

Mean-field and beyond in the 2D BCS-BEC crossover

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Summary

- Condensation and superfluidity in 2D systems
- 2D Fermi gas with pairing
- Mean-field
- Zero-temperature
- Finite-temperature
- Beyond mean-field
- Open problems

Condensation and superfluidity in 2D systems

According to the **Mermin-Wagner theorem**¹ in a 2D uniform system one can find **true condensation**, i.e. off-diagonal-long-range-order (ODLRO), only at zero temperature ($T = 0$).

Nevertheless, as shown by Hohenberg² the 2D uniform system can have **quasi condensation**, i.e. algebraic-long-range-order (ALRO), below a critical finite temperature. This critical temperature is usually identified with the Berezinskii-Kosterlitz-Thouless temperature³ below which the 2D system has a finite **superfluidity**.

¹N.D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 133 (1966).

²P.C. Hohenberg, Phys. Rev. **158**, 383 (1967).

³V.L. Berezinskii, Sov. Phys. JEPT **34**, 610 (1972); J.M. Kosterlitz and D.J. Thouless, J. Phys. C **6**, 1181 (1973).

2D Fermi gas with pairing (I)

We consider a **2D neutral Fermi gas with attractive s-wave interaction**. The **partition function** \mathcal{Z} of the system at temperature T , in a region of area L^2 , and with chemical potential μ can be written as

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

where

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

is the **Euclidean action functional** and \mathcal{L} is given by

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

with $g < 0$ is the attractive strength of the s-wave coupling. Notice that $\beta = 1/(k_B T)$ with k_B the Boltzmann constant.

2D Fermi gas with pairing (II)

The **Lagrangian density** \mathcal{L} is quartic in the fermionic fields ψ_s , but one can reduce the problem to a quadratic Lagrangian density by introducing an auxiliary complex scalar field $\Delta(\mathbf{r}, \tau)$ via **Hubbard-Stratonovich transformation**⁴, which gives

$$\mathcal{Z} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \mathcal{D}[\Delta, \bar{\Delta}] \exp \{-S_e/\hbar\}, \quad (4)$$

where

$$S_e = \int_0^{\hbar\beta} d\tau \int_{L^2} d^2\mathbf{r} \mathcal{L}_e \quad (5)$$

and the (exact) **effective Euclidean Lagrangian density** \mathcal{L}_e reads

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

⁴H.T.C. Stoof, K.B. Gubbels, D.B.M. Dickerscheid, Ultracold Quantum Fields (Springer, Dordrecht, 2009).

2D Fermi gas with pairing (III)

It is a standard procedure to integrate out the quadratic fermionic fields and to get a **new effective action** S_{eff} which depends only on the auxiliary field $\Delta(\mathbf{r}, \tau)$. In this way we obtain

$$\mathcal{Z} = \int \mathcal{D}[\Delta, \bar{\Delta}] \exp \{ -S_{eff} / \hbar \} , \quad (7)$$

where

$$S_{eff} = -Tr[\ln(G^{-1})] - \int_0^{\hbar\beta} d\tau \int_{L^2} d^2\mathbf{r} \frac{|\Delta|^2}{g} \quad (8)$$

with

$$G^{-1} = \begin{pmatrix} \hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu & \Delta \\ \bar{\Delta} & \hbar\partial_\tau + \frac{\hbar^2}{2m}\nabla^2 + \mu \end{pmatrix} \quad (9)$$

We stress that at this level the effective action S_{eff} is formally exact.

Mean-field (I)

In the **mean-field approximation** one considers a constant and real gap parameter, i.e.

$$\Delta(\mathbf{r}, \tau) = \Delta_0, \quad (10)$$

and the **partition function** becomes

$$\mathcal{Z}_{mf} = \exp \{ -S_{mf} / \hbar \} = \exp \{ -\beta \Omega_{mf} \}, \quad (11)$$

where

$$\Omega_{mf} = - \sum_{\mathbf{k}} \frac{1}{\beta} [2 \ln(2 \cosh(\beta E_{\mathbf{k}}/2)) - \beta \xi_{\mathbf{k}}] - L^2 \frac{\Delta_0^2}{g} \quad (12)$$

with $\xi_{\mathbf{k}} = \hbar^2 k^2 / (2m) - \mu$ and

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_0^2}. \quad (13)$$

Mean-field (II)

The constant and real gap parameter Δ_0 is obtained from

$$\frac{\partial \Omega_{mf}}{\partial \Delta_0} = 0, \quad (14)$$

which gives the **gap equation**

$$-\frac{1}{g} = \frac{1}{L^2} \sum_{\mathbf{k}} \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}. \quad (15)$$

The integral on the right side of this equation is divergent. However, in two dimensions quite generally a **bound-state energy** ϵ_B exists. For the contact potential the bound-state equation is

$$-\frac{1}{g} = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{1}{2\frac{\hbar^2 k^2}{2m} + \epsilon_B}. \quad (16)$$

Mean-field (III)

In this way one obtains the **regularized gap equation**⁵

$$\sum_{\mathbf{k}} \left(\frac{\tanh(\beta E_{\mathbf{k}}/2)}{\frac{\hbar^2 k^2}{2m} + \frac{\epsilon_B}{2}} - \frac{1}{E_{\mathbf{k}}} \right) = 0, \quad (17)$$

which can be used to study the BCS-BEC crossover by varying the **binding energy** ϵ_B .

We observe that the binding energy ϵ_B can be written as $\epsilon_B \simeq \hbar^2/(ma_{2D})$, where a_{2D} is the 2D s-wave scattering length, such that $a_{2D} \simeq a_z \exp(-a_z/a_{3D})$ with a_{3D} the 3D scattering length and a_z the characteristic length of the transverse confinement.⁶

⁵M. Randeria, J-M. Duan, L-Y. Shieh, Phys. Rev. B **41**, 327 (1990).

⁶G. Bertaina and S. Giorgini, Phys. Rev. Lett. **106**, 110403 (2011).

Mean-field (IV)

From the thermodynamic formula

$$N = - \left(\frac{\partial \Omega_{mf}}{\partial \mu} \right)_{L^2, T} \quad (18)$$

we obtain the equation for the **total number of fermions**

$$N = \sum_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh(\beta E_{\mathbf{k}}/2) \right) . \quad (19)$$

Moreover, the equation for the $T = 0$ number of **quasi-condensed fermionic atoms**⁷ reads

$$N_0 = 2 \int d^2\mathbf{r} d^2\mathbf{r}' |\langle \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}') \rangle|^2 = \sum_{\mathbf{k}} \frac{\Delta_0^2}{2E_{\mathbf{k}}^2} \tanh(\beta E_{\mathbf{k}}/2) . \quad (20)$$

⁷LS, N. Manini, A. Parola, Phys. Rev. A **72**, 023621 (2005).

Zero-temperature properties (I)

At $T = 0$ the **grand potential** is given by

$$\Omega_{mf} = -\frac{m}{4\pi\hbar^2} L^2 \left(\mu^2 + \mu \sqrt{\mu^2 + \Delta_0^2} \right), \quad (21)$$

where the **chemical potential** μ reads

$$\mu = \epsilon_F - \frac{1}{2}\epsilon_B, \quad (22)$$

with $\epsilon_F = \pi\hbar^2 n/m$ the 2D Fermi energy, and the **gap parameter** Δ_0 is instead

$$\Delta_0 = \sqrt{2\epsilon_F\epsilon_B}. \quad (23)$$

In addition, we find⁸ this nice formula for the **condensate fraction**

$$\frac{N_0}{N} = \frac{1}{2} \frac{\frac{\pi}{2} + \arctan\left(\frac{\mu}{\Delta}\right)}{\frac{\mu}{\Delta} + \sqrt{1 + \frac{\mu^2}{\Delta^2}}}. \quad (24)$$

⁸LS, Phys. Rev. A **76**, 015601 (2007).

Zero-temperature properties (II)

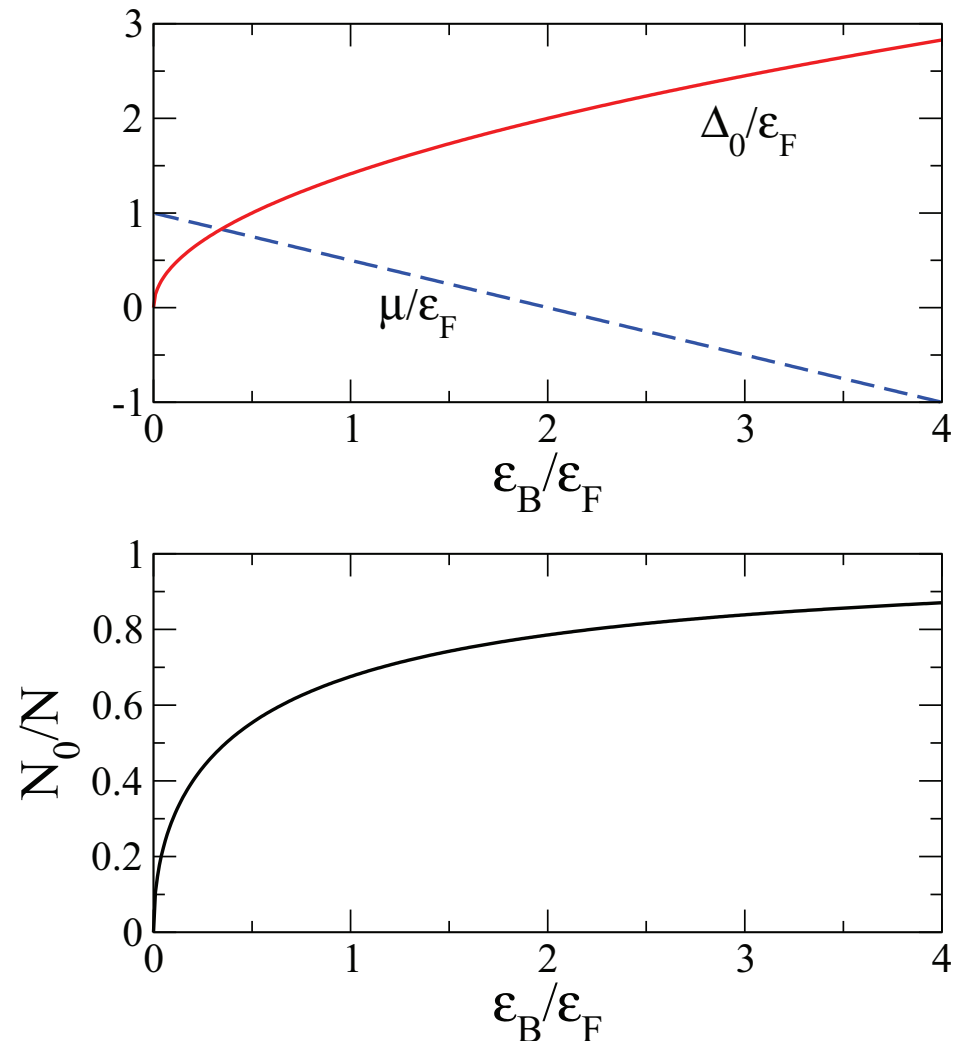


Figure: Upper panel: chemical potential μ and energy gap Δ_0 as a function of the binding energy ϵ_B of pairs. Lower panel: Bose-condensate fraction N_0/N of fermionic atoms as a function of the binding energy ϵ_B of pairs.

Zero-temperature properties (III)

According to Landau⁹ the **first sound velocity** c_s is given by

$$m c_s^2 = \left(\frac{\partial P}{\partial n} \right)_{L^2, \bar{S}}, \quad (25)$$

where P is the pressure and $\bar{S} = S/N$ is the entropy per particle of the superfluid. Moreover, at zero temperature it holds the following equality

$$\left(\frac{\partial P}{\partial n} \right)_{L^2, 0} = n \left(\frac{\partial \mu}{\partial n} \right)_{L^2}. \quad (26)$$

Using the 2D zero-temperature mean-field result

$$\mu = \epsilon_F - \frac{1}{2} \epsilon_B, \quad (27)$$

where $\epsilon_F = (\pi \hbar^2 / m) n = m v_F^2 / 2$, we finally obtain

$$c_s = \frac{v_F}{\sqrt{2}}. \quad (28)$$

⁹L.D. Landau, Journal of Physics USSR **5**, 71 (1941).

Finite-temperature properties (I)

One can explicitly calculate the temperature T^* at which $\Delta_0 = 0$. In particular, one obtains¹⁰ the following equations

$$\mu(T^*) = k_B T^* \ln \left(e^{\epsilon_F / (k_B T^*)} - 1 \right), \quad (29)$$

$$\epsilon_B = k_B T^* \frac{\pi}{\gamma} \exp \left(- \int_0^{\mu(T^*) / (2k_B T^*)} \frac{\tanh(u)}{u} du \right), \quad (30)$$

which determine T^* and $\mu(T^*)$ as a function of the binding energy ϵ_B , with $\gamma = 1.781$.

¹⁰V.P. Gusynin, V.M. Loktev, and Sharapov, J. Exp. Theor. Phys. **88**, 685 (1999).

Finite-temperature properties (II)

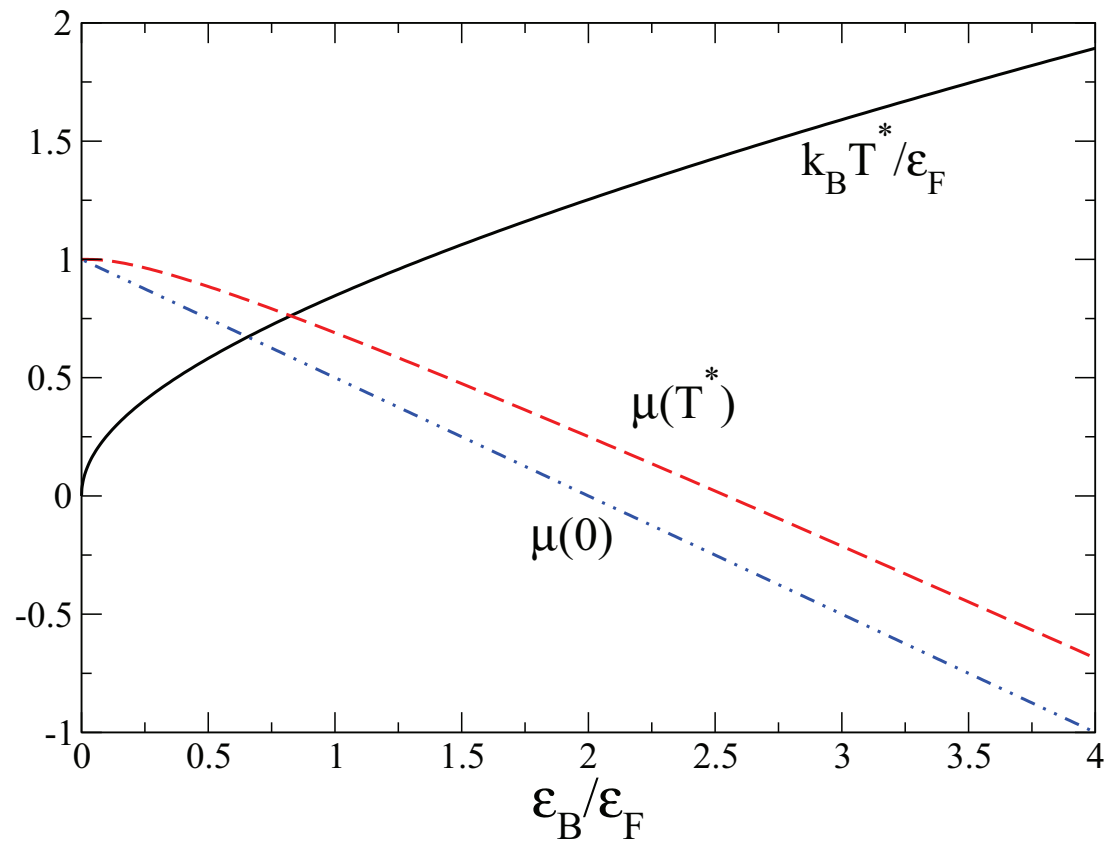


Figure: Critical temperature T^* (solid line), critical chemical potential $\mu(T^*)$ (dashed line), and zero-temperature chemical potential $\mu(0)$ as a function of the binding energy ϵ_B of pairs.

Beyond mean-field (I)

Let us now consider **beyond mean-field** effects. We have seen that the exact partition function can be written as

$$\mathcal{Z} = \int \mathcal{D}[\Delta, \bar{\Delta}] \exp \left\{ -S_{\text{eff}}[\Delta, \bar{\Delta}] / \hbar \right\} , \quad (31)$$

where $S_{\text{eff}}[\Delta, \bar{\Delta}]$ is the effective action, which is a functional of the complex bosonic auxiliary field $\Delta(\mathbf{r}, \tau)$ of pairing.

We impose that

$$\Delta(\mathbf{r}, \tau) = (\Delta_0 + \sigma(\mathbf{r}, \tau)) e^{i\theta(\mathbf{r}, \tau)} . \quad (32)$$

The partition function can be then formally written as

$$\mathcal{Z} = e^{-\beta\Omega_{mf}(\Delta_0)} \int \mathcal{D}[\sigma, \theta] \exp \left\{ -S_{\text{bmf}}[\sigma, \theta; \Delta_0] / \hbar \right\} . \quad (33)$$

Beyond mean-field (II)

Expanding $S_{bmf}[\sigma, \theta; \Delta_0]$ at the second order and functional-integrating over the **amplitude field** $\sigma(\mathbf{r}, \tau)$ one obtains¹¹

$$\mathcal{Z} = e^{-\beta\Omega_{mf}(\Delta_0)} \int \mathcal{D}[\theta] \exp \{ -S_\theta[\theta; \Delta_0]/\hbar \} , \quad (34)$$

where

$$S_\theta[\theta; \Delta_0] = \int_0^{\hbar\beta} d\tau \int_{L^2} d^2\mathbf{r} \left\{ \frac{J}{2} (\nabla\theta)^2 + \frac{K}{2} (\partial_\tau\theta)^2 \right\} \quad (35)$$

is the action functional of the **phase field** (**Goldstone field**) with J the phase stiffness and K the phase susceptibility.

At $T = 0$ we find

$$J = \frac{\epsilon_F}{4\pi} , \quad K = \frac{m}{4\pi} , \quad (36)$$

and the velocity c_θ of the Goldstone field reads

$$c_\theta = \sqrt{\frac{J}{K}} = \frac{v_F}{\sqrt{2}} = c_s . \quad (37)$$

¹¹A.M.J. Schakel, Ann. Phys. (N.Y.) **326**, 193 (2011).

Beyond mean-field (III)

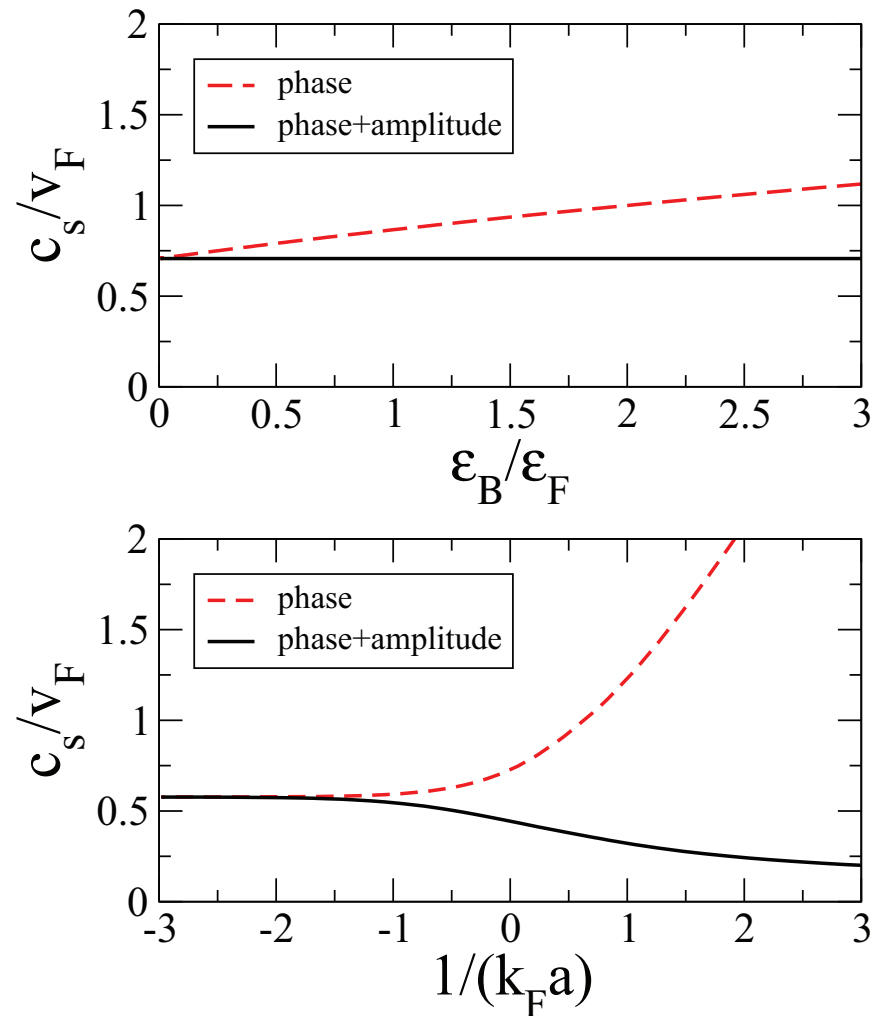


Figure: Upper panel: 2D scaled sound velocity c_s/v_F vs scaled binding energy ϵ_B/ϵ_F . Lower panel: 3D scaled sound velocity c_s/v_F vs scaled inverse interaction strength $1/(k_F a)$.

Beyond mean-field (IV)

The renormalization-group theory¹² dictates that for our 2D system the **superfluid density** n_s is zero above the **Berezinskii-Kosterlitz-Thouless critical temperature** T_{BKT} . Moreover below T_{BKT} the superfluid density can be written as

$$n_s(T) = \frac{4m}{\hbar^2} J(T) \quad \text{for } T < T_{BKT}, \quad (38)$$

and the critical temperature T_{BKT} can be estimated by solving self-consistently

$$k_B T_{BKT} = \frac{\pi}{2} J(T_{BKT}), \quad (39)$$

where $J(T)$ is the finite-temperature stiffness of our action functional S_θ of the phase.

¹²H.T.C. Stoof, K.B. Gubbels, D.B.M. Dickerscheid, Ultracold Quantum Fields (Springer, Dordrecht, 2009).

Beyond mean-field (V)

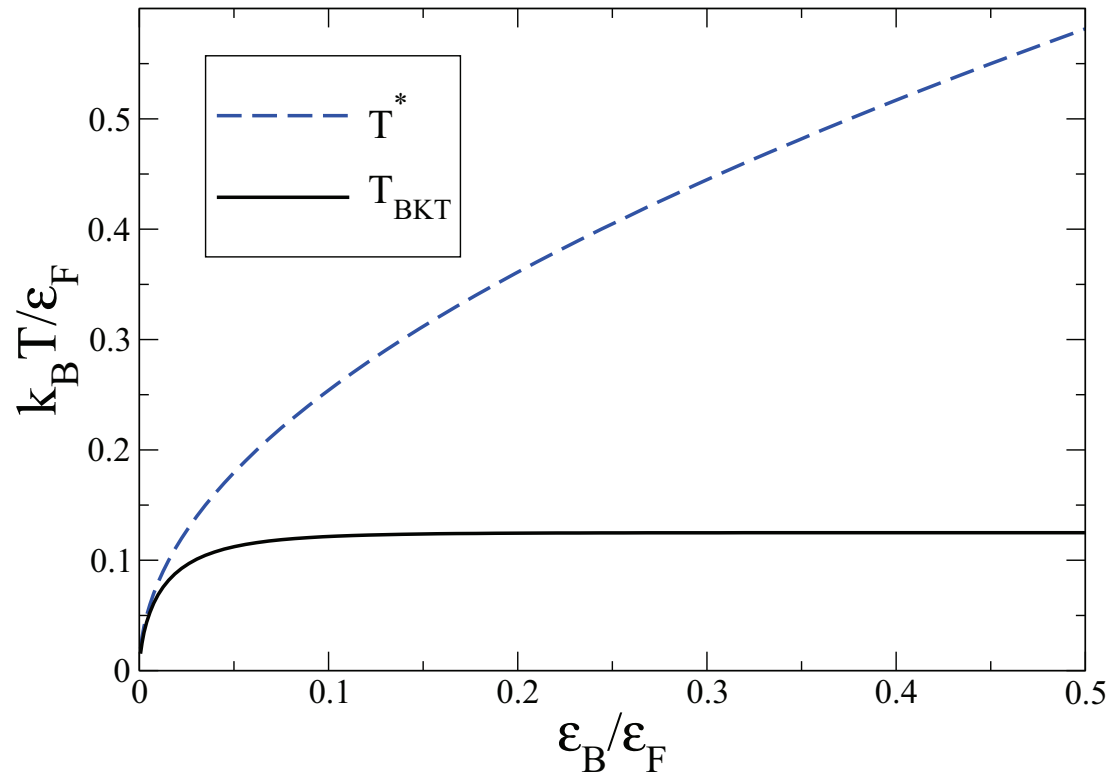


Figure: Dashed line: temperature T^* above which Δ_0 is zero; solid line: Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT} .

Beyond mean-field (VI)

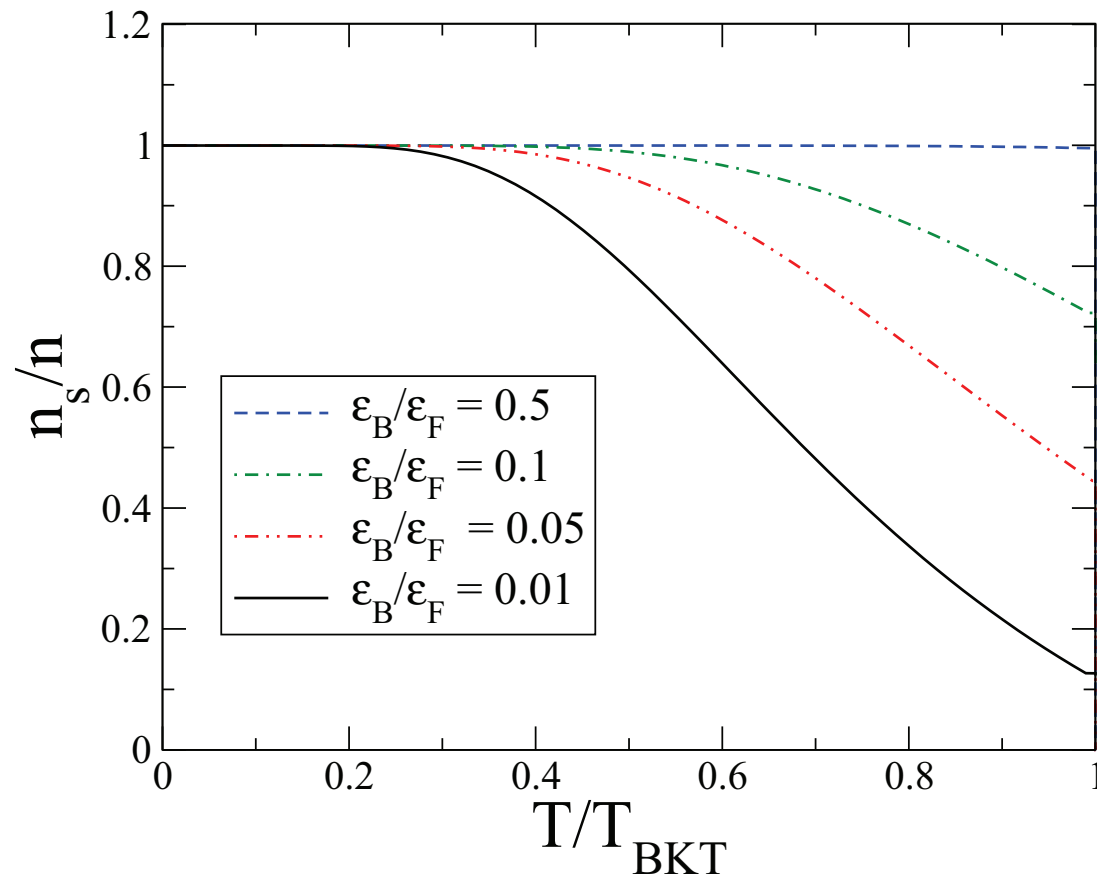


Figure: Superfluid fraction n_s/n as a function of the scaled temperature T/T_{BKT} for different values of the scaled binding energy ϵ_B/ϵ_F , where $\epsilon_F = (\hbar^2/m)\pi n$ is the Fermi energy. Above T_{BKT} one has $n_s = 0$.

Beyond mean-field (VII)

In our system the **two-body density matrix**

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \langle \bar{\psi}_\uparrow(\mathbf{r}_1, 0) \bar{\psi}_\downarrow(\mathbf{r}_2, 0) \psi_\downarrow(\mathbf{r}_3, 0) \psi_\uparrow(\mathbf{r}_4, 0) \rangle$$

shows **algebraic-long-range-order** for $0 < T < T_{BKT}$.

In particular, introducing the center-of-mass positions of the two Cooper pairs, given by $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{R}' = (\mathbf{r}_3 + \mathbf{r}_4)/2$, and their relative distances $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and $\mathbf{r}' = \mathbf{r}_4 - \mathbf{r}_3$, for $|\mathbf{R} - \mathbf{R}'| \rightarrow \infty$ we find¹

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \simeq F^*(\mathbf{r}) F(\mathbf{r}') \left(\frac{R_0}{|\mathbf{R} - \mathbf{R}'|} \right)^{\frac{k_B T}{8\pi J}}$$

where

$$F(\mathbf{r}') = \frac{1}{L^2} \sum_{\mathbf{k}} \frac{\Delta_0}{2E_k} \tanh(\beta E_k/2) e^{i\mathbf{k} \cdot \mathbf{r}'}$$

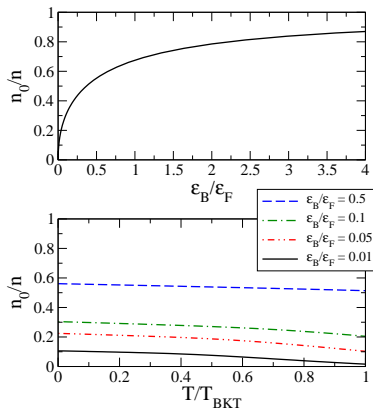
is the **mean-field wavefunction** of the **Cooper pair**.

¹LS, P.A. Marchetti, F. Toigo, arXiv:1309.7459.

Beyond mean-field (VIII)

The finite-temperature **quasi-condensate density** of atoms in the 2D superfluid is then given by

$$n_0 = 2 \int d^2\mathbf{r}' |F(\mathbf{r}')|^2 = \frac{\Delta_0^2}{2L^2} \sum_{\mathbf{k}} \frac{\tanh^2(\beta E_{\mathbf{k}}/2)}{E_{\mathbf{k}}^2}.$$



Open problems

There are several open problems regarding our 2D Fermi superfluid in the BCS-BEC crossover. Among them we mention:

- first and second sound at finite temperature
- beyond mean-field equation of state: comparison with MC results
Bertaina and Giorgini, PRL **106**, 110403 (2011)
- unbalanced system

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