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

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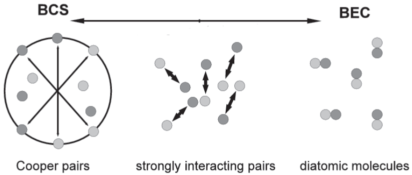
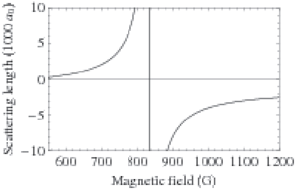
Summary

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

BCS-BEC crossover in 2D (I)

In 2004 the 3D BCS-BEC crossover has been observed with **ultracold gases made of two-component fermionic ^{40}K or ^{6}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

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

where B is the external magnetic field.

[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).

BCS-BEC crossover in 2D (II)

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

$$\epsilon_B \simeq \frac{\hbar^2}{m{a_s}^2} \,, \tag{2}$$

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

$$E_{sp}(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2} \,, \tag{3}$$

where Δ 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 $\mu \to -\epsilon_B/2$.

[2] V. Makhalov et al. PRL **112**, 045301 (2014); M.G. Ries et al., PRL **114**, 230401 (2015); I. Boettcher et al., PRL **116**, 045303 (2016).

BCS-BEC crossover in 2D (III)

To study the 2D BCS-BEC crossover we adopt the formalism of functional integration[3]. 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

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

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

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

is the Euclidean action functional with Lagrangian density

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

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

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

BCS-BEC crossover in 2D (IV)

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

$$\mathcal{L}_e = \bar{\psi}_s \left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_s + \bar{\Delta}\, \psi_\downarrow\, \psi_\uparrow + \Delta \bar{\psi}_\uparrow\, \bar{\psi}_\downarrow - \frac{|\Delta|^2}{\mathbf{g}} \; . \qquad (7)$$

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

$$\Delta(\mathbf{r}, \tau) = \Delta_0 + \eta(\mathbf{r}, \tau) \; , \qquad (8)$$

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

BCS-BEC crossover in 2D (V)

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

$$\Omega = -\frac{1}{\beta}\ln\left(\mathcal{Z}\right) \simeq -\frac{1}{\beta}\ln\left(\mathcal{Z}_{mf}\mathcal{Z}_{g}\right) = \Omega_{mf} + \Omega_{g} \ , \tag{9}$$

where

$$\mathcal{Z}_{mf} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \ \mathrm{exp}\left\{-\frac{S_e(\psi_s, \bar{\psi}_s, \Delta_0)}{\hbar}\right\} \tag{10}$$

is the mean-field partition function and

$$\mathcal{Z}_{g} = \int \mathcal{D}[\psi_s, \bar{\psi}_s]\, \mathcal{D}[\eta, \bar{\eta}] \ \ \mathrm{exp}\left\{-\frac{S_g(\psi_s, \bar{\psi}_s, \eta, \bar{\eta}, \Delta_0)}{\hbar}\right\} \tag{11}$$

is the partition function of Gaussian pairing fluctuations.

BCS-BEC crossover in 2D (VI)

After functional integration over quadratic fields, one finds that the mean-field grand potential reads[4]

$$\Omega_{mf} = -\frac{\Delta_0^2}{\mathbf{g}} L^2 + \sum_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} - \mu - E_{sp}(\mathbf{k}) - \frac{2}{\beta} \ln\left(1 + e^{-\beta E_{sp}(\mathbf{k})}\right) \right) \quad (12)$$

where

$$E_{sp}(\mathbf{k}) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu \right)^2 + \Delta_0^2} \quad (13)$$

is the spectrum of fermionic single-particle excitations.

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

BCS-BEC crossover in 2D (VII)

The Gaussian grand potential is instead given by

$$\Omega_g = \frac{1}{2\beta} \sum_Q \ln \det(\mathbf{M}(Q)) \ , \tag{14}$$

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.[5]
The sum over Matsubara frequencies is quite complicated and it does not give a simple expression. An approximate formula[6] is

$$\Omega_g \simeq \frac{1}{2} \sum_{\mathbf{q}} E_{col}(\mathbf{q}) + \frac{1}{\beta} \sum_{\mathbf{q}} \ln\left(1 - e^{-\beta\, E_{col}(\mathbf{q})}\right) \ , \tag{15}$$

where

$$E_{col}(\mathbf{q}) = \hbar\, \omega(\mathbf{q}) \tag{16}$$

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

$$\det(\mathbf{M}(\mathbf{q}, \omega)) = 0 \ . \tag{17}$$

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

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

$$M_{11}(\mathbf{q}, \mathrm{i}\Omega_m) = -\frac{1}{\mathbf{g}} + \sum_{\mathbf{k}} \frac{\tanh(\beta E_{sp}(\mathbf{k})/2)}{2E_{sp}(\mathbf{k})} \times$$
$$\times \left[\frac{(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) + \frac{\hbar^2(\mathbf{k}+\mathbf{q})^2}{2m} - \mu)(E_{sp}(\mathbf{k}) + \frac{\hbar^2 k^2}{2m} - \mu)}{(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))} \right.$$
$$\left. - \frac{(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) + \frac{\hbar^2(\mathbf{k}+\mathbf{q})^2}{2m} - \mu)(E_{sp}(\mathbf{k}) - \frac{\hbar^2 k^2}{2m} + \mu)}{(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))} \right] , \quad (18)$$

and

$$M_{12}(\mathbf{q}, \mathrm{i}\Omega_m) = -\Delta_0^2 \sum_{\mathbf{k}} \frac{\tanh(\beta E_{sp}(\mathbf{k})/2)}{2E_{sp}(\mathbf{k})} \times$$
$$\times \left[\frac{1}{(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m - E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))} \right.$$
$$\left. + \frac{1}{(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) - E_{sp}(\mathbf{k}+\mathbf{q}))(\mathrm{i}\Omega_m + E_{sp}(\mathbf{k}) + E_{sp}(\mathbf{k}+\mathbf{q}))} \right] . \quad (19)$$

BCS-BEC crossover in 2D (IX)

In our approach (Gaussian pair fluctuation theory[7]), given the grand potential

$$\Omega(\mu, L^2, T, \Delta_0) = \Omega_{mf}(\mu, L^2, T, \Delta_0) + \Omega_g(\mu, L^2, T, \Delta_0) \ , \tag{20}$$

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

$$\frac{\partial \Omega_{mf}(\mu, L^2, T, \Delta_0)}{\partial \Delta_0} = 0 \ . \tag{21}$$

The number density n is instead obtained from the number equation

$$n = -\frac{1}{L^2} \frac{\partial \Omega(\mu, L^2, T, \Delta_0(\mu, T))}{\partial \mu} \tag{22}$$

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[8] is quite similar but in the number equation it forgets that Δ_0 depends on μ.

[7] H. Hu, X-J. Liu, P.D. Drummond, EPL **74**, 574 (2006).
[8] 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[9], the binding energy $\epsilon_B > 0$ of two fermions can be written in terms of the positive 2D fermionic scattering length a_s as

$$\epsilon_B = \frac{4}{e^{2\gamma}} \frac{\hbar^2}{m{a_s}^2} \, , \tag{23}$$

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[10]

$$-\frac{1}{\mathbf{g}} = \frac{1}{2L^2} \sum_{\mathbf{k}} \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2}\epsilon_B} \, . \tag{24}$$

[9] C. Mora and Y. Castin, 2003, PRA **67**, 053615.
[10] 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[11] ($\epsilon_B > 0$)

$$\Omega_{mf} = -\frac{mL^2}{2\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_B)^2 \ . \tag{25}$$

Using

$$n = -\frac{1}{L^2}\frac{\partial\Omega_{mf}}{\partial\mu} \tag{26}$$

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

$$\mu = \frac{\pi\hbar^2}{m}n - \frac{1}{2}\epsilon_B \ . \tag{27}$$

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 $\mu \simeq -\epsilon_B/2 < 0$.

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

Zero-temperature results (III)

At zero temperature, including Gaussian fluctuations

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

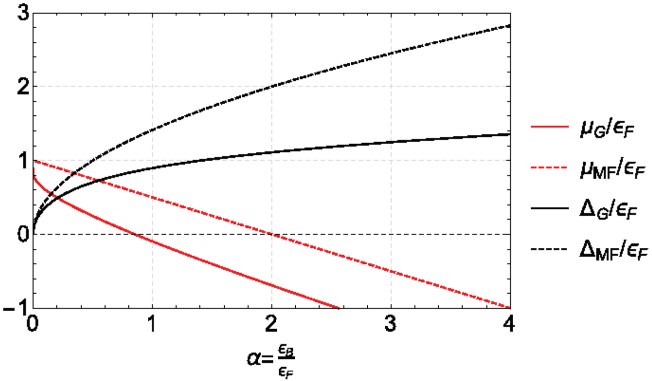
The corresponding total pressure reads

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

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

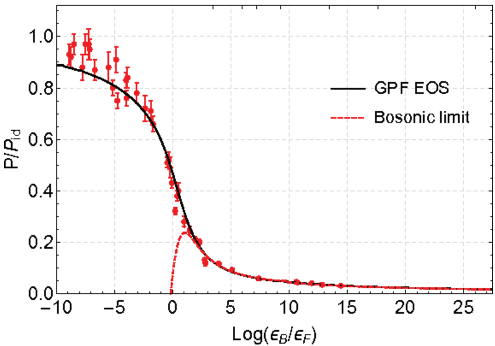
[12] G. Bighin and LS, PRB **93**, 014519 (2016).
[13] L. He, H. Lu, G. Cao, H. Hu, X.-J. Liu, PRA **92**, 023620 (2015).

Zero-temperature results (IV)



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 (V)



Scaled pressure P/P_{id} vs scaled binding energy ϵ_B/ϵ_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)

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

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

where

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

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

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

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

[16] LS and F. Toigo, PRA **91**, 011604(R) (2015); LS, PRL **118**, 130402 (2017).

Finite-temperature results (I)

Following Laudau, we write the bare superfluid density as[17]

$$n_s^{(bare)}(T) = n - n_{n,sp}(T) - n_{n,col}(T) \ , \tag{33}$$

where

$$n_{n,sp}(T) = \beta \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} k^2 \frac{e^{\beta E_{sp}(\mathbf{k})}}{(e^{\beta E_{sp}(\mathbf{k})}+1)^2} \tag{34}$$

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

$$n_{n,col}(T) = \frac{\beta}{2} \int \frac{\mathrm{d}^2\mathbf{q}}{(2\pi)^2} q^2 \frac{e^{\beta E_{col}(\mathbf{q})}}{(e^{\beta E_{col}(\mathbf{q})}-1)^2} \tag{35}$$

is the normal density due to collective bosonic excitations.[18]

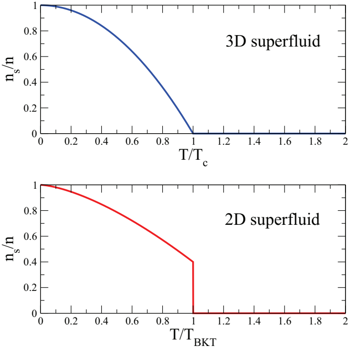
[17] G. Bighin and LS, PRB **93**, 014519 (2016).

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

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

Finite-temperature results (II)

From the bare superfluid density $n_s^{(bare)}(T)$ and taking into account quantized vortices and anti-vortices we obtain[19] 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.

[19] G. Bighin and LS, Sci. Rep. **7**, 45702 (2017).

Finite-temperature results (III)

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

$$H = \frac{J^{(bare)}(T)}{2} \int \mathrm{d}^2\mathbf{r}\, (\boldsymbol{\nabla}\theta(\mathbf{r}))^2 \ , \tag{36}$$

where $\theta(\mathbf{r})$ is the phase angle of the pairing field $\Delta(\mathbf{r}) = |\Delta(\mathbf{r})|e^{\mathrm{i}\theta(\mathbf{r})}$ and

$$J^{(bare)}(T) = \frac{\hbar^2}{4m} n_s^{(bare)}(T) \tag{37}$$

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

$$\theta(\mathbf{r}) = \theta_0(\mathbf{r}) + \theta_v(\mathbf{r}) \ , \tag{38}$$

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

$$H = \frac{J(T)}{2} \int \mathrm{d}^2\mathbf{r}\, (\boldsymbol{\nabla}\theta_0(\mathbf{r}))^2 \ , \tag{39}$$

where $J(T)$ is the renormalized phase stiffness.

Finite-temperature results (IV)

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

$$\frac{\mathrm{d}}{\mathrm{d}\ell}K(\ell) = -4\pi^3 K(\ell)^2 y(\ell)^2 \quad (40)$$

$$\frac{\mathrm{d}}{\mathrm{d}\ell}y(\ell) = (2 - \pi K(\ell))\, y(\ell) \quad (41)$$

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

The renormalized phase stiffness is then

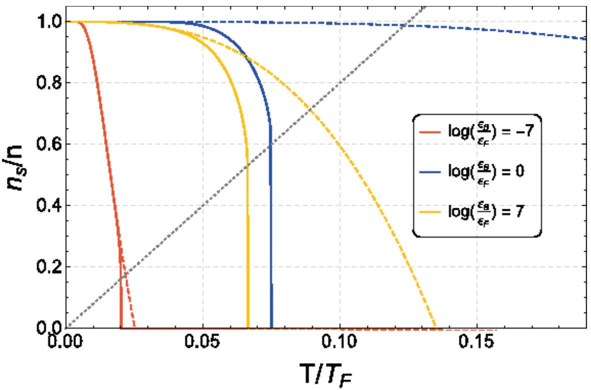
$$J(T) = \frac{K(\ell = +\infty)}{k_B T} \, , \quad (42)$$

and the corresponding renormalized superfluid density reads

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

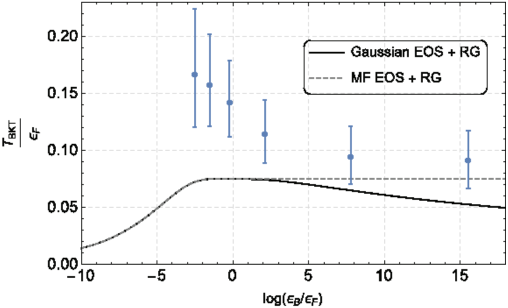
[20] D.R. Nelson and J.M. Kosterlitz, PRL **39**, 1201 (1977)
[21] W. Zhang, G.D. Lin, and L.M. Duan, PRA **78**, 043617 (2008).

Finite-temperature results (V)



Superfluid fraction n_s/n vs scaled temperature T/T_F for three different values of the adimensional binding energy ϵ_B/ϵ_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[22] for the Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT} (at which $n_s(T) = 0$) compared to recent experimental observation[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.

[22] G. Bighin and LS, Sci. Rep. **7**, 45702 (2017).

[23] P.A. Murthy et al., PRL **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}

[24] 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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