to. In fact time invariance is different with a magnetic field. If the time reversed orbit is $\mathbf{x}_r(t) := \mathbf{x}(-t)$, then the time reversed velocity is $\mathbf{v}_r(t) := \dot{\mathbf{x}}_r(t) = -\dot{\mathbf{x}}(-t)$. If the force is given only by a scalar potential, then $(\mathbf{x}_r, \mathbf{v}_r)$ satisfy Newton's equations. But if there is a magnetic field $\mathbf{B}(\mathbf{x})$ this also needs to be changed to $-\mathbf{B}(\mathbf{x})$.

Hence the S-matrix defined as $\left(\Omega_+^d\right)^* \Omega_-^d$ is unitary on $L^2((E_d, \infty) \times \mathbb{T})$. Our wave operators have a simple transformation law under a time independent gauge transformation. If

$$\mathbf{a} \to \mathbf{a} + \nabla f,\ H \to e^{if} H e^{-if} \text{ and } S \to S + f,$$

then

$$\Omega_\pm^d \to e^{if} \Omega_\pm^d.$$

It follows that the S-matrix is gauge invariant.

In the gauge we use here there is no asymptotic momentum and we conjecture that there does not exist a gauge where an asymptotic momentum exists. This would mean that no momentum preserving approximate dynamics is available. This partially motivates our choice of approximate dynamics (3.22) which is not momentum preserving. For a comparative discussion of various types of wave operators as used in [54], [59] and [104], see [28].

4 Thermodynamic behavior of large magnetic quantum systems

4.1 Diamagnetic expansions for perfect quantum gases: Gibbs semigroups

The magnetic properties of a charged perfect quantum gas in the independent electron approximation and confined to a box Λ have been extensively studied in the literature. One of the central problems has been to establish the thermodynamic limit for the magnetization and magnetic susceptibility, see e.g. [1], [2], [13], [14] ,[21], [20], [72] and references therein.

Briefly, the technical question is whether the thermodynamic limit ($\Lambda \to \mathbb{R}^3$) commutes with the derivatives of the grand-canonical pressure with respect to the external constant magnetic field B.

A general way of proving the thermodynamic limit has been outlined in [13] and [20], and the main ingredient consisted in applying the magnetic perturbation theory to a certain Gibbs semigroup. The strategy of the proof, which works not only for the first two derivatives, but also for derivatives of all orders, was explained in [13]. In [14] we proved in detail the pointwise thermodynamic limit near $z = 0$, and the main ideas of this proof will be explained in the next subsection. Here we start by explaining how we can obtain the uniform bounds on compacts needed in order to apply the Vitali Convergence Theorem (see [103]).

Now let us formulate the mathematical problem. The box which contains the quantum gas will be the cube $\Lambda \subset \mathbb{R}^3$ of side length $L > 0$ centered at 0. The constant magnetic field is $\mathbf{B} = (0, 0, B)$, with $B \geq 0$, oriented parallel to the third component of the canonical basis in $\mathbb{R}^3$.

We associate to $\mathbf{B}$ the magnetic vector potential $B\mathbf{a}(\mathbf{x}) = \frac{B}{2}(-x_2, x_1, 0)$ and the cyclotronic frequency $\omega = \frac{e}{c}B$. In the rest of the paper, ω will be a real parameter. The one particle Hamiltonian we consider is the self-adjoint operator densely defined in $L^2(\Lambda)$:

$$H_L(\omega) := \frac{1}{2}(-i\nabla - \omega\mathbf{a})^2, \tag{4.1}$$

corresponding to Dirichlet boundary conditions.

One denotes by $B_1(L^2(\Lambda))$ the Banach space of trace class operators. At $\omega \geq 0$ fixed, the magnetic Schrödinger operator $H_L(\omega)$ generates a Gibbs semigroup $\{W_L(\beta, \omega)\}_{\beta \geq 0}$ where:

$$W_L(\beta, \omega) := e^{-\beta H_L(\omega)}, \quad \|W_L(\beta, \omega)\|_{B_1} \leq \frac{L^3}{(2\pi\beta)^{\frac{3}{2}}}, \quad \beta > 0. \tag{4.2}$$

Now let us introduce the grand-canonical formalism. Let $\beta = 1/(kT) > 0$ be the inverse temperature, $\mu \in \mathbb{R}$ the chemical potential and $z = e^{\beta\mu}$ the fugacity. Let K be a compact included in the domain $D_+ := \mathbb{C} \setminus [e^{\frac{\beta\omega}{2}}, \infty[$ for the Bose statistics and $D_- := \mathbb{C} \setminus]-\infty, -e^{\frac{\beta\omega}{2}}]$ for the Fermi case.

Fix $\omega_0 > 0$ and a compact real interval Ω containing ω_0. For a fixed $\beta > 0$, one can find a simple, positively oriented, closed contour $\mathcal{C}_K \subset D_\pm$ whose interior does not contain 1 in the Bose case or -1 in the Fermi case, and such that

$$\sup_{L>1} \sup_{\omega\in\Omega} \sup_{\xi\in\mathcal{C}_K} \sup_{z\in K} \left\| [\xi - zW_L(\beta,\omega)]^{-1} \right\| = M < \infty. \tag{4.3}$$

Details may be found in [21] for the Bose case, but the main idea is that the spectrum of $W_L(\beta,\omega)$ is always contained in the interval $[0, e^{-\beta\omega/2}]$ and one can apply the spectral theorem.

We then can express the grand canonical pressure at ω_0 as follows (see e.g. [21] for the Bose case):

$$P_L(\beta, z, \omega_0) = \frac{-\epsilon}{2i\pi\beta L^3} \int_{\mathcal{C}_K} d\xi \, \frac{\ln(1-\epsilon\xi)}{\xi} \mathrm{Tr}\left[(\xi - zW_L(\beta,\omega_0))^{-1} zW_L(\beta,\omega_0) \right]. \tag{4.4}$$

where $\epsilon = 1$ for the Bose gas, and $\epsilon = -1$ for the Fermi gas.

For $\omega \in \mathbb{R}$, $\xi \in \mathcal{C}_K$ and $z \in K$, introduce the operator:

$$g_L(\beta, z, \xi, \omega) := [\xi - zW_L(\beta,\omega)]^{-1} zW_L(\beta,\omega). \tag{4.5}$$

This is a trace class operator which obeys (use (4.3) and (4.2)):

$$\|g_L(\beta,\omega,\xi,\omega)\|_{B_1} \leq (\sup_{z\in K}|z|) \, \frac{L^3 M}{(2\pi\beta)^{\frac{3}{2}}}. \tag{4.6}$$

uniformly in $\omega \in \Omega$. According to the next theorem, the map $\omega \to W_L(\beta,\omega)$ is a B_1-entire operator valued function in ω (this result was first obtained in [1] and then refined in [14]):

Theorem 4.1. *Let $\beta > 0$. Then the map $\mathbb{R} \ni \omega \to W_L(\beta,\omega) \in B_1(L^2(\mathbb{R}^3))$ is real analytic. For each open set $\mathcal{K}$ whose closure is compact and $\overline{\mathcal{K}} \subset \mathbf{D}_\epsilon$, $\epsilon = -1, +1$, there exists an open neighborhood $\mathcal{N}$ of the real axis such that the pressure at finite volume $P_L(\beta, z, \omega)$ is analytic w.r.t. (ω, z) on $\mathcal{N} \times \mathcal{K}$.*

Using (4.3) one can show that the map

$$]0,\infty[\ni \omega \mapsto \mathrm{Tr}\; g_L(\beta, z, \xi, \omega) \in \mathbb{C}$$

is smooth, with derivatives which are uniformly bounded in ξ and z. Thus for every $N \geq 1$ and $z \in K$ we can define the generalized susceptibilities at ω_0 by

$$\begin{aligned} \chi_L^N(\beta, z, \omega_0) &:= \frac{\partial^N P_L}{\partial \omega^N}(\beta, z, \omega_0) \\ &= \frac{-\epsilon}{2i\pi\beta L^3} \int_{\mathcal{C}_K} d\xi \, \frac{\ln(1-\epsilon\xi)}{\xi} \, \frac{\partial^N \mathrm{Tr}\; g_L}{\partial \omega^N}(\beta, z, \xi, \omega_0). \end{aligned} \tag{4.7}$$

From this discussion one can see that the pressure as well $\chi_L^N(\beta,\cdot,\omega_0), N\geq 1$ are analytic functions on D_+ (or D_-). If $|z|<1$, then for every $N\geq 0$ we have:

$$\chi_L^N(\beta,\omega,z)=\frac{\epsilon}{\beta|\Lambda_L|}\sum_{k\geq 1}\frac{(-\epsilon z)^k}{k}\quad \mathrm{Tr}\left\{\frac{\partial^N W_L(k\beta,\omega)}{\partial\omega^N}\right\}. \tag{4.8}$$

Now let us describe the case when $L=\infty$. Denote by $W_\infty(\beta,\omega),\beta\geq 0$ the semigroup generated by $H_\infty(\omega)$. Then $W_\infty(\beta,\omega)$ has an explicit integral kernel $G_\infty(\mathbf{x},\mathbf{x}';\beta,\omega)$ whose diagonal satisfies:

$$G_\infty(\mathbf{x},\mathbf{x};\beta,\omega)=\frac{1}{(2\pi\beta)^{3/2}}\frac{\omega\beta/2}{\sinh(\omega\beta/2)},\quad \forall\mathbf{x}\in\mathbb{R}^3. \tag{4.9}$$

Note that the right hand side is independent of $\mathbf{x}$. Let $\beta>0,\omega\geq 0$ and $|z|<1$. In view of (4.8), define:

$$P_\infty(\beta,z,\omega):=\frac{\epsilon}{\beta}\sum_{k\geq 1}\frac{(-\epsilon z)^k}{k}G_\infty(\mathbf{0},\mathbf{0};k\beta,\omega), \tag{4.10}$$

which is well defined because of the estimate $\sinh(t)\geq t$ if $t\geq 0$. One can in fact write (see [2]):

$$P_\infty(\beta,z,\omega_0)=\omega_0\frac{1}{(2\pi\beta)^{3/2}}\sum_{k=0}^{\infty}f_{3/2}^{\epsilon}\left(ze^{-(k+1/2)\omega_0\beta}\right), \tag{4.11}$$

where $f_\sigma^\epsilon(\zeta)$ are the usual Bose (or Fermi) functions for $\epsilon=1$ (or $\epsilon=-1$):

$$f_\sigma^\epsilon(\zeta):=\frac{\zeta}{\Gamma(\sigma)}\int_0^\infty dt\,\frac{t^{\sigma-1}e^{-t}}{1-\zeta\epsilon e^{-t}}, \tag{4.12}$$

analytic in $\mathbb{C}\setminus[1,\infty[$ (or $\mathbb{C}\setminus]-\infty,-1]$) if $\epsilon=1$ (or $\epsilon=-1$). If $|\zeta|<1$, they are given by the following expansion:

$$f_\sigma^\epsilon(\zeta)=\sum_{n=1}^{\infty}\frac{\epsilon^{n-1}\zeta^n}{n^\sigma}\ .$$

We can verify that for any $N\geq 0$, the multiple derivative $\partial_\omega^N P_\infty(\beta,\cdot,\omega_0)$ exists and defines an analytic function on D_+ (or D_-). The main result of [14] establishes the following pointwise convergence:

Theorem 4.2. *Fix $N\geq 1$ and define*

$$\chi_\infty^N(\beta,z,\omega):=\frac{\partial^N P_\infty}{\partial\omega^N}(\beta,z,\omega). \tag{4.13}$$

Then if $|z|<1$ we have the equality:

$$\chi_\infty^N(\beta,z,\omega)=\frac{\epsilon}{\beta}\sum_{k\geq 0}\frac{(-\epsilon z)^k}{k}\frac{\partial^N G_\infty}{\partial\omega^N}(\mathbf{0},\mathbf{0};k\beta,\omega), \tag{4.14}$$

and moreover,

$$\lim_{L\to\infty} \chi_L^N(\beta, z, \omega,) = \chi_\infty^N(\beta, z, \omega) \tag{4.15}$$

uniformly on $[\beta_0, \beta_1] \times [\omega_0, \omega_1]$, $0 < \beta_0 < \beta_1 < \infty$ *and* $0 < \omega_0 < \omega_1 < \infty$.

Remember that we want to apply the Vitali Convergence Theorem (see [103] or [13]). Therefore, in order to conclude that $\chi_L^N(\beta, z, \omega_0)$ converges uniformly to $\chi_\infty^N(\beta, z, \omega_0)$ for all $z \in K$, the only remaining point is to get the uniform boundedness with respect to L. More precisely, we prove the following theorem:

Theorem 4.3. *For all* $N \geq 1$, *for all* $\beta > 0$ *and for all* $\omega > 0$,

$$\sup_{L>1} \sup_{z\in K} \left|\chi_L^N(\beta, z, \omega)\right| \leq \text{ const}(\beta, K, \omega, N). \tag{4.16}$$

Then putting this together with the pointwise convergence result near $z = 0$ of Theorem 4.2, the final conclusion is:

$$\lim_{L\to\infty} \sup_{z\in K} \left|\chi_L^N(\beta, z, \omega_0) - \chi_\infty^N(\beta, z, \omega_0)\right| = 0. \tag{4.17}$$

Remark 4.4. Having uniform convergence (4.17) with respect to z allows us to prove the existence of the thermodynamic limit for canonical susceptibilities (see [13, 20]).

Note that Theorem 4.3 is an immediate consequence of the following estimate:

$$\sup_{\xi\in\mathcal{C}_K} \sup_{z\in K} \left|\frac{\partial^N \text{Tr } g_L}{\partial\omega^N}(\beta, \xi, z, \omega_0)\right| \leq L^3 \,\text{const}(\beta, K, N, \omega_0), \tag{4.18}$$

which implies via (4.7) that the generalized susceptibilities are uniformly bounded in L.

4.1.1 The strategy

Here we omit the parameters ξ and z in the definition of g_L in order to simplify notation. Fix $\beta > 0$ and $\omega_0 \geq 0$. Let $\Omega \subset \mathbb{R}$ be a compact interval containing ω_0. If $\omega \in \Omega$, we denote by $\delta\omega := \omega - \omega_0$. The main idea of the proof is to derive an equality of the following type:

$$\text{Tr } g_L(\beta, \omega) = \text{Tr } g_L(\beta, \omega_0) + \sum_{j=1}^{N} (\delta\omega)^j a_j(\beta, \omega_0) + (\delta\omega)^{N+1} \mathcal{R}_L(\beta, \omega, N), \tag{4.19}$$

where the coefficients $a_j(\beta, \omega_0)$ grow at most like L^3 uniformly in ξ and z, while the remainder $\mathcal{R}_L(\beta, \cdot, N)$ is a smooth function near ω_0. Then since we know that Tr $g_L(\beta, \cdot)$ is smooth, we must have

$$\frac{\partial^N \text{Tr } g_L}{\partial\omega^N}(\beta, \omega_0) = N! a_N(\beta, \omega_0),$$

and this would finish the proof. In order to achieve this program, we will have to do two things.

First step: with the help of magnetic perturbation theory we find a regularized expansion in $\delta\omega$ for g_L of the form

$$g_L(\beta,\omega) = \sum_{n=0}^{N} (\delta\omega)^n g_{L,n}(\beta,\omega) + R_{L,N}(\beta,\omega,N), \tag{4.20}$$

which holds in the sense of trace class operators, and the remainder has the property that $\frac{1}{(\delta\omega)^{N+1}} R_{L,N}(\beta,\omega)$ is smooth near ω_0 in the trace class topology. The operator-coefficients $g_{L,n}(\beta,\omega)$ *will still depend on* ω, but in a more convenient way. That is, they are sums, products, or integrals of products of *magnetic regularized operators*.

Second step: show that for each $0 \leq n \leq N$ we can write

$$\mathrm{Tr}\; g_{L,n}(\beta,\omega) = \sum_{j=0}^{N} (\delta\omega)^j s_{L,j,n}(\beta,\omega_0) + (\delta\omega)^{N+1} \mathcal{R}_{L,N}(\beta,\omega,N), \tag{4.21}$$

where the remainder $\mathcal{R}_{L,n}(\beta,\cdot)$ is smooth near ω_0. Now the coefficients $s_{L,j,n}(\beta,\omega_0)$ are finally independent of ω, and grow at most like L^3.

Finally, if we combine (4.21) with (4.20), we immediately obtain (4.19).

Now let us discuss why a more direct approach only based on trace norm estimates cannot work. Recall that the map $\omega \to W_L(\beta,\omega) \in B_1$ is real analytic, hence $\frac{\partial^N W_L}{\partial \omega^N}$ is well defined in $B_1(L^2(\Lambda))$, and we have the estimate (see [1] and [14]) :

$$\left\| \frac{1}{N!} \frac{\partial^N W_L}{\partial \omega^N}(\beta,\omega_0) \right\|_{B_1} \leq c_N \frac{L^{3+N} (1+\beta)^{sN}}{\beta^{\frac{3}{2}} \left[\frac{N-1}{4}\right]!}, \tag{4.22}$$

where c_N is a positive constant which depends on N, ω_0 and s. Now if we use the Leibniz rule of differentiation for the product which defines the operator $g_L(\beta,\omega)$ (see (4.5)), and estimate traces by trace norms we obtain:

$$\left| \frac{\partial^N \mathrm{Tr}\; g_L}{\partial \omega^N}(\beta,\omega_0) \right| \leq \left\| \frac{\partial^N g_L}{\partial \omega^N}(\beta,\omega_0) \right\|_{B_1} \leq L^{3+N} \mathrm{const}\,(\beta,K,\omega_0,N). \tag{4.23}$$

This is definitely not good enough, and we have to find a more convenient expansion, as described in (4.21).

4.1.2 Relation with the de Haas-van Alphen effect

Our results can be easily extended to the case of more general Bloch electrons, that is when one has a background smooth and periodic electric potential V. More precisely, $V \in C^\infty(\mathbb{R}^3)$, $V \geq 0$, and if Γ is a periodic lattice in $\mathbb{R}^3$ then $V(\cdot) = V(\cdot + \gamma)$ for all $\gamma \in \Gamma$.

Denote by Ω the elementary cell of Γ. In this case, the grandcanonical pressure at the thermodynamic limit will be given by (we work with fermions thus $\epsilon = 1$)

$$P_\infty(\beta, \omega, z) = \frac{1}{\beta} \sum_{k \geq 1} \frac{(-z)^k}{k} \frac{1}{|\Omega|} \int_\Omega G_\infty(\mathbf{x}, \mathbf{x}; k\beta, \omega) d\mathbf{x}, \tag{4.24}$$

where $G_\infty(\mathbf{x}, \mathbf{x}'; k\beta, \omega)$ is the smooth integral kernel of the semigroup generated by $\frac{1}{2}(-i\nabla + \omega\mathbf{a})^2 + V$. This formula only holds for $|z| < 1$, but it can be analytically continued to $\mathbb{C} \setminus (-\infty, -1]$, see [2], [50] or [BCS 2].

Now one can start looking at the behavior of $P_\infty(\beta, \omega, z)$ as function of ω, in particular around the point $\omega_0 = 0$. Working in canonical conditions, that is when z is a function of β, ω and the fixed particle density ρ, then one is interesting in the object

$$p_\infty(\beta, \omega, \rho) := P_\infty(\beta, \omega, z(\beta, \omega, \rho)).$$

A thorough analysis of the ω behavior near 0, involving derivatives with respect to ω of the above quantity, has been considered by Helffer and Sjöstrand in [50], and by us in [BCS 2].

Alternatively, one can start from the finite volume quantities, and define a $z_L(\beta, \omega, \rho)$ as the unique solution of the equation $\rho_L := \beta z \partial_z P_L(\beta, \omega, z_L) = \rho$ and $p_L(\beta, \omega, \rho) := P_L(\beta, \omega, z_L(\beta, \omega, \rho))$. Is it still true that at large volumes we have for example that

$$\partial_\omega^n p_L(\beta, \omega, \rho) \sim \partial_\omega^n p_\infty(\beta, \omega, \rho), \quad n \geq 1\ ?$$

Our answer is yes, for all $z \in \mathbb{C} \setminus (-\infty, -1]$.

4.2 Diamagnetic expansions for perfect quantum gases: singular potentials

Here we examine the case in which both the magnetic field and the electric potential can have singularities, such that the magnetic and scalar singular perturbations are relatively bounded in the form sense with respect to the purely magnetic Schrödinger operator with constant magnetic field. The results are taken from [BCS 1].

Now let us introduce some notation and give the main theorem. Consider a magnetic vector potential $\mathbf{a} = (a_1, a_2, a_3) = \mathbf{a}_c + \mathbf{a}_p$ where $B\mathbf{a}_c := \frac{B}{2}\mathbf{e} \times \mathbf{x}$, $\mathbf{e} = (0, 0, 1)$ is the usual symmetric gauge generated by a constant magnetic field $\mathbf{B} = B\mathbf{e}, B > 0$ and $\mathbf{a}_p$ is $\mathbb{Z}^3$-periodic satisfying $|\mathbf{a}_p|^2 \in \mathcal{K}_{loc}(\mathbb{R}^3)$. The notation $\mathcal{K}_{loc}$ denotes the usual Kato class [27, 98]. Relations between these assumptions on magnetic potentials and related choices of periodic magnetic fields are discussed in [57]. Assume that V is also $\mathbb{Z}^3$-periodic such that $V \in \mathcal{K}_{loc}(\mathbb{R}^3)$. Later on we will give a rigorous sense to the operator (here $\omega := eB/c \in \mathbb{R}$)

$$H_\infty(\omega, V) := \frac{1}{2}(-i\nabla - \omega\mathbf{a})^2 + V$$

corresponding to the obvious quadratic form initially defined on $C_0^\infty(\mathbb{R}^3)$. If Λ is a bounded open and simply connected subset of $\mathbb{R}^3$ we denote by $H_\Lambda(\omega, V)$ the operator obtained by restricting the above mentioned quadratic form to $C_0^\infty(\Lambda)$. The operator $H_\Lambda(\omega, V)$ has purely discrete spectrum.

Set $e_0 = e_0(\omega)$ to be $\inf \sigma(H_\infty(\omega, V))$. Introduce the following complex domains

$$D_{+1}(e_0) := \mathbb{C} \setminus (-\infty, -e^{\beta e_0}], \quad D_{-1}(e_0) := \mathbb{C} \setminus [e^{\beta e_0}, \infty) \tag{4.25}$$

The grand canonical finite volume pressure is given by (see also (4.4)):

$$P_\Lambda(\beta, z, \omega) = \frac{\epsilon}{\beta|\Lambda|} \mathrm{Tr}_{L^2(\Lambda)} \big\{ \ln(\mathrm{Id} + \epsilon z e^{-\beta H_\Lambda(\omega, V)}) \big\} \tag{4.26}$$

where as before, $\epsilon = +1$ corresponds to the Fermi case and $\epsilon = -1$ corresponds to the Bose case. In (4.26) the fugacity $z \in D_\epsilon(e_0) \cap \mathbb{R}$. The operator $\ln(\mathrm{Id} + \epsilon z e^{-\beta H_\Lambda(\omega, V)})$ in the right hand side of (4.26) is defined via functional calculus. Due to some trace class estimates which we will state later on, the pressure P_Λ in (4.26) is well defined. Define the following complex domains

$$\mathbf{D}_\epsilon := \bigcap_{\omega \in \mathrm{Re}} D_\epsilon(e_0(\omega)) = D_\epsilon(e_0(0)), \quad \epsilon = \pm 1 \tag{4.27}$$

The first part of our main result establishes some regularity properties of the pressure at finite volume, seen as a function of z and ω. The second part will identify the thermodynamic limit of the pressure. Assume that the domain Λ is obtained by dilating a given set $\Lambda_1 \subset \mathbb{R}^3$ which is supposed to be bounded, open, simply connected and with smooth boundary. More precisely:

$$\Lambda_L := \{\mathbf{x} \in \mathbb{R}^3 : \ \mathbf{x}/L \in \Lambda_1, \quad L > 1\}.$$

Theorem 4.5. *Let $\beta > 0$.*

(i). *For each open set $K \subset \mathbb{C}$ with the property that $\overline{K}$ is compact and included in $\mathbf{D}_\epsilon$, there exists a complex neighborhood $\mathcal{N}$ of the real axis such that $\mathcal{N} \,\mathrm{x}\, K \ni (\omega, z) \mapsto P_\Lambda(\beta, z, \omega)$ is analytic.*

(ii). *Let $\omega \in \mathbb{R}$ and choose a compact set $K \subset D_\epsilon(e_0(\omega))$. Then uniformly in $z \in K$*

$$P_\infty(\beta, z, \omega) := \lim_{\Lambda \to \mathbb{R}^3} P_\Lambda(\beta, z, \omega)$$

exists and defines a smooth function of ω.

The main idea of the proof is to find for any compact subset K of $D_\epsilon(e_0)$ a cleverly chosen contour Γ_K which surrounds the spectrum of H_{Λ_L} uniformly in L so that we can write using the analytic functional calculus:

$$P_{\Lambda_L}(\beta, z, \omega) = \frac{i\epsilon}{2\beta\pi|\Lambda_L|} \mathrm{Tr}_{L^2(\Lambda_L)} \int_{\Gamma_K} \mathrm{d}\xi \, \ln\big(1 + \epsilon z e^{-\beta\xi}\big)\big(H_{\Lambda_L}(\omega, V) - \xi\big)^{-1}. \tag{4.28}$$

The integral will be trace class, even if the integrand is not. If ω is real, one can prove that the thermodynamic limit is given by:

$$P_\infty(\beta, z, \omega) = \frac{i\epsilon}{2\beta\pi|\Omega|} \mathrm{Tr}_{L^2(\mathbb{R}^3)} \int_{\Gamma_K} \mathrm{d}\xi \, \ln\big(1 + \epsilon z e^{-\beta\xi}\big)\chi_\Omega\big(H_\infty(\omega, V) - \xi\big)^{-1}\chi_\Omega. \tag{4.29}$$

The above integral defines a trace class operator on $L^2(\mathbb{R}^3)$ because after a use of the resolvent identity we can change the integrand into:

$$(\xi-\xi_0)\ln\big(1+\epsilon z e^{-\beta\xi}\big)\chi_\Omega\big(H_\infty(\omega,V)-\xi\big)^{-1}\big(H_\infty(\omega,V)-\xi_0\big)^{-1}\chi_\Omega$$

where ξ_0 is some fixed and negative enough number. Using the Laplace transform and the properties of the semigroup e^{-tH_∞} one can prove that $\chi_\Omega\big(H_\infty(\omega,V)-\xi\big)^{-1}$ and $\big(H_\infty(\omega,V)-\xi_0\big)^{-1}\chi_\Omega$ are Hilbert-Schmidt operators whose norms grow polynomially with $\mathrm{Re}\,\xi$.

The fact that ω must be real is an important ingredient of the proof of (4.29) where one extensively uses the gauge invariance of the operators and the fact that H_∞ commutes with the magnetic translations generated by $\mathbb{Z}^3$. It is shown in [97] that if $\mathbf{a}_c=0$ i.e. the magnetic vector potential is periodic, then the limit in (4.29) holds true for every ω is a small ball around every $\omega_0\in\mathrm{Re}$, provided that z and β are fixed. The explanation is that the analyticity ball in ω which we have constructed for each P_{Λ_L} would be independent of L. If $\mathcal{C}_r(\omega_0)$ denotes the positively oriented circle with radius r and center at ω_0, then for any real ω inside $\mathcal{C}_r(\omega_0)$ and for r small enough we can write:

$$P_{\Lambda_L}(\omega)=\frac{1}{2\pi i}\int_{\mathcal{C}_r(\omega_0)}\frac{P_{\Lambda_L}(\omega')}{\omega'-\omega}d\omega',\quad \chi^N_{\Lambda_L}(\omega)=\frac{N!}{2\pi i}\int_{\mathcal{C}_r(\omega_0)}\frac{P_{\Lambda_L}(\omega')}{(\omega'-\omega)^{N+1}}d\omega'$$

The last integral representation of $\chi^N_{\Lambda_L}(\omega)$ tells us that if the pressure admits the thermodynamic limit, the same property holds true for all generalized susceptibilities. Thus the existence of the thermodynamic limit of the generalized susceptibilities follows easily if there is no linear growth in the magnetic potential generated by the magnetic field.

If $\mathbf{a}_c$ is not zero, then the above argument breaks down because r (the analyticity radius in ω of P_{Λ_L}) goes to zero with L. In fact one cannot hope to prove in general that P_∞ is real analytic in ω, although one can prove that it is smooth in $\omega\in\mathbb{R}$. In order to achieve that, one needs to use the methods of [25].

4.3 The Faraday effect: thermodynamic limit of the transverse conductivity

The rotation of the polarization of a plane-polarized electromagnetic wave passing through a material immersed in a homogeneous magnetic field oriented parallel to the direction of propagation, is known in physics as the Faraday effect (sometimes also called Faraday rotation). The experiment consists in sending a monochromatic light wave, parallel to the $0z$ direction and linearly polarized in the plane $x0z$. When the light enters the sample, the polarization plane starts rotating. A simple argument based on (classical) Maxwell equations shows that there exists a linear relation between the angle θ of rotation of the plane of polarization per unit length and the transverse component of the conductivity tensor of the material (see e.g. formula (1) in [94]). For most materials - and we will restrict ourselves to this case - the transverse component of the conductivity tensor vanishes when the magnetic field is absent and is no longer zero when the magnetic field is turned on.

Under the proviso that the dependence of the conductivity tensor upon the strength B of the magnetic field is smooth, for weak fields one expands the conductivity tensor to the first order and neglect the higher terms. The coefficient of the linear term is known as the Verdet constant of the corresponding material.

It follows that the basic object is the conductivity tensor and the main goal of the theory (classical or quantum) is to provide a workable formula for it, in particular for the Verdet constant. The problem has a long and distinguished history in solid state physics theory and the spectrum of possible applications ranges from astrophysics to optics and general quantum mechanics (see e.g. [94, 85, 107, 24, 71, 38, 61] and references therein).

Using quantum theory in the setting in which the sample is modeled by a system of independent electrons subjected to a periodic electric potential, Laura Roth [94] obtained (albeit only at a formal level) a formula for the Verdet constant in full generality and applied it to metals as well as semiconductors. Roth's method is based on an effective Hamiltonian approach for Bloch electrons in the presence of a weak constant magnetic field (see [96] and references therein) which in turn is based on a (proto) magnetic pseudodifferential calculus (for recent mathematical developments see [58] and references therein).

But Roth's theory is far from being free of difficulties. Due to her highly formal way of doing computations, it seems almost hopeless - even with present day mathematical tools - to control the errors or push the computations to higher orders in B except maybe the case of simple bands. Even more, the final formula contains terms which are singular at the crossings of Bloch bands. Accordingly, in spite of the fact that it has been considered a landmark of the subject, it came as no surprise that at the practical level this theory only met a moderate success and a multitude of unrelated, simplified models have been tailored for specific cases.

We have completed a series of three papers aiming at a self-contained and mathematically sound theory of Faraday effect having the same generality as Roth's theory (i.e. a theory of the conductivity tensor for electrons subjected to a periodic electric potential and to a constant magnetic field in the linear response approximation), but free of its shortcomings. More precisely in the first paper [24] we started by a rigorous derivation of the transverse component of the conductivity tensor in the linear response regime for a finite sample. It is given as the formula 4.39 below. To proceed further, we employ a method going back at least Sondheimer and Wilson [99] and which has been also used in the rigorous study of the Landau magnetism [1, 21, 12, 13, 14]. The basic idea is that the traces involved in computing various physical quantities can be written as integrals involving Green functions (i.e. integral kernels in the configuration space of either the resolvent or the semi-group of the Hamiltonian of the system), which are more robust and easier to control.

As it stands, the conductivity tensor depends upon the shape of the sample and of boundary conditions which define the quantum Hamiltonian. The physical idea of the thermodynamic limit for an intensive physical quantity is that in the limit of large samples it approaches a limit which is independent upon the shape of the sample, boundary conditions etc. The existence of the thermodynamic limit is one of the basic (and far from trivial) problem of statistical mechanics (see e.g. [95, 10]). In [24] we took for granted that the thermodynamic limit of the the transverse component of the conductivity tensor exists and the limit is smooth as a function of the magnetic field strength B. Moreover, we assumed that the thermodynamic limit commuted with taking the derivative with respect to B. Under these assumptions, we gave - among other things - explicit formulas for the Verdet constant in terms of zero magnetic field Green functions, free of any divergences.

The proof of the thermodynamic limit, which from the mathematical point of view is the most delicate part of the theory of the Faraday effect, was left aside in [24], and is the content of [CN 1]. The mathematical problem behind it is hard due to the singularity induced by the long range magnetic perturbation. Even for a simpler problem involving constant magnetic field - namely the Landau diamagnetism of free electrons - the existence of the thermodynamic limit leading to a correct thermodynamic behavior was a long standing problem. Naive computations led to unphysical and contradictory results (see [1] for historical remarks). Accordingly, the first rigorous results came as late as 1975 [1] and were based on various identities expressing the gauge invariance which was crucial in dealing with the singular terms appearing in the thermodynamic limit. Even though the importance of gauge invariance was already highlighted in [1], an efficient way to implement this idea at a technical level was still lacking. Only recently a regularized magnetic perturbation theory based on factorizing the (singular in the thermodynamic limit) magnetic phase factor has been fully developed in [21, 22, 23, 80]. This regularized magnetic perturbation theory has been already used in [21, 12, 13, 14], as we have seen in the previous sections.

Coming back to the Faraday effect, we would like to stress that the object at hand is much more singular than the one encountered in the Landau diamagnetism. This adds an order of magnitude to the mathematical difficulty and requires an elaborate and tedious combination of regularized magnetic perturbation theory with techniques like Combes-Thomas exponential decay, trace norm estimates and elliptic regularity.

The method developed here in order to control the thermodynamic limit in the presence of an extended magnetic field is also useful in related problems, e.g. to obtain an elegant and complete study of the diamagnetism of Bloch electrons in metals.

In the rest of this description we will state the mathematical problem, give the main result in Theorem 4.6, and then outline the strategy of the proof.

4.3.1 The main result

Consider a simply connected open and bounded set $\Lambda_1 \subset \mathbb{R}^3$, which contains the origin. We assume that the boundary $\partial\Lambda_1$ is smooth. Consider again a family of scaled domains

$$\Lambda_L = \{\mathbf{x} \in \mathbb{R}^3 : \ \mathbf{x}/L \in \Lambda_1\}, \ L > 1. \tag{4.30}$$

We have the estimates

$$\mathrm{Vol}(\Lambda_L) \sim L^3, \quad \mathrm{Area}(\partial\Lambda_L) \sim L^2. \tag{4.31}$$

The thermodynamic limit will mean $L \to \infty$, thus Λ_L will fill out the whole space. The one particle Hilbert space is $\mathcal{H}_L := L^2(\Lambda_L)$. This notation includes the case $L = \infty$.

The one body Hamiltonian of a non-confined particle, subjected to a constant magnetic field $(0, 0, B)$, in an external potential V, formally looks like this:

$$H_\infty(B) = \mathbf{P}^2(B) + V, \tag{4.32}$$

with

$$\mathbf{P}(B) = -i\nabla + B\mathbf{a} = \mathbf{P}(0) + B\mathbf{a}. \tag{4.33}$$

Let us explain the various terms. Here $\mathbf{a}(\mathbf{x})$ is a smooth magnetic vector potential which generates a magnetic field of intensity $B = 1$ i.e. $\nabla \wedge \mathbf{a}(\mathbf{x}) = (0, 0, 1)$. Let us give once again the magnetic vector potential in the symmetric gauge:

$$\mathbf{A}(\mathbf{x}) = \frac{1}{2}\mathbf{n}_3 \wedge \mathbf{x} = (-x_2/2, x_1/2, 0), \tag{4.34}$$

where $\mathbf{n}_3$ is the unit vector along the z axis. We neglect the spin structure since it only complicates the notation and does not influence the mathematical problem.

On components, (4.33) reads as:

$$P_j(B) = D_j + Ba_j =: P_j(0) + Ba_j, \quad j \in \{1, 2, 3\}. \tag{4.35}$$

We will from now on assume that V is a $C^\infty(\mathbb{R}^3)$ function, periodic with respect to the lattice $\mathbb{Z}^3$. Standard arguments then show that $H_\infty(B)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

When $L < \infty$ we need to specify a boundary condition. We will only consider Dirichlet boundary conditions, that is we start with the same expression as in (4.32), defined on $C_0^\infty(\Lambda_L)$, and we define $H_L(B)$ to be the Friedrichs extension of it. This is indeed possible, because our operator can be written as $-\Delta_D + W$, where Δ_D is the Dirichlet Laplacian and W is a first order differential operator, relatively bounded to $-\Delta_D$ (remember that $L < \infty$). The form domain of $H_L(B)$ is the Sobolev space $H_0^1(\Lambda_L)$, while the operator domain (use the estimates in section 10.5, Lemma 10.5.1, in [56]) is $H^2(\Lambda_L) \cap H_0^1(\Lambda_L)$. Moreover, $H_L(B)$ is essentially self-adjoint on $C_{(0)}^\infty(\overline{\Lambda_L})$, i.e. functions with support in $\overline{\Lambda_L}$ and indefinitely differentiable in Λ_L up to the boundary.

Another important operator is $(-i\nabla + B\mathbf{a})_D^2$, i.e. the usual free magnetic Schrödinger operator defined with Dirichlet boundary conditions. We know that its spectrum is non-negative for all $L > 1$. By adding a positive constant, we can always assume that the spectrum of $H_L(B)$ is non-negative, uniformly in $L > 1$.

Let us now introduce the physical quantity we want to study. Consider a complex frequency $\nu \in \mathbb{C}$ and $\mathrm{Im}(\nu) < 0$. For some fixed $\mu \in \mathbb{R}$ and $\beta > 0$, consider the Fermi-Dirac function on its maximal domain of analyticity:

$$f_{FD}(z) = \frac{1}{e^{\beta(z-\mu)} + 1}. \tag{4.36}$$

Define

$$d := \min\left\{\frac{\pi}{2\beta}, \frac{|\mathrm{Im}\,\nu|}{2}\right\}, \tag{4.37}$$

and introduce a counter-clockwise oriented contour given by

$$\Gamma_\nu = \{x \pm id : \ a \leq x < \infty\} \bigcup \{a + iy : \ -d \leq y \leq d\} \tag{4.38}$$

where $a+1$ lies below the spectrum of $H_L(B)$. *Note that this is not the same contour as Γ_K of the previous section.* By adding a positive constant to V, we can take $a = -1$ uniformly in $L \geq 1$ and $B \in [0,1]$.

We introduce the transverse component of the conductivity tensor (see [94, 24]) as

$$\sigma_L(B) = -\frac{1}{\mathrm{Vol}(\Lambda_L)} \mathrm{Tr} \int_{\Gamma_\nu} f_{FD}(z) \left\{ P_1(B)(H_L(B) - z)^{-1} P_2(B)(H_L(B) - z - \nu)^{-1} \right.$$
$$\left. + P_1(B)(H_L(B) - z + \nu)^{-1} P_2(B)(H_L(B) - z)^{-1} \right\} dz. \tag{4.39}$$

Here *Tr* assumes that the integral is a trace-class operator. Now we are prepared to formulate our main result.

Theorem 4.6. *The above defined transverse component of the conductivity tensor admits the thermodynamic limit; more precisely:*

i. *The following operator, defined by a $B(L^2(\Lambda_L))$- norm convergent Riemann integral,*

$$F_L := \int_{\Gamma_\nu} f_{FD}(z) \{P_1(B)(H_L(B) - z)^{-1} P_2(B)(H_L(B) - z - \nu)^{-1}$$
$$+ P_1(B)(H_L(B) - z + \nu)^{-1} P_2(B)(H_L(B) - z)^{-1}\} dz, \tag{4.40}$$

is in fact trace-class;

ii. *Consider the operator F_∞ defined by the same integral but with $H_\infty(B)$ instead of $H_L(B)$, and defined on the whole space. Then F_∞ is an integral operator, with a kernel $\mathcal{F}(\mathbf{x}, \mathbf{x}')$ which is jointly continuous on its variables. Moreover, the continuous function defined by $\mathbb{R}^3 \ni \mathbf{x} \to s_B(\mathbf{x}) := \mathcal{F}(\mathbf{x}, \mathbf{x}) \in \mathbb{R}$ is periodic with respect to $\mathbb{Z}^3$;*

iii. *Denote by Ω the unit cube in $\mathbb{R}^3$. The thermodynamic limit exists:*

$$\sigma_\infty(B) := \lim_{L \to \infty} \sigma_L(B) = -\int_\Omega s_B(\mathbf{x}) d\mathbf{x}. \tag{4.41}$$

Moreover, the mapping $B \to s_B \in L^\infty(\Omega)$ is differentiable at $B = 0$ and:

$$\partial_B \sigma_\infty(0) = -\int_\Omega \partial_B s_B \bigg|_{B=0} (\mathbf{x}) d\mathbf{x} = \lim_{L \to \infty} \partial_B \sigma_L(0). \tag{4.42}$$

Remark 1. The formula (4.41) is only the starting point in the study of the Faraday rotation. A related problem is the diamagnetism of Bloch electrons, where the main object is the integrated density of states of magnetic Schrödinger operators (see [50, 48, 57]). For a systematic treatment of magnetic pseudo-differential operators which generalizes our magnetic perturbation theory, see [58, 73, 74, 75].

Remark 2. The Dirichlet boundary conditions are important for us. Even though we suspect that our main result should also hold for Neumann conditions and for less regular domains (see [9, 33]), we do not see an easy way to prove it.
Remark 3. We believe that the method we use in the proof of (4.42) can be used in order to obtain a stronger result: the mapping $B \to s_B \in L^\infty(\Omega)$ is smooth and for any $n \geq 1$:

$$\partial_B^n \sigma_\infty(B) = -\int_\Omega \partial_B^n s_B(\mathbf{x}) d\mathbf{x} = \lim_{L\to\infty} \partial_B^n \sigma_L(B). \tag{4.43}$$

This statement is left as an open problem.

4.3.2 The strategy

Let us start with some general considerations about the thermodynamic limit.

If we are interested in the thermodynamic limit of a quantum physical quantity, the object we need to control is the trace of the operator representing the corresponding quantity. The basic ideea consists in writing this trace as an integral of the diagonal value of the operator's integral kernel (Schwartz kernel) over the confining box. This procedure makes the quantum thermodynamic limit look very similar to what happens in classical statistical mechanics. More precisely, we need to show that the difference between the integral kernel for the finite box and the one for the entire space decays sufficiently rapidly with the distance from the boundary of the box, so that the replacement of the integral kernel for the box with the one corresponding to the entire space gives an error term increasing slower than the volume, which then disappears in the limit.

It turns out that for the transverse conductivity this kernel is far more complicated than say the heat kernel - whose behavior has been extensively studied in the literature. Notice for example, that the integrand in (4.39) contains two resolvents sandwiched with magnetic momentum operators. Thus we need a good control of their integral kernels, in particular when the distance between their arguments increases to infinity, and all that uniformly in the spectral parameter z. Since a constant magnetic field is present, the biggest difficulty is to deal with the linear growth of the vector potential. Here, the use of gauge covariance is crucial. Now let us list the main ideas of the proof.

i. For the first statement of the theorem one simply uses integration by parts with respect to z in order to transform the integrand into a product of Hilbert-Schmidt operators.

ii. The proof of the second statement is based on elliptic regularity. The main technical difficulty is to control the z behavior of all our bounds, especially the exponential localization of the magnetic resolvents sandwiched with momentum operators. We also have to control the linear growth of the magnetic potential. We turn the operator norm bounds into pointwise bounds for certain integral kernels. It is a long road using magnetic perturbation theory, but nevertheless, we use nothing more than well-known Combes-Thomas exponential bounds, local gauge covariance, the Cauchy-Schwarz inequality, and integration by parts.

*iii.*The third statement of Theorem 4.6 contains the main result. We start with a bit strange three-layered partition of unity, where the idea goes back at least to [11, 12]. The main effort consists in isolating the bulk of Λ_L - where only operators defined in the whole space will act - from the region close to the boundary. Note that in the absence of the magnetic field, it would be enough to work with only two cut-off functions: one isolating the bulk from the boundary, and the other one supported in a tubular neighborhood of the boundary. When long-range magnetic fields are present, this is not enough. The tubular neigborhood needs to be chopped up in many small pieces, in order to apply local gauge transformations (see below why we need them).

The central idea in proving (4.41) is to show that the contribution to the total trace of the region close to the boundary grows slower than the volume. Technically, this is obtained by approximating the true resolvent $(H_L(B) - z)^{-1}$ with an operator $U_L(B, z)$ which contains the bulk term, plus a boundary contribution which consists from a sum of terms each *locally* approximating $(H_L(B) - z)^{-1}$ and containing a specially tailored local gauge. These locally defined vector potentials are made *globally* bounded with the help of our third layer of cut-off functions $\tilde{\tilde{g}}_\gamma$'s. The switch to the local gauge is performed through the central identity (4.44):

$$\{\mathbf{P}_\mathbf{x}(0) + B\mathbf{A}(\mathbf{x})\}e^{iB\varphi_0(\mathbf{x},\mathbf{y})} = e^{iB\varphi_0(\mathbf{x},\mathbf{y})}\{\mathbf{P}_\mathbf{x}(0) + B\mathbf{A}(\mathbf{x} - \mathbf{y})\}. \tag{4.44}$$

The proof of (4.42) is heavily based on magnetic perturbation theory. Although the technical estimates are considerably more involved than at the previous point, the main idea is the same: the boundary terms can be discarded but not without using the full power of the magnetic phase factorization.

5 A rigorous derivation of the Landau-Peierls formula

Understanding the zero-field magnetic susceptibility of a Bloch electron gas is one of the oldest problems in quantum statistical mechanics.

The story began in 1930 with a paper by L. Landau [67], in which he computed the diamagnetic susceptibility of a free degenerate gas. (Note that the rigorous proof of Landau's formula for free electrons was given by Angelescu *et al* [1] and came as late as 1975.) For Bloch electrons (which are subjected to a periodic background electric potential), the problem is much harder and -to our best knowledge- it has not been solved yet in its full generality.

The first important contribution to the periodic problem came in 1933, when R. Peierls [87] introduced his celebrated Peierls substitution and constructed an effective band Hamiltonian which permitted to reduce the problem to free electrons. Needless to say that working with only one energy band instead of the full magnetic Schrödinger operator is an important simplification.

In 1957, Kjeldaas and Kohn [62] were probably the first ones who suggested that the Landau-Peierls formula (see below (5.21) and (5.22)) has to be corrected with some higher order terms in the particle density, and these terms must come from the bands not containing the Fermi energy.

The first attempt to address the full quantum mechanical problem -even though the carriers were boltzons and not fermions- was made by Hebborn and Sondheimer [44, 45] in 1960. Unlike the previous authors, they try to develop a magnetic perturbation theory for the trace per unit volume defining the pressure. The biggest problem of their formalism is that they assume that all Bloch energy bands are not overlapping (this is generically false; for a proof of the Bethe-Sommerfeld conjecture in dimension 3 see e.g. [47]), and that the Bloch basis is smooth in the quasi-momentum variables. This assumption also fails at the points where the energy bands cross each other. Not to mention that no convergence issues were addressed in any way.

In 1962, L. Roth [96] developed a magnetic pseudodifferential calculus starting from the ideas of Peierls, Kjeldaas and Kohn. She used this formalism in order to compute local traces and magnetic expansions. Similar results are obtain by E.I. Blunt [7]. Their formal computations can most probably be made rigorous in the case of simple bands.

In 1964, Hebborn *et.al* [43] simplified the formalism developed in [45] and gave for the first time a formula for the zero-field susceptibility of a boltzon gas. Even though the proofs lack any formal rigor, we believe that their derivation could be made rigorous for systems where the Bloch bands do not overlap. But this is generically not the case.

The same year, Wannier and Upadhyaya [105] go back to the method advocated by Peierls, and replace the true magnetic Schrödinger operator with a (possibly infinite) number of bands modified with the Peierls phase factor. They claim that their result is equivalent with that one of Hebborn and Sondheimer [45], but no details are given. Anyhow, the result uses in an essential way the non-overlapping of Bloch bands.

In 1969, Misra and Roth [77] combined the method of [96] with the ideas of Wannier in order to include the core electrons in the computation.

In 1972, Misra and Kleinman [76] had the very nice idea of using sum-rules in order to replace derivatives with respect to the quasi-momentum variables, with matrix elements of the "true" momentum operator. They manage in this way to rewrite the formulas previously derived by Misra and Roth (which only made sense for non-overlapping bands) in a form which might also hold for overlapping bands.

As we have already mentioned, the first serious mathematical approach on the zero-field susceptibility appeared as late as 1975, due to Angelescu *et. al.* [1]. Then in 1990, Helffer and Sjöstrand [50] developed for the first time a rigorous theory based on the Peierls substitution and considered the connection with the de Haas-Van Alphen effect. These and many more results were reviewed by G. Nenciu in 1991 [83].

A related semiclassical problem in which the electron gas is confined by a trapping potential was considered by Combescure and Robert in 2001 [19]. They obtained the Landau formula in the limit $\hbar \to 0$.

The results we obtain in Theorem 5.2 give a complete answer to the problem of zero-field susceptibility in the canonical conditions. Let us now discuss the setting and properly formulate the mathematical problem.

5.1 The setting

Consider a confined quantum gas of charged particles obeying the Fermi-Dirac statistics. The spin is not considered since we are only interested in orbital magnetism. Assume that the gas is subjected to a constant magnetic field and an external periodic electric potential. The interactions between particles are neglected and the gas is at thermal equilibrium.

The gas is trapped in a large cubic box, which is given by $\Lambda_L = \big(-\frac{L}{2}, \frac{L}{2}\big)^3$, $L \geq 1$.

Let us introduce our one-body Hamiltonian. We consider a uniform magnetic field $\mathbf{B} = (0, 0, B)$ with $B \geq 0$, parallel to the third direction of the canonical basis of $\mathbb{R}^3$. Let $\mathbf{a}(\mathbf{x})$ be the symmetric (transverse) gauge.

We again consider that the background electric potential V is smooth, i.e. $V \in \mathcal{C}^\infty(\mathbb{R}^3)$ is a real-valued function and periodic with respect to a (Bravais) lattice Υ with unit cell Ω. Without loss of generality, we assume that Υ is the cubic lattice $\mathbb{Z}^3$, thus Ω is the unit cube centered at the origin of coordinates.

When the box is finite i.e. $1 \leq L < \infty$, the dynamics of each particle is determined by a Hamiltonian defined in $L^2(\Lambda_L)$ with Dirichlet boundary conditions on $\partial\Lambda_L$:

$$H_L(\omega) = \frac{1}{2}\big(-i\nabla_{\mathbf{x}} - \omega\mathbf{a}(\mathbf{x})\big)^2 + V_L(\mathbf{x})$$

where V_L stands for the restriction of V to the box Λ_L. Here $\omega := \frac{e}{c}B \in \mathbb{R}$ denotes the cyclotron frequency.

When $L = \infty$ we denote by $H_\infty(\omega)$ the unique self-adjoint extension of the operator

$$\frac{1}{2}\big(-i\nabla_{\mathbf{x}} - \omega\mathbf{a}(\mathbf{x})\big)^2 + V(\mathbf{x})$$

initially defined on $\mathcal{C}_0^\infty(\mathbb{R}^3)$. Then $H_\infty(\omega)$ is bounded from below and only has essential spectrum.

For the moment we use the grand canonical formalism. We already know that the pressure and the density can be expressed as:

$$P_L(\beta,z,\omega) = \frac{1}{\beta|\Lambda_L|}\mathrm{Tr}_{L^2(\Lambda_L)}\big\{\ln\left(\mathrm{Id}+z\mathrm{e}^{-\beta H_L(\omega)}\right)\big\} = \frac{1}{\beta|\Lambda_L|}\sum_{j=1}^{\infty}\ln\left(1+z\mathrm{e}^{-\beta e_j(\omega)}\right) \quad (5.1)$$

$$\rho_L(\beta,z,\omega) = \beta z\frac{\partial P_L}{\partial z}(\beta,z,\omega) = \frac{1}{|\Lambda_L|}\sum_{j=1}^{\infty}\frac{z\mathrm{e}^{-\beta e_j(\omega)}}{1+z\mathrm{e}^{-\beta e_j(\omega)}}. \quad (5.2)$$

Since the function $\mathbb{R}\ni\omega\mapsto P_L(\beta,z,\omega)$ is smooth, we can define the finite volume diamagnetic susceptibility as the second derivative of the pressure with respect to the intensity B of the magnetic field at $B=0$ (see e.g. [1]):

$$\mathcal{X}_L^{GC}(\beta,z) := \left(\frac{e}{c}\right)^2\frac{\partial^2 P_L}{\partial\omega^2}(\beta,z,0). \quad (5.3)$$

When Λ_L fills the whole space, we proved that the thermodynamic limits of the three grand canonical quantities defined above exist. By denoting $P_\infty(\beta,z,\omega) := \lim_{L\to\infty}P_L(\beta,z,\omega)$, we proved moreover the following pointwise convergence:

$$\rho_\infty(\beta,z,\omega) := \beta z\frac{\partial P_\infty}{\partial z}(\beta,z,\omega) = \lim_{L\to\infty}\beta z\frac{\partial P_L}{\partial z}(\beta,z,\omega) \quad (5.4)$$

$$\mathcal{X}_\infty^{GC}(\beta,z) := \left(\frac{e}{c}\right)^2\frac{\partial^2 P_\infty}{\partial\omega^2}(\beta,z,0) = \lim_{L\to\infty}\left(\frac{e}{c}\right)^2\frac{\partial^2 P_L}{\partial\omega^2}(\beta,z,0) \quad (5.5)$$

and the limit commutes with the first derivative (resp. the second derivative) of the grand canonical pressure with respect to the fugacity z (resp. to the external magnetic field B).

Now assume that our fixed external parameter is the density of particles $\rho_0>0$. We prefer to see ρ_∞ as a function of the chemical potential μ instead of the fugacity z; the density is a strictly increasing function with respect to both μ and z. Denote by $\mu_\infty(\beta,\rho_0)\in\mathbb{R}$ the unique solution of the equation:

$$\rho_0 = \rho_\infty\left(\beta, e^{\beta\mu_\infty(\beta,\rho_0)},0\right). \quad (5.6)$$

The diamagnetic susceptibility at $\beta>0$ and fixed density $\rho_0>0$ defined from (5.5) is defined as:

$$\mathcal{X}(\beta,\rho_0) := \mathcal{X}_\infty^{GC}\left(\beta,e^{\beta\mu_\infty(\beta,\rho_0)}\right). \quad (5.7)$$

In fact one can also show that $\mathcal{X}(\beta,\rho_0) = -\left(\frac{e}{c}\right)^2\frac{\partial^2 f_\infty}{\partial\omega^2}(\beta,\rho_0,0)$ where $f_\infty(\beta,\rho_0,\omega)$ is the thermodynamic limit of the reduced free energy defined as the Legendre transform of the thermodynamic limit of the pressure (see e.g.[95]). Note that for a perfect quantum gas, (5.7) is nothing but the Landau susceptibility [1].

In order to formulate our main result, we need to introduce some more notation. In the case in which $\omega=0$, the Floquet theory for periodic operators (see e.g. [8], [66]) allows one to use the band structure of the spectrum of $H_\infty(0)$. Denote by $\Omega^* = 2\pi\Omega$ the Brillouin zone of the dual lattice $\Upsilon^* \equiv 2\pi\mathbb{Z}^3$.

If the dimension is $d \geq 1$, the Bloch-Floquet unitary is (see e.g. [92]):

$$\begin{aligned} &U : L^2(\mathbb{R}^d) \mapsto \int_{\Omega^*}^{\oplus} L^2(\Omega) d\mathbf{k}, \\ &(Uf)(\mathbf{x}, \mathbf{k}) := \frac{1}{(2\pi)^{d/2}} \sum_{\gamma \in \mathbb{Z}^d} e^{-i\mathbf{k}\cdot(\mathbf{x}+\gamma)} f(\mathbf{x}+\gamma), \quad \mathbf{k} \in \Omega^*, \quad \mathbf{x} \in \Omega, \quad f \in C_0^\infty(\mathbb{R}^d). \end{aligned} \tag{5.8}$$

Then $H_\infty(0)$ can be written as a fiber integral $H_\infty(0) = \int_{\Omega^*}^{\oplus} h(\mathbf{k}) d\mathbf{k}$ where the fiber operator

$$h(\mathbf{k}) = \frac{1}{2} \left(-i\nabla_p + \mathbf{k}\right)^2 + V, \tag{5.9}$$

is defined in $L^2(\Omega)$ with periodic boundary conditions, and its domain is the periodic Sobolev space $H^2(\Omega_p)$. Here $-i\nabla_p$ denotes the momentum operator in $L^2(\Omega)$ with periodic boundary conditions. The operator $h(\mathbf{k})$ has compact resolvent and purely discrete spectrum $\{E_j(\mathbf{k})\}_{j\geq 1}$. We can choose a set of eigenfunctions $\{u_j(\cdot, \mathbf{k})\}_{j\geq 1}$ which form an orthonormal basis of $L^2(\Omega)$ and obey the equation:

$$h(\mathbf{k}) u_j(\cdot, \mathbf{k}) = E_j(\mathbf{k}) u_j(\cdot, \mathbf{k}). \tag{5.10}$$

We label $E_j(\mathbf{k})$ in *increasing* order. We have to remember that due to this choice, $E_j(\mathbf{k})$ are not differentiable with respect to $\mathbf{k}$ at crossing points. The eigenfunctions $u_j(\mathbf{x}, \mathbf{k})$ can even loose their continuity in $\mathbf{k}$ near crossing points. Without loss of generality, we may also assume that $h(\mathbf{k}) \geq 1$ for all $\mathbf{k}$ which implies:

$$E_j(\mathbf{k}) \geq 1, \quad \mathbf{k} \in \Omega^*, \quad j \geq 1. \tag{5.11}$$

One can introduce the Bloch functions:

$$\Psi_j(\mathbf{x}, \mathbf{k}) := \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{d}{2}}} u_j(\mathbf{x}, \mathbf{k}), \quad \mathbf{x} \in \mathbb{R}^d \tag{5.12}$$

which form a basis of generalized eigenfunctions of $H_\infty(0)$ in $L^2(\mathbb{R}^d)$, i.e. in distributional sense we have:

$$\int_{\Omega^*} \sum_{j\geq 1} \Psi_j(\mathbf{x}, \mathbf{k}) \overline{\Psi_j}(\mathbf{y}, \mathbf{k}) d\mathbf{k} = \delta(\mathbf{x} - \mathbf{y}).$$

Using Bloch functions, one can express the integral kernel of any function of $H_\infty(0)$ in terms of the fiber $h(\mathbf{k})$. For example, the Green function (i.e. the integral kernel of the resolvent) writes as:

$$G_\infty(\mathbf{x}, \mathbf{y}; z) = \int_{\Omega^*} \sum_{j\geq 1} \frac{\Psi_j(\mathbf{x}, \mathbf{k}) \overline{\Psi_j(\mathbf{y}, \mathbf{k})}}{E_j(\mathbf{k}) - z} d\mathbf{k}, \tag{5.13}$$

The above formula has to be understood in the distributional sense since the series on the right hand side is typically not absolutely convergent.

If $j \geq 1$, the jth Bloch band function is defined by $\mathcal{E}_j := [\min_{\mathbf{k}\in\Omega^*} E_j(\mathbf{k}), \max_{\mathbf{k}\in\Omega^*} E_j(\mathbf{k})]$. The spectrum of $H_\infty(0)$ is absolutely continuous and given (as a set of points) by $\sigma(H_\infty(0)) = \bigcup_{j=1}^\infty \mathcal{E}_j$. Note that the sets $\mathcal{E}_j$ can overlap each other in many ways, and some of them can even coincide even though they are images of increasingly ordered functions. The energy bands are disjoint unions of $\mathcal{E}_j$'s. Moreover, if $\max\mathcal{E}_j < \min\mathcal{E}_{j+1}$ for some $j \geq 1$ then we have a spectral gap. The number of spectral gaps is finite if not zero, see e.g. [47].

It remains to introduce the integrated density of states of the operator $H_\infty(0)$. Recall its definition. For any $E \in \mathbb{R}$, let $N_L(E)$ be the number of eigenvalues of $H_L(0)$ not greater than E. The integrated density of states of $H_\infty(0)$ is defined by the limit (see [30]):

$$n_\infty(E) := \lim_{L\to\infty} \frac{N_L(E)}{|\Lambda_L|} = \lim_{L\to\infty} \frac{\mathrm{Tr}\{\chi_{(-\infty,E]}(H_L(0))\}}{|\Lambda_L|} \tag{5.14}$$

and $n_\infty(\cdot)$ is a positive continuous and non-decreasing function (see e.g. [8]). In this case one can express $n_\infty(E)$ with the help of the Bloch energies in the following way:

$$n_\infty(E) = \frac{1}{(2\pi)^3} \sum_{j\geq 1} \int_{\Omega^*} \chi_{[E_0,E]}(E_j(\mathbf{k}))\, d\mathbf{k} \tag{5.15}$$

where $\chi_{[E_0,E]}(\cdot)$ is the characteristic function of the interval $[E_0, E]$. Thus n_∞ is clearly continuous in E due to the continuity of the Bloch bands. Moreover, this function is piecewise constant when E belongs to a spectral gap.

5.2 The statements of our main results

The first theorem is not directly related to the magnetic problem, and it deals with the rigorous definition of the Fermi energy for Bloch electrons. Even though these results are part of the 'physics folklore', we have not found a serious mathematical treatment in the literature.

Theorem 5.1. *Let $\rho_0 > 0$ be fixed. If $\mu_\infty(\beta, \rho_0)$ is the unique real solution of the equation $\rho_\infty\left(\beta, e^{\beta\mu}, 0\right) = \rho_0$ (see (5.6)), then the limit:*

$$\mathcal{E}_F(\rho_0) := \lim_{\beta\to\infty} \mu_\infty(\beta, \rho_0) \tag{5.16}$$

exists and defines an increasing function of ρ_0 called the Fermi energy. There can only occur two cases:

SC *(semiconductor/insulator/semimetal): Suppose that there exists some $N \in \mathbb{N}^*$ such that $\rho_0 = n_\infty(E)$ for all $E \in [\max\mathcal{E}_N, \min\mathcal{E}_{N+1}]$. Then:*

$$\mathcal{E}_F(\rho_0) = \frac{\max\mathcal{E}_N + \min\mathcal{E}_{N+1}}{2}. \tag{5.17}$$

M *(metal): Suppose that there exists a unique solution E_M of the equation $n_\infty(E_M) = \rho_0$ which belongs to $(\min \mathcal{E}_N, \max \mathcal{E}_N)$ for some (possibly not unique) N. Then :*

$$\mathcal{E}_F(\rho_0) = E_M. \tag{5.18}$$

Remark 1. In other words, a semiconductor/semimetal either has its Fermi energy in the middle of a non-trivial gap (this occurs if $\max \mathcal{E}_N < \min \mathcal{E}_{N+1}$), or where the two consecutive Bloch bands touch each other closing the gap (this occurs if $\max \mathcal{E}_N = \min \mathcal{E}_{N+1}$). As for a metal, its Fermi energy lies in the interior of a Bloch band.
Remark 2. According to the above result, $\mathcal{E}_F$ is discontinuous at all values of ρ_0 for which the equation $n_\infty(E) = \rho_0$ does not have a unique solution. Each open gap gives such a discontinuity.

Now here is our main result concerning the susceptibility of a Bloch electrons gas at fixed density and zero temperature:

Theorem 5.2. *Denote by $E_0 := \inf \sigma(H_\infty(0))$.*

(i). *Assume that the Fermi energy is in the middle of a non-trivial gap (see (5.17)). Then there exist $2N$ functions $\mathfrak{c}_j(\cdot), \mathfrak{d}_j(\cdot)$, with $1 \leq j \leq N$, defined on Ω^* outside a set of Lebesgue measure zero, such that the integrand in (5.19) can be extended by continuity to the whole of Ω^* and:*

$$\mathcal{X}_{\mathrm{SC}}(\rho_0) := \lim_{\beta\to\infty} \mathcal{X}(\beta,\rho_0) = \left(\frac{e}{c}\right)^2 \frac{1}{2}\frac{1}{(2\pi)^3} \int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{j=1}^{N} \Big\{ \mathfrak{c}_j(\mathbf{k}) + \big\{E_j(\mathbf{k}) - \mathcal{E}_F(\rho_0)\big\}\mathfrak{d}_j(\mathbf{k}) \Big\}. \tag{5.19}$$

(ii). *Suppose that there exists a unique $N \geq 1$ such that $\mathcal{E}_F(\rho_0) \in (\min \mathcal{E}_N, \max \mathcal{E}_N)$. Assume that the Fermi surface $\mathcal{S}_F := \{\mathbf{k} \in \Omega^* \,:\, E_N(\mathbf{k}) = \mathcal{E}_F(\rho_0)\}$ is smooth and non-degenerate. Then there exist $2N+1$ functions $\mathcal{F}_N(\cdot), \mathfrak{c}_j(\cdot), \mathfrak{d}_j(\cdot)$ with $1 \leq j \leq N$, defined on Ω^* outside a set of Lebesgue measure zero, in such a way that they are all continuous on $\mathcal{S}_F$ while the second integrand in (5.20) can be extended by continuity to the whole of Ω^*:*

$$\begin{aligned}
&\mathcal{X}_{\mathrm{M}}(\rho_0) := \lim_{\beta\to\infty} \mathcal{X}(\beta,\rho_0) = -\left(\frac{e}{c}\right)^2 \frac{1}{12}\frac{1}{(2\pi)^3} \qquad\qquad (5.20)\\
&\Bigg\{ \int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_N(\mathbf{k})|} \left[\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}\right)^2 - 3\mathcal{F}_N(\mathbf{k}) \right] \\
&- 6 \int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{j=1}^{N} \Big[\chi_{[E_0,\mathcal{E}_F(\rho_0)]}\big(E_j(\mathbf{k})\big)\mathfrak{c}_j(\mathbf{k}) + \big\{E_j(\mathbf{k}) - \mathcal{E}_F(\rho_0)\big\} \chi_{[E_0,\mathcal{E}_F(\rho_0)]}\big(E_j(\mathbf{k})\big)\mathfrak{d}_j(\mathbf{k}) \Big] \Bigg\}.
\end{aligned}$$

Here $\chi_{[E_0,\mathcal{E}_F(\rho_0)]}(\cdot)$ denotes the characteristic function of the interval $E_0 \leq t \leq \mathcal{E}_F(\rho_0)$.

(iii). *Let* $k_F := (6\pi^2\rho_0)^{\frac{1}{3}}$ *be the Fermi wave vector. Then in the limit of small densities,* (5.20) *gives the Landau-Peierls formula:*

$$\mathcal{X}_{\mathrm{M}}(\rho_0) = -\frac{e^2}{24\pi^2 c^2}\frac{(m_1^* m_2^* m_3^*)^{\frac{1}{3}}}{m_1^* m_2^*} k_F + o(k_F); \tag{5.21}$$

here $\left[\frac{1}{m_i^*}\right]_{1\leq i\leq 3}$ *are the eigenvalues of the positive definite Hessian matrix* $\{\partial_{ij}^2 E_1(\mathbf{0})\}_{1\leq i,j\leq 3}$.

Remark 1. The functions $\mathfrak{c}_j(\cdot)$ and $\mathfrak{d}_j(\cdot)$ with $1 \leq j \leq N$ which appear in (5.19) are the same as the ones in (5.20). All of them can be explicitely written down in terms of Bloch energy functions and their associated eigenfunctions. One can notice in (5.20) the appearance of an explicit term associated with the Nth Bloch energy function; it is only this term which will generate the linear k_F behavior in the Landau-Peierls formula.
Remark 2. The functions $\mathfrak{c}_j(\cdot)$ and $\mathfrak{d}_j(\cdot)$ might have local singularities at a set of Lebesgue measure zero where the Bloch bands might touch each other. But their combinations entering the integrands above are always bounded because the individual singularities get canceled by the sum.
Remark 3. When $m_1^* = m_2^* = m_3^* = m^*$ holds in (iii), (5.21) is nothing but the usual Landau-Peierls susceptibility formula:

$$\mathcal{X}_{\mathrm{M}}(\rho_0) \sim -\frac{e^2}{24\pi^2 m^* c^2} k_F \quad \text{when} \quad k_F \to 0. \tag{5.22}$$

Note that our expression is twice smaller than the one in [87] since we do not take into account the degeneracy related to the spin of the Bloch electrons.
Remark 4. The assumption $V \in \mathcal{C}^\infty(\mathbb{T}^3)$ can be relaxed to $V \in \mathcal{C}^r(\mathbb{T}^3)$ with $r \geq 23$. The smoothness of V plays an important role in the absolute convergence of the series defining $\mathcal{X}(\beta, \rho_0)$, before the zero-temperature limit; see [26] for a detailed discussion on sum rules and local traces for periodic operators.
Remark 5. The role of magnetic perturbation theory (see Section 3) is *crucial* when one wants to write down a formula for $\mathcal{X}(\beta, \rho_0)$ which contains no derivatives with respect to the quasi-momentum $\mathbf{k}$. Remember that the Bloch energies ordered in increasing order and their corresponding eigenfunctions are not necessarily differentiable at crossing points.
Remark 6. We do not treat the semi-metal case, in which the Fermi energy equals $\mathcal{E}_F(\rho_0) = \max \mathcal{E}_N = \min \mathcal{E}_{N+1}$ for some $N \geq 1$ (see (5.17)). This remains as a challenging open problem.

5.3 Traces per unit volume and sum rules

This subsection is devoted to another convergence issue left open in [24], and also used in the derivation of the Landau-Peierls formula. More precisely, when expressing the relevant quantities in terms of Bloch eigenfunctions and eigenvalues one arrives, by formal computations, at expressions containing multiple sums over the band indices as well as integrals over Brillouin and unit cells. The point is that the order of summation is crucial since the sums might not be absolutely convergent. The problem is more than an academic one since in practical computations finite bands models are used which amounts to truncate the infinite sums so that the question whether the sums are absolutely convergent is a crucial one. The main result of this paper is that the smoothness of the periodic potential V guarantees that such series are always absolutely convergent. The smoothness of V is not superfluous as shown by an example. Since the same kind of series appear very oftenly in solid state physics (e.g. when computing derivatives of dispersion laws) and are related to sum rules concerning various observables, we present our main technical result Theorem 5.3 in a general setting.

5.3.1 Perturbation theory and sum rules

By writing (see (5.9))

$$h(\mathbf{k}) = h(\mathbf{k}_0) + (\mathbf{k} - \mathbf{k}_0) \cdot [-i\nabla_p + \mathbf{k}_0] + \frac{1}{2}(\mathbf{k} - \mathbf{k}_0)^2 =: h(\mathbf{k}_0) + W,$$

we see that W is a regular perturbation for $h(\mathbf{k}_0)$. Assume that $E_1(\mathbf{k}_0)$ is non-degenerate. Then according to the analytic perturbation theory, $E_1(\mathbf{k})$ remains non-degenerate in a neighborhood of $\mathbf{k}_0$. Keeping $|\mathbf{k} - \mathbf{k}_0|$ small enough and using the Feshbach formula with the projection $\Pi_0 = |u_1(\cdot, \mathbf{k}_0)\rangle\langle u_1(\cdot, \mathbf{k}_0)|$ we obtain:

$$\begin{aligned} E_1(\mathbf{k}) &= \lambda(\mathbf{k}_0) + \langle u_1(\cdot, \mathbf{k}_0), W u_1(\cdot, \mathbf{k}_0)\rangle \\ &\quad - \langle W u_1(\cdot, \mathbf{k}_0), \left\{\Pi_0^\perp [h(\mathbf{k}) - E_1(\mathbf{k})]\Pi_0^\perp\right\}^{-1} W u_1(\cdot, \mathbf{k}_0)\rangle. \end{aligned} \tag{5.23}$$

By iterating the above formula we can identify in an efficient way the full Taylor expansion of E_1 around $\mathbf{k}_0$. Let us first introduce the notation:

$$\hat{\pi}_{ij}(\alpha, \mathbf{k}) := \langle u_i(\cdot, \mathbf{k}), (-i\partial_\alpha + k_\alpha) u_j(\cdot, \mathbf{k})\rangle_{L^2(\Omega)} = \int_\Omega u_i(\mathbf{x}, \mathbf{k}) \overline{[(-i\partial_\alpha + k_\alpha) u_j]}(\mathbf{x}, \mathbf{k}) d\mathbf{x}. \tag{5.24}$$

If we are interested for example in $\frac{\partial^4 E_1}{\partial k_\alpha^4}$, one of the terms building it will be proportional with:

$$\sum_{j_1 \geq 2} \hat{\pi}_{1j_1}(\alpha, \mathbf{k}) \sum_{j_2 \geq 2} \frac{\hat{\pi}_{j_1 j_2}(\alpha, \mathbf{k})}{E_{j_2}(\mathbf{k}) - E_1(\mathbf{k})} \sum_{j_3 \geq 2} \frac{\hat{\pi}_{j_2 j_3}(\alpha, \mathbf{k})}{E_{j_3}(\mathbf{k}) - E_1(\mathbf{k})} \hat{\pi}_{j_3 1}(\alpha, \mathbf{k}), \tag{5.25}$$

where the order of the sums is crucial. Each series generates an $l^2(\mathbb{N})$-summable vector for the next one. The multiple series is convergent, but not apriori absolutely convergent. This is because the inner $\hat{\pi}$'s can grow in absolute value with the energy. But we will prove in this paper that such series are always absolutely convergent if V is smooth.

Before giving some more precise results, let us make the connection with the notion of sum rules and argue why the above matrix elements may have a rapid decay with the energy if one index is kept fixed. We work in $L^2(\Omega)$ and let us omit $\mathbf{k}$ in order to simplify notation. If A is an operator which is relatively bounded to h, then we can write the identity ($t \geq 0$):

$$i\langle [A, e^{ith}Ae^{-ith}]u_m, u_m\rangle = 2\sum_{n\geq 1} |\langle Au_m, u_n\rangle|^2 \sin\{t(E_m - E_n)\}. \tag{5.26}$$

The commutator on the left hand side is well defined as a quadratic form on functions belonging to the domain of h. Now if we assume that hAh^{-N} is bounded for some $N \geq 1$, then we obtain the bound

$$|\langle Au_m, u_n\rangle| = \frac{E_m^N}{E_n}|\langle hAh^{-N}u_m, u_n\rangle|$$

which when applied to (5.26) would insure that the series defines a differentiable function at all t. If in addition we assume that we can make sense out of the double commutator $[A, [h, A]]$, then a typical sum rule would be:

$$\langle [A, [h, A]]u_m, u_m\rangle = 2\sum_{n\geq 1} |\langle Au_m, u_n\rangle|^2 \cdot (E_n - E_m). \tag{5.27}$$

If A does not commute well with h, it can happen that even if the function of t in (5.26) is continuous on $\mathbb{R}$, we cannot be sure that it is also differentiable. It is possible to give examples of Schrödinger operators which make appear the Riemann function on the right hand side of (5.26). This function is known to be everywhere continuous, but differentiable only at certain rational points not including $t = 0$.

The connection between the Faraday effect and various sum rules associated to the conductivity tensor is carefully explained in section IV of [6]. For many more rigorous aspects and applications of sum rules, see [40].

5.3.2 Traces per unit volume

Let us consider the Fermi-Dirac distribution function:

$$f_{FD}(x) = \frac{1}{e^{\beta(x-\mu)} + 1}, \quad x \in \mathbb{R}, \beta > 0, \mu \in \mathbb{R},$$

and choose the following path in the complex plane (see for comparison (4.38)):

$$\Gamma = \{x \pm i\delta :\ -1 \leq x < \infty\} \bigcup \{-1 + iy :\ -\delta \leq y \leq \delta\} \tag{5.28}$$

with a fixed $\delta \in (0, \frac{\pi}{2\beta}]$. Introduce the notation:

$$R_\infty(z) := (H_\infty - z)^{-1}. \tag{5.29}$$

The quantity we are interested in this time is a trace-per-unit-volume (provided it exists):

$$I_{\alpha_1,\ldots,\alpha_n} := \frac{1}{|\Omega|}\int_\Omega d\mathbf{x}\left\{\int_\Gamma dz f_{FD}(z)P_{\alpha_1}R_\infty(z)P_{\alpha_2}R_\infty(z)\ldots P_{\alpha_n}R_\infty(z)\right\}(\mathbf{x},\mathbf{x}). \quad (5.30)$$

We want to express the above quantity only with the help of Bloch functions and energies. The fact that the operator

$$\int_\Gamma \{P_{\alpha_1}R_\infty(z)P_{\alpha_2}R_\infty(z)\ldots P_{\alpha_n}R_\infty(z)\}\, f_{FD}(z)dz \quad (5.31)$$

has a jointly continuous integral kernel if V is smooth, can be proved with the same methods as in for example [23], even in the presence of constant magnetic fields and without any periodicity condition on V. In the periodic case the situation is somewhat simpler.

Now let us use (5.13) and (5.12) in (5.30) and perform formal computations using the completeness of Bloch functions and freely interchanging the order of various integrals and series. We would arrive at an expression as follows:

$$I_{\alpha_1,\ldots,\alpha_n} = \frac{1}{(2\pi)^d}\int_{\Omega^*} d\mathbf{k} \quad (5.32)$$
$$\left\{\sum_{j_1,\ldots,j_n\geq 1}\hat{\pi}_{j_1j_2}(\alpha_1,\mathbf{k})\ldots\hat{\pi}_{j_nj_1}(\alpha_n,\mathbf{k})\int_\Gamma \frac{f_{FD}(z)}{(E_{j_1}(\mathbf{k})-z)\ldots(E_{j_n}(\mathbf{k})-z)}dz\right\}.$$

The first question is why is (5.32) convergent? The answer is not obvious. Moreover, if we look at $\hat{\pi}_{ij}(\alpha,\mathbf{k})$ alone (assume without loss that $E_j \geq E_i$), we see that using Cauchy's inequality we obtain that it could grow like $||(-i\partial_\alpha + k_\alpha)u_i|| \sim \sqrt{E_i}$, which is not very encouraging. For some more physical background on such problems see [86].

But it turns out that if the potential is smooth enough, then we can control the growth of the momentum coefficients at least with respect to one energy. Here is our main estimate:

Theorem 5.3. *Let $M \geq 1$ be an integer and assume that $V \in C^{2M-1}(\mathbb{R}^d)$ is a Ω-periodic potential with $V \geq 1$. Then for every integer $0 \leq N \leq M$ there exists a constant C_N such that uniformly in $\mathbf{k} \in \Omega^*$, $\alpha \in \{1,\ldots,d\}$ and $s,t \geq 1$ we have the estimate (we assume without loss of generality that $E_s(\mathbf{k}) \leq E_t(\mathbf{k})$):*

$$|\hat{\pi}_{st}(\alpha,\mathbf{k})| = |\hat{\pi}_{ts}(\alpha,\mathbf{k})| \leq C_N\frac{E_s(\mathbf{k})^{N+\frac{1}{2}}}{E_t(\mathbf{k})^N}. \quad (5.33)$$

It turns out that one can use the estimate in (5.33) in order to prove absolute convergence for series like the one in (5.32). Details can be found in [CN 2].

6 Dansk résumé

Denne doktorafhandling består af fire kapitler:

1. *Spektral teori for Schrödinger og Harper operatorer med konstante magnetiske felter.* Vi er interesserede i magnetiske perturbationer, som ikke er relativt begrænsede til de uperturberede operatorer. I artiklen præsenteret her [C], betragter vi en stor klasse af diskrete Harper-lignende og kontinuerte magnetiske Schrödinger operatorer, hvis spektrale båndkanter er Lipschitz kontinuerte med hensyn til intensiteten af det konstante magnetfelt.

2. *Spredningsteori af to dimensionelle partikler under påvirkning af magnetiske felter med lang rækkevidde.* I papiret præsenteret her [CHS] ser vi på den asymptotiske opførsel af en klassisk/kvante partikel i en $2D$ magnetfelt, der er homogen af grad -1. Vi antager, at det magnetiske felt bliver aldrig nul, og at over en vis energi, den tilsvarende klassiske dynamisk system har en globalt tiltrækkende periodisk bane i en reduceret faserum. I denne energi regime, konstruerer vi en simpel evolution baseret på denne attraktor, og beviser, at den beskriver kvantedynamikken i vores system når tiden går mod uendelig.

3. *Termodynamisk opførsel af store magnetiske kvantesystemer.* I [BCL 1] og [BCL 2] beskæftiger vi os med en perfekt kvantegas i den effektive masse approksimation, og i det makrokanoniske tilstandsrum. Vi beviser, at den generelle magnetiske susceptibilitet har en termodynamisk grænse for alle tilladte kemiske potentialer, som er uniformt på kompakte mængder inkluderet i analyticitetsområdet af det makro-kanoniske tryk. Mere præcist, i [BCL 1] viser vi, at den generelle magnetiske susceptibilitet har en punktvis termodynamisk grænse i $z = 0$. [BCL2] giver beviset for, at susceptibiliteten er uniformt begrænset på kompakte mængder, som er nødvendigt for at kunne anvende Vitali's konvergens sætning. I en nyere papir [BCS 1] viser vi hvordan man kan udvide nogle af de tidligere resultater i det tilfælde hvor man arbejder med singulære potentialer.

Den næste artikel om den termodynamiske grænse for magnetiske systemer er [CN 1], og det handler om Faraday rotationen. Vi formulerer og beviser den termodynamiske grænse for den elektriske ledningsevne af Bloch systemer, samt for Verdet konstanten. I modsætning til [BCL 1,2] hvor vi anvendte magnetiske semigrupper, i [CN 1] bruger vi en metode som er baseret p magnetisk perturbationsteori for resolventer. Et andet vigtigt værktøj er den geometriske perturbationsteori kombineret med Agmon-Combes-Thomas eksponentiel lokalisering.

4. *En stringent bevis for Landau-Peierls formlen.* I [BCS 2] præsenterer vi en komplet matematisk behandling af den magnetiske susceptibilitet ved nul magnetisk felt, for en ikke-vekselvirkende Bloch elektrongas, ved en givet temperatur og partikeltæthed, for både metaller og halvledere (isolatorer). Især får vi Landau-Peierls formlen i den lave temperatur og tæthedsgrænse, som var formodet af Kjeldaas og Kohn i 1957. Nogle vigtige tekniske resultater er forklaret i [CN 2].

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