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
In 2004 the 3D BCS-BEC crossover has been observed with ultracold gases made of two-component fermionic $^{40}\text{K}$ or $^{6}\text{Li}$ alkali-metal atoms.¹

This crossover is obtained by using a Fano-Feshbach resonance to change the 3D s-wave scattering length $a_s$ of the inter-atomic potential

$$a_s = a_{bg} \left( 1 + \frac{\Delta_B}{B - B_0} \right),$$

where $B$ is the external magnetic field.

¹C.A. Regal et al., PRL 92, 040403 (2004); M.W. Zwierlein et al., PRL 92, 120403 (2004); J. Kinast et al., PRL 92, 150402 (2004).
Recently also the 2D BEC-BEC crossover has been achieved experimentally\(^2\) with a Fermi gas of two-component \(^6\text{Li}\) atoms. In 2D attractive fermions \textit{always} form biatomic molecules with bound-state energy

\[
\epsilon_B \simeq \frac{\hbar^2}{ma_s^2},
\]

(2)

where \(a_s\) is the 2D s-wave scattering length, which is experimentally tuned by a Fano-Feshbach resonance. The fermionic single-particle spectrum is given by

\[
E_{sp}(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2},
\]

(3)

where \(\Delta\) is the energy gap and \(\mu\) 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 \(\mu \to -\epsilon_B/2\).

To study the 2D BCS-BEC crossover we adopt the formalism of functional integration\(^3\). The partition function \(Z\) of the uniform system with fermionic fields \(\psi_s(r, \tau)\) at temperature \(T\), in a 2-dimensional volume \(L^2\), and with chemical potential \(\mu\) reads

\[
Z = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \exp \left\{ -\frac{S}{\hbar} \right\}, \tag{4}
\]

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

\[
S = \int_0^{\hbar \beta} d\tau \int_{L^2} d^2r \mathcal{L} \tag{5}
\]

is the Euclidean action functional with Lagrangian density

\[
\mathcal{L} = \bar{\psi}_s \left[ \hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \tag{6}
\]

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

\(^3\)N. Nagaosa, Quantum Field Theory in Condensed Matter Physics (Springer, 1999)
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

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

(7)

We investigate the effect of fluctuations of the **pairing field** $\Delta(\mathbf{r}, t)$ around its mean-field value $\Delta_0$ which may be taken to be real. For this reason we set

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

(8)

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

$$\Omega = \frac{-1}{\beta} \ln (Z) \simeq \frac{-1}{\beta} \ln (Z_{mf} Z_g) = \Omega_{mf} + \Omega_g ,$$

(9)

where

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

(10)

is the mean-field partition function and

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

(11)

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

$$\Omega_{mf} = -\frac{\Delta^2_0}{g} L^2 + \sum_k \left( \frac{\hbar^2 k^2}{2m} - \mu - E_{sp}(k) - \frac{2}{\beta} \ln \left( 1 + e^{-\beta E_{sp}(k)} \right) \right) \tag{12}$$

where

$$E_{sp}(k) = \sqrt{\left( \frac{\hbar^2 k^2}{2m} - \mu \right)^2 + \Delta^2_0} \tag{13}$$

is the spectrum of fermionic single-particle excitations.

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\(^4\)A. Altland and B. Simons, Condensed Matter Field Theory (Cambridge Univ. Press, 2006).
The Gaussian grand potential is instead given by

\[ \Omega_g = \frac{1}{2\beta} \sum_Q \ln \det(M(Q)), \quad (14) \]

where \( M(Q) \) is the inverse propagator of Gaussian fluctuations of pairs and \( Q = (q, i\Omega_m) \) is the 4D wavevector with \( \Omega_m = 2\pi m/\beta \) the Matsubara frequencies and \( q \) the 3D wavevector.5

The sum over Matsubara frequencies is quite complicated and it does not give a simple expression. An approximate formula6 is

\[ \Omega_g \approx \frac{1}{2} \sum_q E_{col}(q) + \frac{1}{\beta} \sum_q \ln (1 - e^{-\beta E_{col}(q)}), \quad (15) \]

where

\[ E_{col}(q) = \hbar \omega(q) \quad (16) \]

is the spectrum of bosonic collective excitations with \( \omega(q) \) derived from

\[ \det(M(q, \omega)) = 0. \quad (17) \]

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

$$M_{11}(q, i\Omega_m) = -\frac{1}{g} + \sum_k \frac{\tanh(\beta E_{sp}(k)/2)}{2E_{sp}(k)} \times$$

$$\times \left[ \frac{(i\Omega_m - E_{sp}(k) + \frac{\hbar^2(k+q)^2}{2m} - \mu)(E_{sp}(k) + \frac{\hbar^2k^2}{2m} - \mu)}{(i\Omega_m - E_{sp}(k) + E_{sp}(k + q))(i\Omega_m - E_{sp}(k) - E_{sp}(k + q))} \right]$$

$$- \frac{(i\Omega_m + E_{sp}(k) + \frac{\hbar^2(k+q)^2}{2m} - \mu)(E_{sp}(k) - \frac{\hbar^2k^2}{2m} + \mu)}{(i\Omega_m + E_{sp}(k) - E_{sp}(k + q))(i\Omega_m + E_{sp}(k) + E_{sp}(k + q))} \right] \right], \quad (18)$$

and

$$M_{12}(q, i\Omega_m) = -\Delta_0^2 \sum_k \frac{\tanh(\beta E_{sp}(k)/2)}{2E_{sp}(k)} \times$$

$$\times \left[ \frac{1}{(i\Omega_m - E_{sp}(k) + E_{sp}(k + q))(i\Omega_m - E_{sp}(k) - E_{sp}(k + q))} \right]$$

$$+ \frac{1}{(i\Omega_m + E_{sp}(k) - E_{sp}(k + q))(i\Omega_m + E_{sp}(k) + E_{sp}(k + q))} \right]. \quad (19)$$
In our approach (Gaussian pair fluctuation theory\(^7\)), given the grand potential

\[ \Omega(\mu, L^2, T, \Delta_0) = \Omega_{mf}(\mu, L^2, T, \Delta_0) + \Omega_g(\mu, L^2, T, \Delta_0) , \]  

the energy gap \(\Delta_0\) is obtained from the (mean-field) gap equation

\[ \frac{\partial \Omega_{mf}(\mu, L^2, T, \Delta_0)}{\partial \Delta_0} = 0 . \]  

The number density \(n\) is instead obtained from the number equation

\[ n = -\frac{1}{L^2} \frac{\partial \Omega(\mu, L^2, T, \Delta_0(\mu, T))}{\partial \mu} \]  

taking into account the gap equation, i.e. that \(\Delta_0\) depends on \(\mu\) and \(T\): \(\Delta_0(\mu, T)\). Notice that the Nozieres and Schmitt-Rink approach\(^8\) is quite similar but in the number equation it forgets that \(\Delta_0\) depends on \(\mu\).

\(^7\)H. Hu, X-J. Liu, P.D. Drummond, EPL 74, 574 (2006).
\(^8\)P. Nozieres and S. Schmitt-Rink, JLTP 59, 195 (1985).
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, the binding energy $\epsilon_B > 0$ of two fermions can be written in terms of the positive 2D fermionic scattering length $a_s$ as

$$\epsilon_B = \frac{4}{e^{2\gamma}} \frac{\hbar^2}{ma_s^2},$$

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

$$-\frac{1}{g} = \frac{1}{2L^2} \sum_k \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2}\epsilon_B}.$$
In the **2D BCS-BEC crossover**, at zero temperature \((T = 0)\) the mean-field grand potential \(\Omega_{mf}\) can be written as\(^{11}\) \((\varepsilon_B > 0)\)

\[
\Omega_{mf} = -\frac{mL^2}{2\pi\hbar^2} \left(\mu + \frac{1}{2} \varepsilon_B\right)^2.
\] (25)

Using

\[
n = -\frac{1}{L^2} \frac{\partial \Omega_{mf}}{\partial \mu}
\] (26)

one immediately finds the chemical potential \(\mu\) as a function of the number density \(n = N/L^2\), i.e.

\[
\mu = \frac{\pi\hbar^2}{m} n - \frac{1}{2} \varepsilon_B.
\] (27)

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

\(^{11}\text{M. Randeria, J-M. Duan, and L-Y. Shieh, PRL 62, 981 (1989).}\)
At zero temperature, including Gaussian fluctuations

\[ \Omega = -\frac{mL^2}{2\pi\hbar^2} (\mu + \frac{1}{2}\epsilon_B)^2 + \Omega_g(\mu, L^2, T = 0). \] (28)

The corresponding total pressure reads

\[ P = - \frac{\Omega}{L^2} = \frac{m}{2\pi\hbar^2} (\mu + \frac{1}{2}\epsilon_B)^2 - \frac{1}{L^2} \Omega_g(\mu, L^2, T = 0). \] (29)

In the full 2D BCS-BEC crossover, from the regularized version of Eq. (14), we obtain numerically the zero-temperature pressure\(^\text{12}\) finding, as expected, the same results of He, Lu, Cao, Hu and Liu\(^\text{13}\).

\(^\text{12}\)G. Bighin and LS, PRB 93, 014519 (2016).
Scaled chemical potential $\mu/\epsilon_F$ and scaled energy gap $\Delta_0/\epsilon_F$ as a function of the scaled binding energy $\epsilon_B/\epsilon_F$. 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).
Scaled pressure $P/P_{id}$ vs scaled binding energy $\epsilon_B/\epsilon_F$. Filled squares with error bars are experimental data of Makhalov et al. $^{14}$ Solid line is obtained with the regularized Gaussian theory$^{15}$. Dashed line is the Popov equation of state of bosons with mass $m_B = 2m$. $P_{id}$ is the pressure of the ideal 2D Fermi gas.

$^{14}$V. Makhalov et al. PRL 112, 045301 (2014)
$^{15}$L. He, H. Lu, G. Cao, H. Hu and X.-J. Liu, PRA 92, 023620 (2015)
In the deep BEC regime of the 2D BCS-BEC crossover, where the chemical potential $\mu$ becomes strongly negative, one finds

$$\Omega = \Omega_{mf} + \Omega_g \simeq \frac{m}{2\pi \hbar^2} (\mu + \frac{1}{2} \epsilon_B)^2 + \frac{1}{2} \sum_q E_{col}(q), \quad (30)$$

where

$$E_{col}(q) \simeq \sqrt{\frac{\hbar^2 q^2}{2m} \left( \lambda \frac{\hbar^2 q^2}{2m} + 2mc_s^2 \right)}, \quad (31)$$

with $\lambda = 1/4$ and $mc_s^2 = \mu + \epsilon_B/2$. The corresponding regularized pressure reads$^{16}$

$$P = \frac{m}{64\pi \hbar^2} (\mu + \frac{1}{2} \epsilon_B)^2 \ln \left( \frac{\epsilon_B}{2(\mu + \frac{1}{2} \epsilon_B)} \right). \quad (32)$$

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

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Finite-temperature results (I)

Following Laudau, we write the bare superfluid density as

\[ n_s^{(\text{bare})}(T) = n - n_{n,sp}(T) - n_{n,col}(T) , \]

where

\[ n_{n,sp}(T) = \beta \int \frac{d^2k}{(2\pi)^2} k^2 \frac{e^\beta E_{sp}(k)}{(e^\beta E_{sp}(k) + 1)^2} \]

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

\[ n_{n,col}(T) = \frac{\beta}{2} \int \frac{d^2q}{(2\pi)^2} q^2 \frac{e^\beta E_{col}(q)}{(e^\beta E_{col}(q) - 1)^2} \]

is the normal density due to collective bosonic excitations.\(^{18}\)

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\(^{17}\)G. Bighin and LS, PRB 93, 014519 (2016).

\(^{18}\)To simplify the calculation of \(n_{n,sp}(T)\) and \(n_{n,col}(T)\) we use the approximation

\[ E_{col}(q; \mu(T), \Delta_0(T)) \simeq E_{col}(q; \mu(0), \Delta_0(0)) \].
Finite-temperature results (II)

From the bare superfluid density $n_s^{(bare)}(T)$ and taking into account quantized vortices and anti-vortices we obtain 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.

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The effective low-energy Hamiltonian can be written as (see, for instance, N. Nagaosa, Quantum Field Theory in Condensed Matter Physics (Springer, 1999))

\[ H = \frac{J^{(\text{bare})}(T)}{2} \int d^2r (\nabla \theta(r))^2 , \]

(36)

where \( \theta(r) \) is the phase angle of the pairing field \( \Delta(r) = |\Delta(r)|e^{i\theta(r)} \) and \( J^{(\text{bare})}(T) = \frac{\hbar^2}{4m} n_s^{(\text{bare})}(T) \)

(37)

is the bare phase stiffness. One can rewrite the phase angle as follows

\[ \theta(r) = \theta_0(r) + \theta_v(r) , \]

(38)

where \( \theta_0(r) \) has zero circulation (no vortices) while \( \theta_v(r) \) encodes the contribution of quantized vortices and anti-vortices, and

\[ H = \frac{J(T)}{2} \int d^2r (\nabla \theta_0(r))^2 , \]

(39)

where \( J(T) \) is the renormalized phase stiffness.
Finite-temperature results (IV)

The renormalized phase stiffness $J(T)$ is obtained from the bare one $J^{(\text{bare})}(T)$ by solving the Kosterlitz renormalization group equations\(^{20}\).

\begin{align}
\frac{d}{d\ell} K(\ell) &= -4\pi^3 K(\ell)^2 y(\ell)^2 \quad (40) \\
\frac{d}{d\ell} y(\ell) &= (2 - \pi K(\ell)) y(\ell) \quad (41)
\end{align}

for the running variables $K(\ell)$ and $y(\ell)$, as a function of the adimensional scale $\ell$ subjected to the initial conditions $K(\ell = 0) = k_B T J^{(\text{bare})}(T)$ and $y(\ell = 0) = \exp(-\mu_c/(k_B T))$, with $\mu_c = \pi^2 J^{(\text{bare})}(T)/4$ the vortex energy\(^{21}\).

The renormalized phase stiffness is then

\[ J(T) = \frac{K(\ell = +\infty)}{k_B T}, \quad (42) \]

and the corresponding renormalized superfluid density reads

\[ n_s(T) = \frac{4m}{\hbar^2} J(T). \quad (43) \]


Superfluid fraction $n_s/n$ vs scaled temperature $T/T_F$ for three different values of the adimensional binding energy $\epsilon_B/\epsilon_F$, ranging from the BCS to the BEC regime. Solid lines: renormalized superfluid density. Dashed lines: bare superfluid density. $T_F = \epsilon_F/k_B$ is the Fermi temperature. G. Bighin and LS, Sci. Rep. 7, 45702 (2017).
Finite-temperature results (VI)

Theoretical predictions\textsuperscript{22} for the Berezinskii-Kosterlitz-Thouless critical temperature $T_{BKT}$ (at which $n_s(T) = 0$) compared to recent experimental observation\textsuperscript{23} (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.

\textsuperscript{23}P.A. Murthy et al., PRL \textbf{115}, 010401 (2015).
Conclusions

- After regularization\(^{24}\) 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 \(n_s^{(bare)}(T)\) and renormalized \(n_s(T)\) superfluid density
  - Berezinskii-Kosterlitz-Thouless critical temperature \(T_{BKT}\)

Thank you for your attention!

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