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Renormalization of the superfluid density in the two-dimensional BCS-BEC crossover

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We analyze the theoretical derivation of the beyond-mean-field equation of state for a two-dimensional gas of dilute, ultracold alkali-metal atoms in the Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein condensate (BEC) crossover. We show that at zero temperature our theory – considering Gaussian fluctuations on top of the mean-field equation of state – is in very good agreement with experimental data. Subsequently, we investigate the superfluid density at finite temperature and its renormalization due to the proliferation of vortex-antivortex pairs. By doing so, we determine the Berezinskii-Kosterlitz-Thouless (BKT) critical temperature – at which the renormalized superfluid density jumps to zero – as a function of the inter-atomic potential strength. We find that the Nelson-Kosterlitz criterion overestimates the BKT temperature with respect to the renormalization group equations, this effect being particularly relevant in the intermediate regime of the crossover.

1. Introduction

In 2004 the three-dimensional crossover between the Bardeen-Cooper-Schrieffer (BCS) regime of weakly attractive fermions to the Bose-Einstein condensate (BEC) regime of strongly-bound bosonic molecules has been realised using ultracold, two-component fermionic ^{40}K or ^6Li atoms^{1,2,3}. The crossover is obtained using a Fano-Feshbach resonance to tune the s-wave scattering length a_F of the inter-atomic potential. Recently, the two-dimensional BEC-BEC crossover has been achieved experimentally^{4,5,6,7} using a two-component fermionic ^6Li atoms confined in a (quasi-) two-dimensional geometry. The properties of two-dimensional fermions are quite different with respect to their three-dimensional counterpart, in particular, in two dimensions, attractive fermions always form a bound-state with energy $\epsilon_B \simeq \hbar^2/(ma_F^2)$, where a_F is the two-dimensional s-wave scattering length. The

fermionic single-particle spectrum is given by

$$E_{sp}(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta_0^2}, \quad (1)$$

where Δ_0 is the energy gap and μ is the chemical potential: $\mu > 0$ corresponds to the BCS regime while $\mu < 0$ corresponds to the BEC regime. Moreover, in the deep BEC regime $\mu \rightarrow -\epsilon_B/2$.

2. Two-dimensional equation of state

To study the two-dimensional BCS-BEC crossover we adopt the formalism of functional integration⁸. The partition function \mathcal{Z} of a uniform system of ultracold, dilute, interacting spin 1/2 fermions at temperature T , in a two-dimensional volume L^2 , with chemical potential μ reads

$$\mathcal{Z} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \exp\left\{-\frac{S}{\hbar}\right\}, \quad (2)$$

where the complex Grassmann field $\psi_s(\mathbf{r}, \tau)$, $\bar{\psi}_s(\mathbf{r}, \tau)$ describes the fermions, $\beta \equiv 1/(k_B T)$ with k_B Boltzmann's constant and

$$S = \int_0^{\hbar\beta} d\tau \int_{L^2} d^2\mathbf{r} \mathcal{L} \quad (3)$$

is the Euclidean action functional with Lagrangian density

$$\mathcal{L} = \bar{\psi}_s \left[\hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \quad (4)$$

g being the attractive strength ($g < 0$) of the s-wave coupling.

Through the usual Hubbard-Stratonovich transformation the Lagrangian density \mathcal{L} – quartic in the fermionic fields – can be rewritten as a quadratic form by introducing the auxiliary complex scalar field $\Delta(\mathbf{r}, \tau)$. After doing so, the effective Euclidean Lagrangian density reads

$$\mathcal{L}_e = \bar{\psi}_s \left[\hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + \bar{\Delta} \psi_\downarrow \psi_\uparrow + \Delta \bar{\psi}_\uparrow \bar{\psi}_\downarrow - \frac{|\Delta|^2}{g}. \quad (5)$$

We investigate the effect of fluctuations of the pairing field $\Delta(\mathbf{r}, t)$ around its mean-field value Δ_0 which may be taken to be real. For this reason we set

$$\Delta(\mathbf{r}, \tau) = \Delta_0 + \eta(\mathbf{r}, \tau), \quad (6)$$

where $\eta(\mathbf{r}, \tau)$ is the complex field describing pairing fluctuations. In particular, we are interested in the grand potential Ω , given by

$$\Omega = -\frac{1}{\beta} \ln(\mathcal{Z}) \simeq -\frac{1}{\beta} \ln(\mathcal{Z}_{mf} \mathcal{Z}_g) = \Omega_{mf} + \Omega_g, \quad (7)$$

where

$$\mathcal{Z}_{mf} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \exp\left\{-\frac{S_e(\psi_s, \bar{\psi}_s, \Delta_0)}{\hbar}\right\} \quad (8)$$

is the mean-field partition function and

$$\mathcal{Z}_g = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \mathcal{D}[\eta, \bar{\eta}] \exp \left\{ -\frac{S_g(\psi_s, \bar{\psi}_s, \eta, \bar{\eta}, \Delta_0)}{\hbar} \right\} \quad (9)$$

is the partition function of Gaussian pairing fluctuations. After functional integration over quadratic fields, one finds that the mean-field grand potential reads⁹

$$\Omega_{mf} = -\frac{\Delta_0^2}{g} L^2 + \sum_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} - \mu - E_{sp}(\mathbf{k}) - \frac{2}{\beta} \ln(1 + e^{-\beta E_{sp}(\mathbf{k})}) \right), \quad (10)$$

where $E_{sp}(\mathbf{k})$ is the spectrum of fermionic single-particle excitations, as defined in Eq. (1). On the other hand, the Gaussian-level grand potential is given by

$$\Omega_g = \frac{1}{2\beta} \sum_Q \ln \det(\mathbf{M}(Q)), \quad (11)$$

where $\mathbf{M}(Q)$ is the inverse propagator of Gaussian fluctuations of pairs and $Q = (\mathbf{q}, i\Omega_m)$ is the $(2+1)$ -dimensional wavevector with $\Omega_m = 2\pi m/\beta$ the Matsubara frequencies and \mathbf{q} the two-dimensional wavevector¹⁰.

The sum over Matsubara frequencies is quite complicated and it does not give a simple expression. An approximate formula¹¹ is

$$\Omega_g \simeq \frac{1}{2} \sum_{\mathbf{q}} E_{col}(\mathbf{q}) + \frac{1}{\beta} \sum_{\mathbf{q}} \ln(1 - e^{-\beta E_{col}(\mathbf{q})}), \quad (12)$$

where

$$E_{col}(\mathbf{q}) = \hbar \omega(\mathbf{q}) \quad (13)$$

is the spectrum of bosonic collective excitations with $\omega(\mathbf{q})$ derived from

$$\det(\mathbf{M}(\mathbf{q}, \omega)) = 0. \quad (14)$$

Notice that very recently a comprehensive experimental study of fermionic and bosonic elementary excitations in a homogeneous 3D strongly interacting Fermi gas through the BCS-BEC crossover has been performed using two-photon Bragg spectroscopy.¹²

In our approach (Gaussian pair fluctuation theory¹³), the grand potential is given by

$$\Omega(\mu, L^2, T, \Delta_0) = \Omega_{mf}(\mu, L^2, T, \Delta_0) + \Omega_g(\mu, L^2, T, \Delta_0), \quad (15)$$

and the energy gap Δ_0 is obtained from the (mean-field) gap equation

$$\frac{\partial \Omega_{mf}(\mu, L^2, T, \Delta_0)}{\partial \Delta_0} = 0. \quad (16)$$

The number density n is instead obtained from the number equation

$$n = -\frac{1}{L^2} \frac{\partial \Omega(\mu, L^2, T, \Delta_0(\mu, T))}{\partial \mu} \quad (17)$$

taking into account the gap equation, i.e. that Δ_0 is a function $\Delta_0(\mu, T)$ of μ and T . Notice that the Nozières-Schmitt-Rink approach¹⁴ is quite similar but neglects, in the number equation, that Δ_0 depends on μ .

3. Zero-temperature results

In the analysis of the two-dimensional attractive Fermi gas one must remember that, as opposed to the three-dimensional case, two-dimensional realistic interatomic attractive potentials always have a bound state. In particular¹⁵, the binding energy $\epsilon_B > 0$ of two fermions can be written in terms of the positive two-dimensional fermionic scattering length a_F as

$$\epsilon_B = \frac{4}{e^{2\gamma}} \frac{\hbar^2}{m a_F^2}, \quad (18)$$

where $\gamma = 0.577\dots$ is the Euler-Mascheroni constant. Moreover, the attractive s-wave interaction strength g appearing in Eq. (4) is related to the binding energy $\epsilon_B > 0$ of a fermion pair in vacuum by the expression^{16,17}

$$-\frac{1}{g} = \frac{1}{2L^2} \sum_{\mathbf{k}} \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2}\epsilon_B}. \quad (19)$$

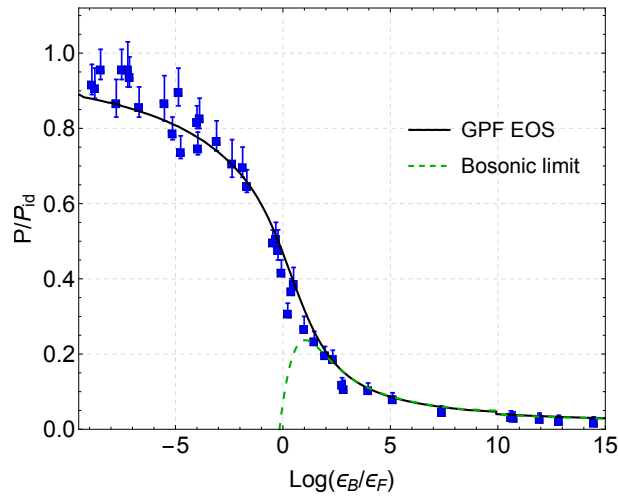


Fig. 1. Scaled pressure P/P_{id} vs scaled binding energy ϵ_B/ϵ_F . Notice that $P = -\Omega/L^2$ and P_{id} is the pressure of the ideal two-dimensional Fermi gas. Filled squares with error bars: experimental data of Makhlov *et al.*⁴. Solid black line: the regularized Gaussian pair (GP) theory¹⁸. Dashed green line: Popov equation of state, Eq. (23), of bosons with mass $m_B = 2m$.

At zero temperature, including Gaussian fluctuations, the pressure is

$$P = -\frac{\Omega}{L^2} = \frac{mL^2}{2\pi\hbar^2} (\mu + \frac{1}{2}\epsilon_B)^2 + P_g(\mu, L^2, T = 0), \quad (20)$$

with

$$P_g(\mu, L^2, T = 0) = -\frac{1}{2} \sum_{\mathbf{q}} E_{col}(\mathbf{q}). \quad (21)$$

In the full two-dimensional BCS-BEC crossover, from the regularized version of Eq. (11), we obtain numerically the zero-temperature pressure¹⁸ (see also Ref. 19). The results are shown in Fig. 1, where the agreement with the experimental data⁴ is very satisfying.

In the deep-BEC regime the chemical potential μ is negative and large in modulus. The energy of bosonic collective excitations becomes

$$E_{col}(\mathbf{q}) = \sqrt{\frac{\hbar^2 q^2}{2m} \left(\lambda \frac{\hbar^2 q^2}{2m} + 2mc_s^2 \right)} \quad (22)$$

with $\lambda = 1/4$ and $mc_s^2 = \mu + \epsilon_B/2$. Moreover, the corresponding regularized pressure – which can be obtained by means of dimensional regularization^{20,21} – reads

$$P = \frac{m}{64\pi\hbar^2} (\mu + \frac{1}{2}\epsilon_B)^2 \ln \left(\frac{\epsilon_B}{2(\mu + \frac{1}{2}\epsilon_B)} \right). \quad (23)$$

This is exactly the Popov equation of state of two-dimensional Bose gas with chemical potential $\mu_B = 2(\mu + \epsilon_B/2)$ and boson mass $m_B = 2m$. In this way we have identified the two-dimensional scattering length a_B of composite bosons as

$$a_B = \frac{1}{2^{1/2}e^{1/4}} a_F. \quad (24)$$

The value $a_B/a_F = 1/(2^{1/2}e^{1/4}) \simeq 0.551$ is in full agreement with the value $a_B/a_F = 0.55(4)$ obtained by Monte Carlo calculations²².

4. Quantized vortices and superfluid density

In Section II we have written the pairing field through Eq. (6). A different parametrisation²³ is provided by

$$\Delta(\mathbf{r}, \tau) = (\Delta_0 + \sigma(\mathbf{r}, \tau)) e^{i\theta(\mathbf{r}, \tau)}, \quad (25)$$

where $\sigma(\mathbf{r}, \tau)$ is the real field of amplitude fluctuations and $\theta(\mathbf{r}, \tau)$ is the angular field of phase fluctuations. However, Taylor-expanding the exponential of the phase, one has

$$(\Delta_0 + \sigma(\mathbf{r}, \tau)) e^{i\theta(\mathbf{r}, \tau)} = \Delta_0 + \sigma(\mathbf{r}, \tau) + i \Delta_0 \theta(\mathbf{r}, \tau) + \dots \quad (26)$$

Thus, at the Gaussian level, we can write

$$\eta(\mathbf{r}, \tau) = \sigma(\mathbf{r}, \tau) + i \Delta_0 \theta(\mathbf{r}, \tau). \quad (27)$$

After functional integration over $\sigma(\mathbf{r}, \tau)$, the Gaussian action becomes

$$S_g = \int_0^{\hbar\beta} d\tau \int_{L^2} d^2\mathbf{r} \left\{ \frac{J}{2} (\nabla\theta)^2 + \frac{\chi}{2} \left(\frac{\partial\theta}{\partial\tau} \right)^2 \right\} \quad (28)$$

where J is the phase stiffness and χ is the compressibility. This is the quantum action of the 2D continuous XY model.⁹ The superfluid density is related to the phase stiffness J by the simple formula

$$n_s = \frac{4m}{\hbar^2} J. \quad (29)$$

At the Gaussian level J depends only on fermionic single-particle excitations $E_{sp}(k)$.²⁴ However, beyond the Gaussian level also bosonic collective excitations $E_{col}(q)$ contribute²⁵. Thus, we assume the following Landau-type formula

$$n_s(T) = n - \beta \int \frac{d^2k}{(2\pi)^2} k^2 \frac{e^{\beta E_{sp}(k)}}{(e^{\beta E_{sp}(k)} + 1)^2} - \frac{\beta}{2} \int \frac{d^2q}{(2\pi)^2} q^2 \frac{e^{\beta E_{col}(q)}}{(e^{\beta E_{col}(q)} - 1)^2} \quad (30)$$

where both fermionic and bosonic elementary excitations are included.

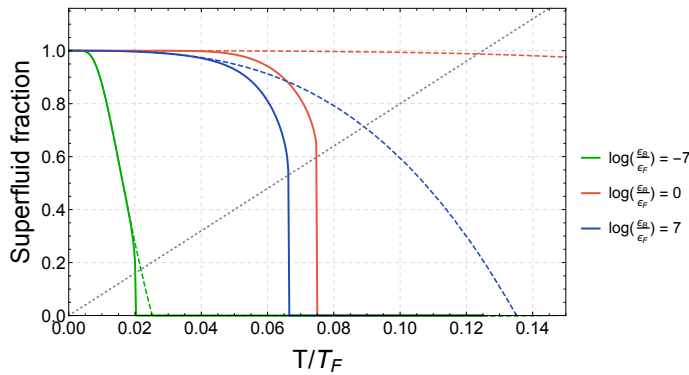


Fig. 2. Superfluid fraction n_s/n vs scaled temperature T/T_F in the two-dimensional BEC-BEC crossover.²⁶ Solid lines: renormalized superfluid density. Dashed lines: bare superfluid density. $T_F = \epsilon_F/k_B$ is the Fermi temperature. Gray dotted line: Nelson-Kosterlitz condition $k_B T = (\pi/2)J(T) = (\hbar^2\pi/(8m))n_s(T)$.

It is important to stress that the compactness of the phase angle $\theta(\mathbf{r}, t)$ implies that

$$\oint_{\mathcal{C}} \nabla \theta(\mathbf{r}, t) \cdot d\mathbf{r} = 2\pi \sum_i q_i, \quad (31)$$

where q_i is the integer number associated to quantized vortices ($q_i > 0$) and anti-vortices ($q_i < 0$) encircled by \mathcal{C} . One can write⁹

$$\nabla \theta(\mathbf{r}, t) = \nabla \theta_0(\mathbf{r}, t) - \nabla \wedge (\mathbf{u}_z \theta_v(\mathbf{r})), \quad (32)$$

where $\nabla \theta_0(\mathbf{r}, t)$ has zero circulation (no vortices) while $\theta_v(\mathbf{r})$ encodes the contribution of quantized vortices and anti-vortices, namely

$$\theta_v(\mathbf{r}) = \sum_i q_i \ln \left(\frac{|\mathbf{r} - \mathbf{r}_i|}{\xi} \right), \quad (33)$$

where \mathbf{r}_i is the position of the i -th vortex and ξ is the cutoff length defining the vortex core size, with μ_v its energy. From Eqs. (28) and (33) one finds that the attractive intraction potential of a vortex-antivortex pair (with $q_i = 1$ and $q_j = -1$) is proportional to the phase stiffness J and is given by⁹

$$V_v(\mathbf{r}_i, \mathbf{r}_j) = -2\pi J \ln \left(\frac{|\mathbf{r}_i - \mathbf{r}_j|}{\xi} \right). \quad (34)$$

The analysis of Kosterlitz and Thouless²⁷ of the two-dimensional XY model shows that:

- As the temperature T increases vortices start to appear in vortex-antivortex pairs (mainly with $q = \pm 1$).
- The pairs are bound at low temperature until, at the critical temperature T_{BKT} of Berezinskii-Kosterlitz-Thouless,^{8,9} an unbinding transition occurs above which a proliferation of free vortices and antivortices is predicted.
- The phase stiffness J and the vortex energy μ_v are renormalized due the screening of other vortex-antivortex pairs on the interaction potential (34).
- The renormalized superfluid density $n_{s,R} = J_R(4m/\hbar^2)$ decreases by increasing the temperature T and jumps to zero at T_{BKT} .
- The renormalized vortex energy $\mu_{v,R}$, that is the energy cost to produce a unbound vortex, is infinity for $T \leq T_{BKT}$.

The renormalized phase stiffness J_R is obtained from the bare one J by solving the renormalization group (RG) equations²⁸

$$\frac{d}{d\ell} K(\ell) = -4\pi^3 K(\ell)^2 y(\ell)^2 \quad (35)$$

$$\frac{d}{d\ell} y(\ell) = (2 - \pi K(\ell)) y(\ell) \quad (36)$$

for the running variables $K(\ell)$ and $y(\ell)$, as a function of the adimensional scale ℓ subjected to the initial conditions $K(\ell = 0) = J/\beta$ and $y(\ell = 0) = \exp(-\beta\mu_v)$, with $\mu_v = \pi^2 J/4$ the vortex energy²⁹. The renormalized phase stiffness is then

$$J_R = \beta K(\ell = +\infty), \quad (37)$$

and the corresponding renormalized superfluid density reads

$$n_{s,R} = \frac{4m}{\hbar^2} J_R. \quad (38)$$

In Fig. 2 we plot the superfluid fraction n_s/n as a function of the temperature T for three strengths of the BEC-BEC crossover. In the figure we report both the bare superfluid density (dashed lines) and the renormalized one (solid lines). Notice that the renormalized superfluid density satisfies the Nelson-Kosterlitz condition²⁸

$$k_B T_{BKT} = \frac{\pi}{2} J_R(T_{BKT}^-) = \frac{\hbar^2 \pi}{8m} n_{s,R}(T_{BKT}^-). \quad (39)$$

In Fig. 3 we report our theoretical predictions for the critical temperature T_{BKT} . Dot-dashed and dotted lines are obtained by using¹⁸ the Nelson-Kosterlitz condition with the bare superfluid density. This approach is called Nelson-Kosterlitz criterion. Solid and dashed lines are instead obtained by using²⁶ the Nelson-Kosterlitz condition on the renormalized superfluid density. The figure clearly shows that the inclusion of bosonic elementary excitations is crucial to get a reduction of T_{BKT}

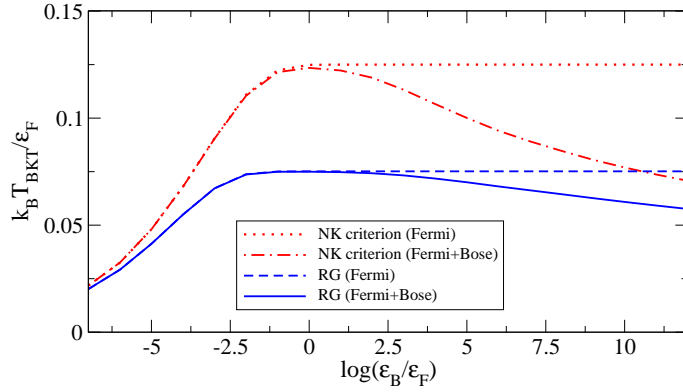


Fig. 3. Theoretical predictions for the Berezinskii-Kosterlitz-Thouless (BTK) critical temperature T_{BKT} . Red dot-dashed and dashed lines obtained by using¹⁸ the Nelson-Kosterlitz (NK) condition on the bare superfluid density (NK criterion): $k_B T_{BKT} = (\hbar^2 \pi / (8m)) n_s(T_{BKT})$. Blue solid and dashed lines obtained by solving²⁶ the renormalization group (RG) equations.

the BEC regime. Moreover, the Nelson-Kosterlitz criterion, based on the Nelson-Kosterlitz condition with the bare superfluid density instead of the renormalized one, is not accurate in the middle of the crossover.

5. Conclusions

We have shown that, after regularization of Gaussian fluctuations (for a recent comprehensive review see Ref. ³⁰), the beyond-mean-field theory of the two-dimensional BCS-BEC crossover is in very good agreement with (quasi) zero-temperature experimental data⁴. Moreover, in the BEC regime of the crossover the equation of state gives the correct logarithmic behavior characteristic of weakly-interacting repulsive bosons²⁰. At finite temperature we have found that beyond-mean-field effects, as well the contribution from quantized vortices and antivortices, determine the properties of the two-dimensional BCS-BEC crossover. In particular, the inclusion of collective bosonic excitations is essential to get a reliable determination of the superfluid density and of Berezinskii-Kosterlitz-Thouless (BKT) critical temperature, across the whole crossover. Moreover, we have shown that, in the intermediate regime of the BCS-BEC crossover, the Nelson-Kosterlitz criterion strongly overestimate the critical temperature with respect to the results obtained through the renormalization group equations.

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