Beyond-mean-field analysis of the 2D BCS-BEC crossover

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Summary

- BCS-BEC crossover in 2D
- Zero-temperature results
- Finite-temperature results
- Conclusions

BCS-BEC crossover in 2D (I)

To study the 2D BCS-BEC crossover we adopt the formalism of functional integration[1]. The partition function $\mathcal{Z}$ of the uniform system with fermionic fields $\psi_s(\mathbf{r},\tau)$ at temperature T, in a 2-dimensional volume L^2, and with chemical potential μ reads

$$\mathcal{Z} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \; \exp\left\{ -\frac{S}{\hbar} \right\} , \qquad (1)$$

where ($\beta \equiv 1/(k_B T)$ with k_B Boltzmann's constant)

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

is the Euclidean action functional with Lagrangian density

$$\mathcal{L} = \bar{\psi}_s \left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_s + \mathbf{g}\, \bar{\psi}_\uparrow \, \bar{\psi}_\downarrow \, \psi_\downarrow \, \psi_\uparrow \qquad (3)$$

where $\mathbf{g}$ is the attractive strength ($\mathbf{g} < 0$) of the s-wave coupling.

[1] N. Nagaosa, Quantum Field Theory in Condensed Matter Physics (Springer, 1999)

BCS-BEC crossover in 2D (II)

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 $\Delta(\mathbf{r}, \tau)$. In this way the effective Euclidean Lagrangian density reads

$$\mathcal{L}_e = \bar{\psi}_s \left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_s + \bar{\Delta}\,\psi_\downarrow\,\psi_\uparrow + \Delta\bar{\psi}_\uparrow\,\bar{\psi}_\downarrow - \frac{|\Delta|^2}{\mathbf{g}} \; . \tag{4}$$

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

$$\Delta(\mathbf{r}, \tau) = \Delta_0 + \eta(\mathbf{r}, \tau) \; , \tag{5}$$

where $\eta(\mathbf{r}, \tau)$ is the complex field which describes pairing fluctuations.

BCS-BEC crossover in 2D (III)

In particular, we are interested in the grand potential Ω, given by

$$\Omega = -\frac{1}{\beta} \ln \left(\mathcal{Z} \right) \simeq -\frac{1}{\beta} \ln \left(\mathcal{Z}_{mf} \mathcal{Z}_g \right) = \Omega_{mf} + \Omega_g \ , \tag{6}$$

where

$$\mathcal{Z}_{mf} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \ \exp \left\{ -\frac{S_e(\psi_s, \bar{\psi}_s, \Delta_0)}{\hbar} \right\} \tag{7}$$

is the mean-field partition function and

$$\mathcal{Z}_g = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \, \mathcal{D}[\eta, \bar{\eta}] \ \exp \left\{ -\frac{S_g(\psi_s, \bar{\psi}_s, \eta, \bar{\eta}, \Delta_0)}{\hbar} \right\} \tag{8}$$

is the partition function of Gaussian pairing fluctuations.

BCS-BEC crossover in 2D (IV)

After functional integration over quadratic fields, one finds that the mean-field grand potential reads[2]

$$\Omega_{mf} = -\frac{\Delta_0^2}{\mathbf{g}} L^2 + \sum_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} - \mu - E_{sp}(\mathbf{k}) - \frac{2}{\beta} \ln \left(1 + e^{-\beta \, E_{sp}(\mathbf{k})}\right) \right) \quad (9)$$

where

$$E_{sp}(\mathbf{k}) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu \right)^2 + \Delta_0^2} \quad (10)$$

is the spectrum of fermionic single-particle excitations.

[2] A. Altland and B. Simons, Condensed Matter Field Theory (Cambridge Univ. Press, 2006).

BCS-BEC crossover in 2D (V)

The Gaussian grand potential is instead given by

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

where $\mathbf{M}(Q)$ is the inverse propagator of Gaussian fluctuations of pairs and $Q = (\mathbf{q}, i\Omega_m)$ is the 4D wavevector with $\Omega_m = 2\pi m/\beta$ the Matsubara frequencies and $\mathbf{q}$ the 3D wavevector.[3]
The sum over Matsubara frequencies is quite complicated and it does not give a simple expression. An approximate formula[4] is

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

where

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

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

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

[3] R.B. Diener, R. Sensarma, M. Randeria, PRA **77**, 023626 (2008).
[4] E. Taylor, A. Griffin, N. Fukushima, Y. Ohashi, PRA **74**, 063626 (2006).

BCS-BEC crossover in 2D (V)

The $\mathbf{M}(Q)$ matrix is the inverse pair fluctuation propagator and describes the dynamics of the bosonic collective excitations of the theory, where

$$M_{11}(\mathbf{q}, \mathrm{i}\Omega_m) = -\frac{1}{\mathbf{g}} + \sum_{\mathbf{k}} \frac{\tanh(\beta E_{sp}(\mathbf{k})/2)}{2E_{sp}(\mathbf{k})} \times$$
$$\times \left[\frac{(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) + \frac{\hbar^2(\mathbf{k}+\mathbf{q})^2}{2m} - \mu)(E_{sp}(\mathbf{k}) + \frac{\hbar^2 k^2}{2m} - \mu)}{(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))} \right.$$
$$\left. - \frac{(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) + \frac{\hbar^2(\mathbf{k}+\mathbf{q})^2}{2m} - \mu)(E_{sp}(\mathbf{k}) - \frac{\hbar^2 k^2}{2m} + \mu)}{(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))} \right] , \quad (15)$$

and

$$M_{12}(\mathbf{q}, \mathrm{i}\Omega_m) = -\Delta_0^2 \sum_{\mathbf{k}} \frac{\tanh(\beta E_{sp}(\mathbf{k})/2)}{2E_{sp}(\mathbf{k})} \times$$
$$\times \left[\frac{1}{(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))} \right.$$
$$\left. + \frac{1}{(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))} \right] . \quad (16)$$

BCS-BEC crossover in 2D (VI)

In our approach (Gaussian pair fluctuation theory[5]), given the grand potential

$$\Omega(\mu, L^2, T, \Delta_0) = \Omega_{mf}(\mu, L^2, T, \Delta_0) + \Omega_g(\mu, L^2, T, \Delta_0) \; , \qquad (17)$$

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

$$\frac{\partial \Omega_{mf}(\mu, L^2, T, \Delta_0)}{\partial \Delta_0} = 0 \; . \qquad (18)$$

The number density n is instead obtained from the number equation

$$n = -\frac{1}{L^2} \frac{\partial \Omega(\mu, L^2, T, \Delta_0(\mu, T))}{\partial \mu} \qquad (19)$$

taking into account the gap equation, i.e. that Δ_0 depends on μ and T: $\Delta_0(\mu, T)$. Notice that the Nozieres and Schmitt-Rink approach[6] is quite similar but in the number equation it forgets that Δ_0 depends on μ.

[5] H. Hu, X-J. Liu, P.D. Drummond, EPL **74**, 574 (2006).
[6] P. Nozieres and S. Schmitt-Rink, JLTP **59**, 195 (1985).

Zero-temperature results (I)

In the analysis of the **two-dimensional attractive Fermi gas** one must remember that, contrary to the 3D case, 2D realistic interatomic attractive potentials have always a bound state. In particular[7], the binding energy $\epsilon_B > 0$ of two fermions can be written in terms of the positive 2D fermionic scattering length a_s as

$$\epsilon_B = \frac{4}{e^{2\gamma}} \frac{\hbar^2}{m{a_s}^2} \, , \tag{20}$$

where $\gamma = 0.577...$ is the Euler-Mascheroni constant. Moreover, the attractive (negative) interaction strength $\mathbf{g}$ of s-wave pairing is related to the binding energy $\epsilon_B > 0$ of a fermion pair in vacuum by the expression[8]

$$-\frac{1}{\mathbf{g}} = \frac{1}{2L^2} \sum_{\mathbf{k}} \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2}\epsilon_B} \, . \tag{21}$$

[7] C. Mora and Y. Castin, 2003, PRA **67**, 053615.

[8] M. Randeria, J-M. Duan, and L-Y. Shieh, PRL **62**, 981 (1989).

Zero-temperature results (II)

In the **2D BCS-BEC crossover**, at zero temperature ($T = 0$) the mean-field grand potential Ω_{mf} can be written as[9] ($\epsilon_B > 0$)

$$\Omega_{mf} = -\frac{mL^2}{2\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_B)^2 \ . \tag{22}$$

Using

$$n = -\frac{1}{L^2}\frac{\partial\Omega_{mf}}{\partial\mu} \tag{23}$$

one immediately finds the chemical potential μ as a function of the number density $n = N/L^2$, i.e.

$$\mu = \frac{\pi\hbar^2}{m}n - \frac{1}{2}\epsilon_B \ . \tag{24}$$

In the BCS regime, where $\epsilon_B \ll \epsilon_F$ with $\epsilon_F = \pi\hbar^2 n/m$, one finds $\mu \simeq \epsilon_F > 0$ while in the BEC regime, where $\epsilon_B \gg \epsilon_F$ one has $\mu \simeq -\epsilon_B/2 < 0$.

[9] M. Randeria, J-M. Duan, and L-Y. Shieh, PRL **62**, 981 (1989).

Zero-temperature results (III)

At zero temperature, including Gaussian fluctuations

$$\Omega = -\frac{mL^2}{2\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_B)^2 + \Omega_g(\mu, L^2, T = 0) \; . \qquad (25)$$

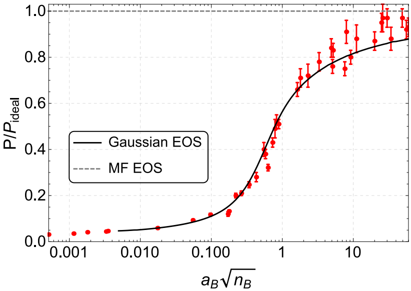
The corresponding total pressure reads

$$P = -\frac{\Omega}{L^2} = \frac{m}{2\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_B)^2 - \frac{1}{L^2}\Omega_g(\mu, L^2, T = 0) \qquad (26)$$

In the full 2D BCS-BEC crossover, from the regularized version of Eq. (11), we obtain numerically the zero-temperature pressure[10] finding, as expected, the same results of He, Lu, Cao, Hu and Liu[11]

[10] G. Bighin and LS, PRB **93**, 014519 (2016).
[11] L. He, H. Lu, G. Cao, H. Hu, X.-J. Liu, PRA **92**, 023620 (2015).

Zero-temperature results (IV)

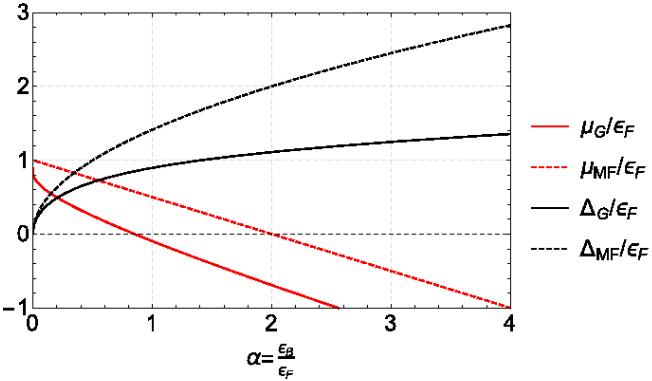


Scaled pressure P/P_{ideal} as a function of the bosonic gas parameter $a_B n_B^{1/2}$, where $P_{ideal} = 2\pi\hbar^2 n_B^2/m_B$ is the pressure of an ideal 2D gas with $m_B = 2m$ the mass of each bosonic particle (made of two fermions with mass m), a_B is the s-wave scattering length of bosons, and $n_B = n/2$ is the bosonic 2D density (with n the fermionic density). Filled squares with error bars are experimental data of Makhalov *et al.* [12]. Solid line is obtained with the regularized Gaussian theory[13]

[12] V. Makhalov et al. PRL **112**, 045301 (2014)

[13] L. He, H. Lu, G. Cao, H. Hu and X.-J. Liu, PRA **92**, 023620 (2015).

Zero-temperature results (V)



Scaled chemical potential μ/ϵ_F and scaled energy gap Δ_0/ϵ_F as a function of the scaled binding energy ϵ_B/ϵ_F. In the plot there are both mean-field results (MF) and mean-field plus Gaussian ones (G).
G. Bighin and LS, J. Phys.: Conf. Ser. **691**, 012018 (2016).

Zero-temperature results (VI)

In the deep BEC regime of the **2D BCS-BEC crossover**, where the chemical potential μ becomes strongly negative, one finds

$$\Omega = \Omega_{mf} + \Omega_g \simeq \frac{m}{2\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_B)^2 + \frac{1}{2}\sum_{\mathbf{q}} E_{col}(\mathbf{q}) \ , \qquad (27)$$

where

$$E_{col}(\mathbf{q}) \simeq \sqrt{\frac{\hbar^2 q^2}{2m}\left(\lambda\frac{\hbar^2 q^2}{2m} + 2mc_s^2\right)} \ , \qquad (28)$$

with $\lambda = 1/4$ and $mc_s^2 = \mu + \epsilon_B/2$. The corresponding regularized pressure reads[14]

$$P = \frac{m}{64\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_B)^2 \ \ln\left(\frac{\epsilon_B}{2(\mu + \frac{1}{2}\epsilon_B)}\right) \ . \qquad (29)$$

This is exactly the Popov equation of state of 2D Bose gas with chemical potential $\mu_B = 2(\mu + \epsilon_B/2)$ and mass $m_B = 2m$.

[14] LS and F. Toigo, PRA **91**, 011604(R) (2015).

Finite-temperature results (I)

Following Laudau, we write the bare superfluid density as[15]

$$n_s^{(bare)} = n - n_{n,sp} - n_{n,col} \ , \tag{30}$$

where

$$n_{n,sp} = \beta \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} k^2 \frac{e^{\beta E_{sp}(\mathbf{k})}}{(e^{\beta E_{sp}(\mathbf{k})}+1)^2} \tag{31}$$

is the normal density due to single-particle fermionic excitations, and

$$n_{n,col} = \frac{\beta}{2} \int \frac{\mathrm{d}^2\mathbf{q}}{(2\pi)^2} q^2 \frac{e^{\beta E_{col}(\mathbf{q})}}{(e^{\beta E_{col}(\mathbf{q})}-1)^2} \tag{32}$$

is the normal density due to collective bosonic excitations.[16]

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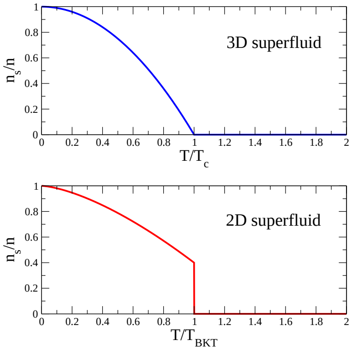
[15] G. Bighin and LS, PRB **93**, 014519 (2016).

[16] To simplify the calculation of $n_{n,sp}$ and $n_{n,col}$ we use the approximation

$$E_{col}(\mathbf{q}; \mu(T), \Delta_0(T)) \simeq E_{col}(\mathbf{q}; \mu(0), \Delta_0(0)) \ .$$

Finite-temperature results (I)

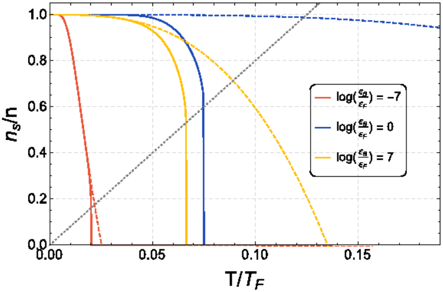
From the bare superfluid density $n_s^{(bare)}(T)$ and taking into account quantized vortices and anti-vortices we obtain[17] a renormalized superfluid density $n_s(T)$, which jumps to zero at the Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT}.



This is in contrast with the 3D case.

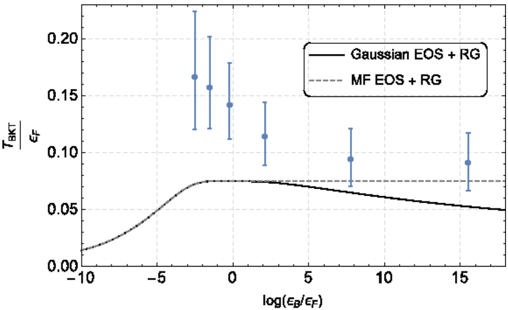
[17] G. Bighin and LS, arXiv:1703.02427, to appear in Sci. Rep. (2017).

Finite-temperature results (II)



Superfluid fraction n_s/n vs scaled temperature T/T_F for three different values of the interaction, ranging from the BCS to the BEC regime. The solid lines represent the results of the renormalization group analysis, whereas the dashed lines represent the unrenormalized result obtained from the single-particle and collective contributions to superfluid density. G. Bighin and LS, arXiv:1703.02427, to appear in Sci. Rep. (2017).

Finite-temperature results (III)



Theoretical predictions[18] for the Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT} (at which vortex-antivortex pairs unbind) compared to recent experimental observation[19] (circles with error bars).

The underestimation of experimental data can be due to:

– absence of harmonic trap in the theory,

– 3D effects in the experiment.

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[18] G. Bighin and LS, arXiv:1703.02427, to appear in Sci. Rep. (2017).

[19] P.A. Murthy et al., PRL **115**, 010401 (2015).

Conclusions

- After regularization[20] beyond-mean-field Gaussian fluctuations give remarkable effects for superfluid fermions in the 2D BCS-BEC crossover at zero temperature:
  – logarithmic behavior of the equation of state in the deep BEC regime
  – good agreement with (quasi) zero-temperature experimental data
- Also at finite temperature beyond-mean-field effects, with the inclusion of quantized vortices and antivortices, become relevant in the strong-coupling regime of 2D BCS-BEC crossover:
  – bare and renormalized superfluid density n_s
  – critical temperature T_{BKT}

[20] For a very recent comprehensive review see:
LS and F. Toigo, Zero-Point Energy of Ultracold Atoms, Phys. Rep. **640**, 1 (2016).

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