Quantized vortices in two-dimensional ultracold Fermi gases

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Summary

- BCS-BEC crossover in 3D and 2D
- 2D equation of state
- Zero-temperature 2D results
- Quantized vortices and 2D superfluid density
- Conclusions
In 2004 the 3D BCS-BEC crossover has been observed with ultracold gases made of two-component fermionic $^{40}$K or $^6$Li atoms.\textsuperscript{1}

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

\textsuperscript{1}C.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 \(^6\)Li atoms. In 2D attractive fermions always form biatomic molecules with bound-state energy

\[ \epsilon_B \simeq \frac{\hbar^2}{ma_F^2}, \tag{1} \]

where \(a_F\) is the 2D s-wave scattering length, which is experimentally tuned by a Fano-Feshbach resonance.

The fermionic single-particle spectrum is given by

\[ E_{sp}(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta_0^2}, \tag{2} \]

where \(\Delta_0\) 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

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

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

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

is the Euclidean action functional with Lagrangian density

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

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

$$\mathcal{L}_e = \bar{\psi}_s \left[ \hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + \bar{\Delta} \psi_\downarrow \psi_\uparrow + \Delta \bar{\psi}_\uparrow \bar{\psi}_\downarrow - \frac{|\Delta|^2}{g}. \quad (6)$$

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

$$\Delta(r, \tau) = \Delta_0 + \eta(r, \tau), \quad (7)$$

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

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

(8)

where

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

(9)

is the mean-field partition function and

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

(10)

is the partition function of Gaussian pairing fluctuations.
After functional integration over quadratic fields, one finds that the mean-field grand potential reads\(^4\)

\[
\Omega_{mf} = -\frac{\Delta_0^2}{g} L^2 + \sum_k \left(\frac{\hbar^2 k^2}{2m} - \mu - E_{sp}(k) - \frac{2}{\beta} \ln \left(1 + e^{-\beta E_{sp}(k)}\right)\right)
\]

(11)

where

\[
E_{sp}(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta_0^2}
\]

(12)

is the spectrum of fermionic single-particle excitations.

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

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

(13)

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 formula\(^6\) is

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

(14)

where

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

(15)

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

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

(16)


In our approach (Gaussian pair fluctuation theory\textsuperscript{7}), given the grand potential

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

(17)

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

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

(18)

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

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

(19)

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\textsuperscript{8} is quite similar but in the number equation it forgets that \( \Delta_0 \) depends on \( \mu \).

\textsuperscript{7}H. Hu, X-J. Liu, P.D. Drummond, EPL 74, 574 (2006).

\textsuperscript{8}P. Nozieres and S. Schmitt-Rink, JLTP 59, 195 (1985).
Scaled pressure $P/P_{id}$ vs scaled binding energy $\epsilon_B/\epsilon_F$. Notice that $P = -\Omega/L^2$ and $P_{id}$ is the pressure of the ideal 2D Fermi gas. Filled squares with error bars: experimental data of Makhalov et al. $^9$. Solid line: the regularized Gaussian theory$^{10}$. Dashed line: Popov equation of state of bosons with mass $m_B = 2m$.

$^9$V. Makhalov et al. PRL 112, 045301 (2014)
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\(^{11}\), the binding energy \(\epsilon_B > 0\) of two fermions can be written in terms of the positive 2D fermionic scattering length \(a_F\) as

\[
\epsilon_B = \frac{4}{e^2\gamma} \frac{\hbar^2}{ma_F^2},
\]

where \(\gamma = 0.577\ldots\) 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\(^{12}\)

\[
-\frac{1}{g} = \frac{1}{2L^2} \sum_k \frac{1}{\hbar^2k^2/2m + 1/2\epsilon_B}.
\]

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\(^{11}\)C. Mora and Y. Castin, 2003, PRA 67, 053615.

At zero temperature, including Gaussian fluctuations, the pressure is

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

with

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

In the full 2D BCS-BEC crossover, from the regularized version of Eq. (13), we obtain numerically the zero-temperature pressure\(^\text{13}\)

Notice that the energy of bosonic collective excitations becomes

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

in the deep BEC regime, with \(\lambda = 1/4\) and \(mc_s^2 = \mu + \epsilon_B/2\).

\(^{13}\)G. Bighin and LS, PRB 93, 014519 (2016).
In the deep BEC regime of the 2D BCS-BEC crossover, where the chemical potential $\mu$ becomes strongly negative, the corresponding regularized pressure (dimensional regularization \(^{14}\)) reads

$$P = \frac{m}{64\pi \hbar^2} (\mu + \frac{1}{2} \epsilon_B)^2 \ln \left( \frac{\epsilon_B}{2(\mu + \frac{1}{2} \epsilon_B)} \right).$$  \hspace{1cm} (25)

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

$$a_B = \frac{1}{2^{1/2} e^{1/4}} a_F. \hspace{1cm} (26)$$

The value $a_B/a_F = 1/(2^{1/2} e^{1/4}) \simeq 0.551$ is in full agreement with $a_B/a_F = 0.55(4)$ obtained by Monte Carlo calculations\(^ {15}\).


At the beginning we have written the pairing field as

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

(27)

where $\eta(r, \tau)$ is the complex field of pairing fluctuations. A quite different approach\textsuperscript{16} is the following

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

(28)

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

$$(\Delta_0 + \sigma(r, \tau)) e^{i\theta(r, \tau)} = \Delta_0 + \sigma(r, \tau) + i \Delta_0 \theta(r, \tau) + \ldots.$$\hspace{1cm}

(29)

Thus, at the Gaussian level, we can write

$$\eta(r, \tau) = \sigma(r, \tau) + i \Delta_0 \theta(r, \tau).$$

(30)

\textsuperscript{16}LS, P.A. Marchetti, and F. Toigo, PRA \textbf{88}, 053612 (2013).
After functional integration over $\sigma(r, \tau)$, the Gaussian action becomes

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

(31)

where $J$ is the phase stiffness and $\chi$ is the compressibility. The superfluid density is related to the phase stiffness $J$ by the simple formula

$$n_s = \frac{4m}{\hbar^2} J.$$  

(32)

At the Gaussian level $J$ depends only on fermionic single-particle excitations $E_{sp}(k)^{17}$ **Beyond the Gaussian level** also bosonic collective excitations $E_{col}(q)$ contribute.$^{18}$ Thus, we assume the following Landau-type formula

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

(33)

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$^{17}$E. Babaev and H.K. Kleinert, PRB 59, 12083 (1999).

It is important to stress that the compactness of the phase angle $\theta(r)$ implies that

$$\oint_C \nabla \theta(r) \cdot dr = 2\pi \sum_i q_i,$$

where $q_i$ is the integer number associated to quantized vortices ($q_i > 0$) and antivortices ($q_i < 0$) encircled by $C$. One can write\(^\text{19}\)

$$\nabla \theta(r) = \nabla \theta_0(r) - \nabla \wedge (u_z \psi_v(r))$$

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

$$\psi_v(r) = \sum_i q_i \ln \left( \frac{|r - r_i|}{\xi} \right),$$

where $r_i$ is the position of the i-th vortex and $\xi$ is a cutoff length.

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\(^\text{19}\)Alternatively, one has $\theta(r) = \theta_0(r) + \theta_v(r)$ with $\theta_v(r) = \sum_i q_i \arctan \left( \frac{y-y_i}{x-x_i} \right)$ because $\nabla \arctan (y/x) = -\nabla \wedge (u_z \ln (\sqrt{x^2 + y^2}/\xi))$.\footnote{Quantized vortices and 2D superfluid density (III)}
The analysis of Kosterlitz and Thouless\textsuperscript{20} on the 2D gas of quantized vortices 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 $T_c = T_{BKT}$ an unbinding transition occurs above which a proliferation of free vortices and antivortices is predicted.
- The phase stiffness $J$ and the vortex energy $\mu_v$ are renormalized.
- The renormalized superfluid density $n_{s,R} = J_R(4m/\hbar^2)$ decreases by increasing the temperature $T$ and jumps to zero at $T_c = T_{BKT}$.

The renormalized phase stiffness $J_R$ is obtained from the bare one $J$ by solving the Kosterlitz renormalization group equations:\(^{21}\)

\[
\frac{d}{d\ell} K(\ell) = -4\pi^3 K(\ell)^2 y(\ell)^2 \tag{37}
\]

\[
\frac{d}{d\ell} y(\ell) = (2 - \pi K(\ell)) y(\ell) \tag{38}
\]

for the running variables $K(\ell)$ and $y(\ell)$, as a function of the adimensional scale $\ell$ subjected to the initial conditions $K(\ell = 0) = J/\beta$ and $y(\ell = 0) = \exp(-\beta \mu_v)$, with $\mu_v = \pi^2 J/4$ the vortex energy.\(^{22}\) The renormalized phase stiffness is then

\[
J_R = \beta K(\ell = +\infty), \tag{39}
\]

and the corresponding renormalized superfluid density reads

\[
n_{s,R} = \frac{4m}{\hbar^2} J_R. \tag{40}
\]


Quantized vortices and 2D superfluid density (VI)

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

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Theoretical predictions for the Berezinskii-Kosterlitz-Thouless (BTK) critical temperature $T_{BKT}$. **Red lines** obtained by using the Nelson-Kosterlitz (NK) criterion on the bare superfluid density: $k_B T_{BKT} = (\hbar^2 \pi/(8m)) n_s(T_{BKT})$. **Blue lines** obtained by solving the renormalization group (RG) equations of Kosterlitz.

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$^{24}$G. Bighin and LS, PRB 93, 014519 (2016).

Conclusions

- After regularization\(^\text{26}\) 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 \(n_s\) and renormalized \(n_{s,R}\) superfluid density
  - Berezinskii-Kosterlitz-Thouless critical temperature \(T_{BKT}\)
- Finite-range effects of the inter-atomic potential could be included within an effective-field-theory (EFT) approach.\(^\text{27}\)

\(^{26}\)For a recent comprehensive review see LS and F. Toigo, Phys. Rep. 640, 1 (2016).
\(^{27}\)EFT for 2D dilute bosons: LS, PRL 118, 130402 (2017).
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