Finite-Size Effects in the 2D BCS-BEC Crossover

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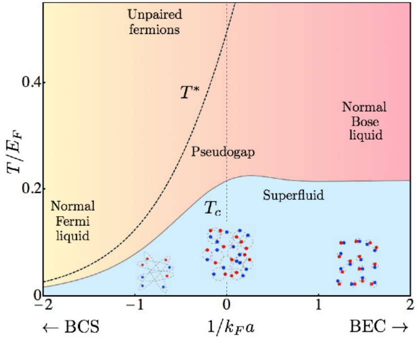
Summary

- 2D Fermi gas in the BCS-BEC crossover
- Superfluid density and BKT
- Finite size effects
- Conclusions

2D Fermi gas in the BCS-BEC crossover (I)

Twenty years ago the 3D BCS-BEC crossover has been observed with **ultracold gases made of two-component fermionic ^{40}K or ^{6}Li atoms.**[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.

[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).

2D Fermi gas in the BCS-BEC crossover (II)

Ten years ago also the 2D BEC-BEC crossover has been achieved experimentally[2] with a **Fermi gas of two-component ^{6}Li atoms**.

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 is related to the 2D scattering length a_F by

$$\epsilon_B = \frac{4}{e^{2\gamma}} \frac{\hbar^2}{m{a_F}^2} \, , \tag{1}$$

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 by the expression[3]

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

[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); K. Fenech et al., PRL **116**, 045302 (2016).

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

2D Fermi gas in the BCS-BEC crossover (III)

To study the 2D BCS-BEC crossover we adopt the formalism of functional integration[4]. 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

$$\mathcal{Z} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \; \exp\left\{ -\frac{S}{\hbar} \right\} , \tag{3}$$

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

$$S = \int_0^{\hbar\beta} d\tau \int_{L^2} d^2\mathbf{r} \; \mathcal{L} \tag{4}$$

is the Euclidean action functional with Lagrangian density

$$\mathcal{L} = \bar{\psi}_s \left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_s + \mathbf{g}\, \bar{\psi}_\uparrow \, \bar{\psi}_\downarrow \, \psi_\downarrow \, \psi_\uparrow \tag{5}$$

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

[4] S. S. Botelho and C. A. R. Sa de Melo, PRL **96**, 040404 (2006)

2D Fermi gas in the BCS-BEC crossover (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

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

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

$$\Delta(\mathbf{r},\tau) = \Delta_0 + \eta(\mathbf{r},\tau) \ , \qquad (7)$$

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

2D Fermi gas in the BCS-BEC crossover (V)

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

$$\Omega = -\frac{1}{\beta} \ln\left(\mathcal{Z}\right) \simeq -\frac{1}{\beta} \ln\left(\mathcal{Z}_{mf} \mathcal{Z}_g\right) = \Omega_{mf} + \Omega_g \ , \tag{8}$$

where

$$\mathcal{Z}_{mf} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \ \exp\left\{ -\frac{S_e(\psi_s, \bar{\psi}_s, \Delta_0)}{\hbar} \right\} \tag{9}$$

is the mean-field partition function and

$$\mathcal{Z}_g = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \, \mathcal{D}[\eta, \bar{\eta}] \ \exp\left\{ -\frac{S_g(\psi_s, \bar{\psi}_s, \eta, \bar{\eta}, \Delta_0)}{\hbar} \right\} \tag{10}$$

is the partition function of Gaussian pairing fluctuations.

2D Fermi gas in the BCS-BEC crossover (VI)

After functional integration over quadratic fields, one finds that the mean-field grand potential[5] reads

$$\Omega_{mf} = -\frac{\Delta_0^2}{\mathbf{g}} L^2 + \sum_{\mathbf{k}} \left(\frac{\hbar^2 k^2}{2m} - \mu - E_{sp}(\mathbf{k}) - \frac{2}{\beta} \ln \left(1 + e^{-\beta\, E_{sp}(\mathbf{k})}\right) \right) \quad (11)$$

where

$$E_{sp}(\mathbf{k}) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} - \mu \right)^2 + \Delta_0^2} \quad (12)$$

is the spectrum of fermionic single-particle excitations.

[5] J. Tempere, S. N. Klimin, J. T. Devreese, PRA **79**, 053637 (2009).

2D Fermi gas in the BCS-BEC crossover (VII)

The Gaussian grand potential is instead given by

$$\Omega_g = \frac{1}{2\beta} \sum_Q \ln \det(\mathbf{M}(Q)) \; , \tag{13}$$

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 2D wavevector.[6]

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

$$\Omega_g \simeq \frac{1}{2} \sum_{\mathbf{q}} E_{col}(\mathbf{q}) + \frac{1}{\beta} \sum_{\mathbf{q}} \ln\left(1 - e^{-\beta\, E_{col}(\mathbf{q})}\right) \; , \tag{14}$$

where

$$E_{col}(\mathbf{q}) = \hbar\, \omega(\mathbf{q}) \tag{15}$$

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

$$\det(\mathbf{M}(\mathbf{q}, \omega)) = 0 \; . \tag{16}$$

[6] H. Kurkjian, S.N. Klimin, J. Tempere, and Y. Castin, PRL **122**, 09340 (2019).

2D Fermi gas in the BCS-BEC crossover (VIII)

In our approach, 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 gap equation

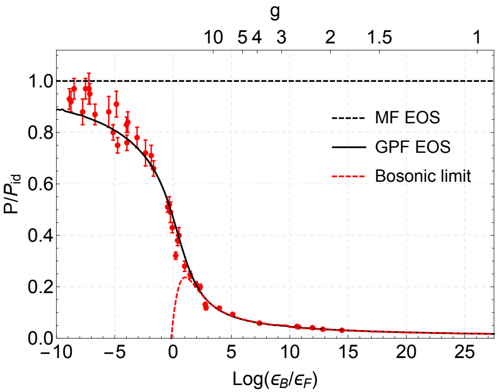
$$\frac{\partial \Omega_{mf}(\mu, L^2, T, \Delta_0)}{\partial \Delta_0} = 0 \ . \qquad (18)$$

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: $\Delta_0(\mu, T)$.

2D Fermi gas in the BCS-BEC crossover (IX)



Zero-temperature scaled pressure P/P_{id} vs scaled binding energy ϵ_B/ϵ_F. Notice that $P = -\Omega/L^2$ and P_{id} is the pressure of the ideal 2D Fermi gas. Filled circles with error bars: experimental data of Makhalov *et al.* [7]. Solid line: our regularized Gaussian theory.[8] Figure adapted from G. Bighin and LS, PRB **93**, 014519 (2016).

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

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

Superfluid density and BKT (I)

We are now interested on the temperature dependence of superfluidy density $n_s(T)$ of the system.
At the Gaussian level $n_s(T)$ depends only on fermionic single-particle excitations $E_{sp}(k)$.[9] **Beyond the Gaussian level** also bosonic collective excitations $E_{col}(q)$ contribute.[10]
Thus, we assume the following Landau-type formula for the superfluid density[11]

$$n_s(T) = n - \beta \int \frac{\mathrm{d}^2 k}{(2\pi)^2} k^2 \frac{e^{\beta E_{sp}(k)}}{(e^{\beta E_{sp}(k)}+1)^2} - \frac{\beta}{2} \int \frac{\mathrm{d}^2 q}{(2\pi)^2} q^2 \frac{e^{\beta E_{col}(q)}}{(e^{\beta E_{col}(q)}-1)^2} \, . \tag{20}$$

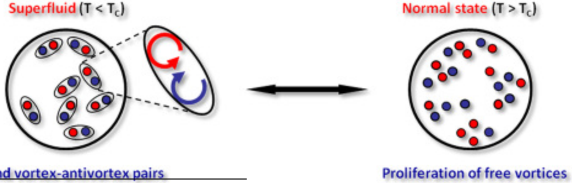
Clearly, this bare superfluid density must be renormalized using the flow equations of Kosterlitz-Thouless-Nelson, which take into account the effect of **quantized vortices and anti-vortices**.

[9] E. Babaev and H.K. Kleinert, PRB **59**, 12083 (1999).
[10] L. Benfatto, A. Toschi, and S. Caprara, PRB **69**, 184510 (2004).
[11] G. Bighin and LS, Phys. Rev. B **93**, 014519 (2016).

Superfluid density and BKT (II)

The analysis of **Kosterlitz** and **Thouless**[12] applied to 2D superfluids shows that:

- As the temperature T increases vortices start to appear in vortex-antivortex pairs.
- The pairs are bound at low temperature until at the Berezinskii-Kosterlitz-Thouless critical temperature $T_c = T_{BKT}$ an unbinding transition occurs above which a proliferation of free vortices and antivortices is predicted.
- The superfluid density $n_s(T)$ is renormalized by the presence of vortex-antivortex pairs.
- The renormalized superfluid density $n_{s,R}(T)$ decreases by increasing the temperature T and jumps to zero at $T_c = T_{BKT}$.



[12] J.M. Kosterlitz and D.J. Thouless, J. Phys. C **6**, 1181 (1973).

Superfluid density and BKT (III)

We have seen that the renormalized superfluid density $n_{s,R}(T)$ jumps to zero at a critical temperature T_{BKT}.
Moreover, one finds the Nelson-Kosterlitz condition[13]

$$k_B T_{BKT} = \frac{\hbar^2 \pi}{8m} n_{s,R}(T_{BKT}^-) \ . \tag{21}$$

Often the following Nelson-Kosterlitz criterion is adopted

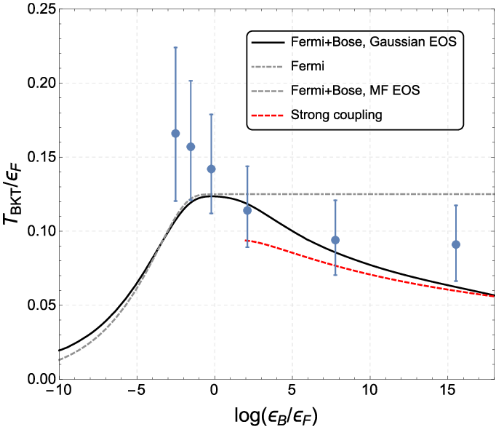
$$k_B T_{BKT} = \frac{\hbar^2 \pi}{8m} n_s(T_{BKT}) \ , \tag{22}$$

with $n_s(T)$ **instead of** $n_{s,R}(T)$. In this way one gets an approximated[14] T_{BKT} without the effort of calculating the renormalized superfluid density $n_{s,R}(T)$.

[13] D.R. Nelson and J.M. Kosterlitz, Phys Rev. Lett. **39**, 1201 (1977).

[14] An improved approach based on the RG equations of Kosterlitz and Thouless can be found in G. Bighin and LS, Sci. Rep. **7**, 45702 (2017).

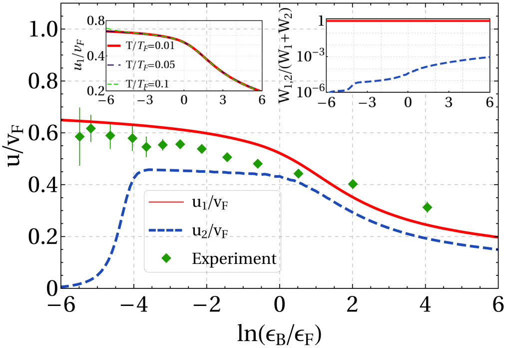
Superfluid density and BKT (IV)



Our theoretical predictions[15] for the Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT} compared to experimental observation[16] (filled circles with error bars).

[15] G. Bighin and LS, Phys. Rev. B **93**, 014519 (2016).
[16] P.A. Murthy et al., PRL **115**, 010401 (2015).

Superfluid density and BKT (V)



First sound velocity u_1 (**red solid line**) and **second sound** velocity u_2 (**blue dashed line**) along the BCS-BEC crossover, at temperature $T/T_F = 0.01$, with $T_F = \epsilon_F/k_B$ and $v_F = \sqrt{2\epsilon_F/m}$. **Green points**: measurements of the first sound [M. Bohlen *et al.* PRL **124**, 240403 (2020).] Right inset: relative contribution to the density response of u_1 (red solid line) and u_2 (blue dashed line). Figure adapted from A. Tononi, A. Capellaro, G. Bighin, and LS, PRA **103**, L061303 (2021).

Finite-size effects (I)

Finite-size effects are included through an infrared cutoff

$$k_{min} = \frac{2\pi}{L} \tag{23}$$

in the wavenumber k of the quantum particle of mass m with L the size of the confined system. We consider a box confinement such that

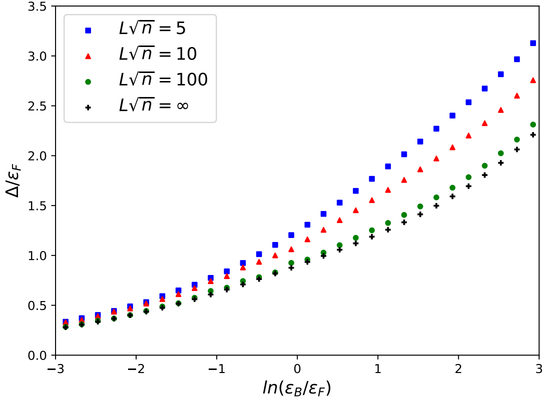
$$\epsilon_{min} = \frac{\hbar^2 k_{min}}{2m} \tag{24}$$

is the lowest single-particle energy of the non-interacting Schrödinger problem.
From the gap equation, in presence of the cutoff, we get

$$\Delta_0 = \sqrt{\epsilon_B^2 + 2(\epsilon_{min} + \mu)\epsilon_B} \tag{25}$$

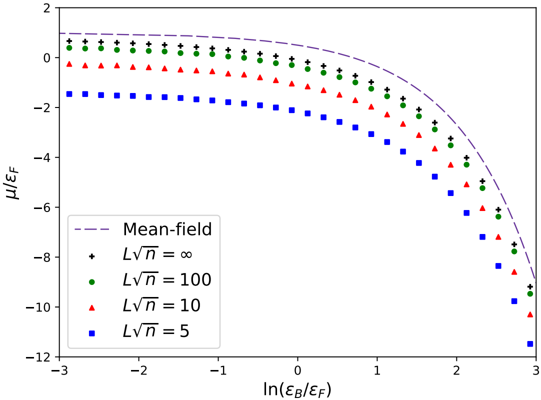
where ϵ_B is the binding energy and μ is the chemical potential, obtained by solving the number equation at the mean-field level supplemented by the Gaussian contribution.

Finite-size effects (II)



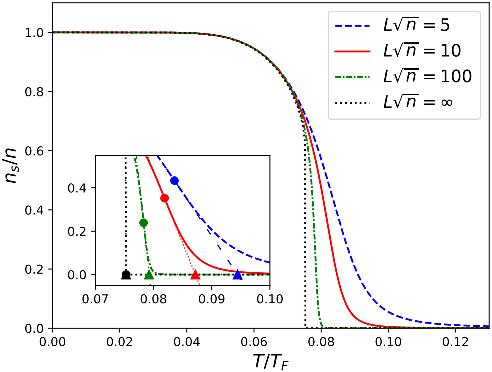
In the panel we show Δ_0/ϵ_F versus ϵ_B/ϵ_F for different values of the cutoff, respectively $L\sqrt{n}$=5 (blue squared points), 10 (red triangled points), 100 (green rounded points) and ∞ (black plus points). Here $L = 2\pi/k_{min}$ with k_{min} the infrared cutoff while $\sqrt{n} = 1/d$, with d inter-particle distance. In this way, $L\sqrt{n}$ is an adimensional quantity. Figure adapted from M. Lanaro, G. Bighin, L. Dell'Anna, and LS, PRB **109**, 104511 (2024).

Finite-size effects (III)



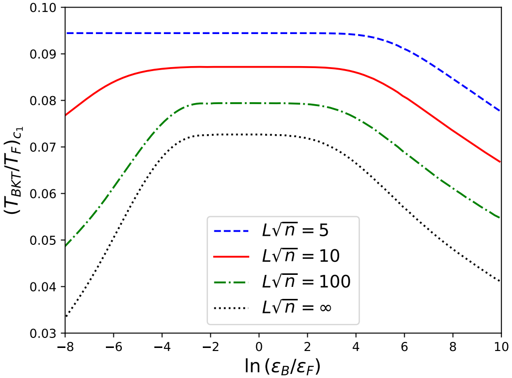
In the panel we show μ/ϵ_F versus ϵ_B/ϵ_F for different values of the cutoff, respectively $L\sqrt{n}$=5 (blue squared points), 10 (red triangled points), 100 (green rounded points) and ∞ (black plus points). We have also included (dashed line) the mean-field chemical potential μ. Figure adapted from M. Lanaro, G. Bighin, L. Dell'Anna, and LS, PRB **109**, 104511 (2024).

Finite-size effects (IV)



(Main plot) The superfluid density n_s/n versus T/T_F at fixed value of $\ln(\epsilon_B/\epsilon_F) = 0.92$, for $L\sqrt{n}$=5 (blue dashed line), 10 (red solid line), 100 (green dashed-dotted line) and ∞ (black dotted line). (Inset) Zoom of the main plot. The inflection points of the superfluid density are depicted by round points while the triangular points are placed at the intersections of the slope at the inflection points with the T-axis. Figure adapted from M. Lanaro, G. Bighin, L. Dell'Anna, and LS, PRB **109**, 104511 (2024).

Finite-size effects (V)



The critical temperature obtained through the intersection between the tangent to the superfluid density at the inflection point and the horizontal line $n_s/n = 0$, i.e. $(T_{BKT}/T_F)_{c_1}$ against $\ln(\epsilon_B/\epsilon_F)$. Figure adapted from M. Lanaro, G. Bighin, L. Dell'Anna, and LS, PRB **109**, 104511 (2024).

Conclusions

- In the **BCS-BEC crossover of the 2D Fermi gas**, to get a good agreement with experimental data for the equation of state, the critical temperature T_{BKT}, and the sound modes, both fermionic single-particle excitations and bosonic collective excitations are needed.
- The **finite size** has been introduced through an infrared cutoff in momentum space. Setting a minimum value to the wave-vector corresponds, indeed, to setting a maximum value to the wave-length, which is the size of the system.
- We have analyzed the effects of the **finite size** in several thermodynamic properties, such as the chemical potential, the energy gap and the superfluid density, going beyond the mean-field level by including Gaussian quantum fluctuations.
- We have also identified the putative Berezinskii-Kosterlitz-Thouless (BTK) phase transition at **finite size**.

Acknowledgements

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