Equation of state of composite bosons in the BCS-BEC crossover

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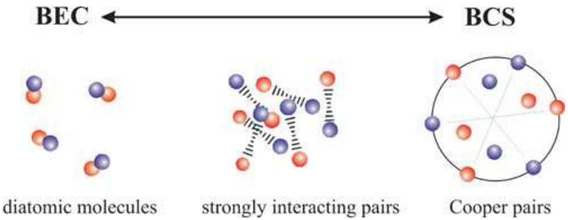
Summary

- The BCS-BEC crossover
- Formalism for a *D*-dimensional Fermi superfluid
- Results of the 3D model at T=0
- Results of the 2D model at T=0
- Conclusions

The BCS-BEC crossover (I)

In 2004 the 3D BCS-BEC crossover has been observed with **ultracold gases made of fermionic ^{40}K and ^{6}Li alkali-metal atoms.**[1]



This crossover is obtained by changing (with a Feshbach resonance) the s-wave scattering length a_F of the inter-atomic potential:
– $a_F \to 0^-$ (BCS regime of weakly-interacting Cooper pairs)
– $a_F \to \pm\infty$ (unitarity limit of strongly-interacting Cooper pairs)
– $a_F \to 0^+$ (BEC regime of bosonic dimers)

[1] C.A. Regal et al., PRL **92**, 040403 (2004); M.W. Zwierlein et al., PRL **92**, 120403 (2004); M. Bartenstein, A. Altmeyer et al., PRL **92**, 120401 (2004); J. Kinast et al., PRL **92**, 150402 (2004).

The BCS-BEC crossover (II)

The crossover from a BCS superfluid ($a_F < 0$) to a BEC of molecular pairs ($a_F > 0$) has been investigated experimentally around a Feshbach resonance, where the s-wave scattering length a diverges, and it has been shown that the system is (meta)stable.
The detection of quantized vortices under rotation[2] has clarified that this dilute gas of ultracold atoms is superfluid.
Usually the BCS-BEC crossover is analyzed in terms of

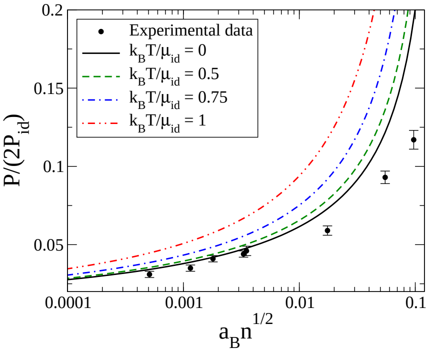
$$y = \frac{1}{k_F a_F} \qquad (1)$$

the inverse scaled interaction strength, where $k_F = (3\pi^2 n)^{1/3}$ is the Fermi wave number and n the total density.
The system is dilute because $r_e k_F \ll 1$, with r_e the effective range of the inter-atomic potential.

[2] M.W. Zwierlein *et al.*, Science **311**, 492 (2006); M.W. Zwierlein *et al.*, Nature **442**, 54 (2006)

The BCS-BEC crossover (III)

In 2014 also the 2D BEC-BEC crossover has been achieved[3] with a **quasi-2D Fermi gas of ^{6}Li atoms** with widely tunable s-wave interaction, measuring the pressure P *vs* the gas parameter $a_B n^{1/2}$.



Filled circles with error bars are **experimental data** while solid lines are obtained with our beyond-mean-field finite-temperature theory[4].

[3] V. Makhalov, K. Martiyanov, and A. Turlapov, PRL **112**, 045301 (2014).
[4] LS and F. Toigo, in preparation.

Formalism for a D-dimensional Fermi superfluid (I)

We adopt the path integral formalism[5]. The partition function $\mathcal{Z}$ of the uniform system with fermionic fields $\psi_s(\mathbf{r},\tau)$ at temperature T, in a D-dimensional volume L^D, and with chemical potential μ reads

$$\mathcal{Z} = \int \mathcal{D}[\psi_s, \bar{\psi}_s] \; \exp\left\{ -\frac{1}{\hbar} \, S \right\} , \tag{2}$$

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

$$S = \int_0^{\hbar\beta} d\tau \int_{L^D} d^D\mathbf{r} \; \mathcal{L} \tag{3}$$

is the Euclidean action functional with Lagrangian density

$$\mathcal{L} = \bar{\psi}_s \left[\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_s + \mathbf{g} \, \bar{\psi}_\uparrow \, \bar{\psi}_\downarrow \, \psi_\downarrow \, \psi_\uparrow \tag{4}$$

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

[5] J. Tempere, in Ultracold Fermi Gases, Proceedings of Enrico Fermi School, Course CLXIV, pp. 639-655 (IOS Press, 2007).

Formalism for a D-dimensional Fermi superfluid (II)

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 $\Delta(\mathbf{r}, \tau)$ so that:

$$\mathcal{Z} = \int \mathcal{D}[\psi_s, \bar{\psi}_s]\, \mathcal{D}[\Delta, \bar{\Delta}]\ \exp\left\{ -\frac{S_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta})}{\hbar} \right\}, \tag{5}$$

where

$$S_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta}) = \int_0^{\hbar\beta} d\tau \int_{L^D} d^D\mathbf{r}\ \mathcal{L}_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta}) \tag{6}$$

and the (exact) effective Euclidean Lagrangian density $\mathcal{L}_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta})$ reads

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

Formalism for a D-dimensional Fermi superfluid (III)

We want to investigate the effect of fluctuations of the gap field $\Delta(\mathbf{r}, t)$ around its mean-field value Δ_0 which may be taken to be real. For this reason we set

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

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

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

where

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

is the mean-field partition function and

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

is the partition function of Gaussian pairing fluctuations.

Formalism for a D-dimensional Fermi superfluid (IV)

One finds that in the gas of paired fermions there are two kinds of elementary excitations: fermionic single-particle excitations with energy

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

where Δ_0 is the pairing gap, and bosonic collective excitations with energy

$$E_{col}(q) = \sqrt{\frac{\hbar^2 q^2}{2m}\left(\lambda\ \frac{\hbar^2 q^2}{2m} + 2\ m\ c_s^2\right)}\ , \tag{13}$$

where λ is the first correction to the familiar low-momentum phonon dispersion $E_{col}(q) \simeq c_s \hbar q$ and c_s is the sound velocity. Notice that both λ and c_s depend on the chemical potential μ.

Formalism for a D-dimensional Fermi superfluid (V)

Moreover, at the Gaussian level, the total grand potential reads

$$\Omega = \Omega_{mf} + \Omega_g \ , \tag{14}$$

where

$$\Omega_{mf} = \Omega_0 + \Omega_F^{(0)} + \Omega_F^{(T)} \tag{15}$$

is the mean-field grand potential with

$$\Omega_0 = -\frac{\Delta_0^2}{\mathbf{g}} L^D \tag{16}$$

the grand potential of the order parameter Δ_0,

$$\Omega_F^{(0)} = -\sum_{\mathbf{k}} \left(E_{sp}(k) - \frac{\hbar^2 k^2}{2m} + \mu \right) \tag{17}$$

the zero-point energy of fermionic single-particle excitations,

$$\Omega_F^{(T)} = \frac{2}{\beta} \sum_{\mathbf{k}} \ln\left(1 + e^{-\beta E_{sp}(k)}\right) \tag{18}$$

the finite-temperature grand potential of the fermionic single-particle excitations.

Formalism for a D-dimensional Fermi superfluid (VI)

The grand-potential of bosonic Gaussian fluctuations reads

$$\Omega_g = \Omega_{g,B}^{(0)} + \Omega_{g,B}^{(T)} \; , \tag{19}$$

where

$$\Omega_{g,B}^{(0)} = \frac{1}{2} \sum_{\mathbf{q}} E_{col}(q) \tag{20}$$

is the zero-point energy of bosonic collective excitations and

$$\Omega_{g,B}^{(T)} = \frac{1}{\beta} \sum_{\mathbf{q}} \ln\left(1 - e^{-\beta\, E_{col}(q)}\right) \tag{21}$$

is the finite-temperature grand potential of the bosonic collective excitations.

Both $\Omega_F^{(0)}$ and $\Omega_{g,B}^{(0)}$ are ultraviolet divergent in any dimension D ($D = 1, 2, 3$) and the regularization of these divergent terms is complicated by the fact that one also must take into account the BCS-BEC crossover.

Results of the 3D model at T=0 (I)

Scattering theory[6] plays an essential role in the 3D BCS-BEC crossover. Indeed, also if $\mathbf{g} < 0$, one can model the change of sign of a_F through

$$\frac{m}{4\pi\hbar^2 a_F} = \frac{1}{\mathbf{g}} - \frac{1}{L^3} \sum_{|\mathbf{k}|<\Lambda} \frac{m}{\hbar^2 k^2} \,, \tag{22}$$

where the ultraviolet cutoff Λ is introduced to avoid the divergence of the second term on the right side. In the continuum limit $\sum_{\mathbf{k}} \to L^3 \int d^3\mathbf{k}/(2\pi)^3$, after integration over momenta, Eq. (22) reads

$$\frac{m}{4\pi\hbar^2 a_F} = \frac{1}{\mathbf{g}} + \frac{m}{2\pi^2\hbar^2}\Lambda \,. \tag{23}$$

In the weak-coupling BCS limit, where $\mathbf{g} \to 0^-$, the first term on the right of Eq. (23) dominates and $a_F = m\mathbf{g}/(4\pi\hbar^2) \to 0^-$. In the strong-coupling BEC limit, where $\mathbf{g} \to -\infty$, the second term on the right of Eq. (23) dominates and $a_F = \pi/(2\Lambda) \to 0^+$ when Λ is sent to infinity.

[6] A.J. Leggett, Quantum Liquids (Oxford Univ. Press, 2006).

Results of the 3D model at T=0 (II)

In the deep BEC regime of the crossover, where the fermionic scattering length a_F becomes positive and the chemical potential μ becomes negative, taking into account the result

$$\Lambda = \frac{\pi}{2\, a_F} \tag{24}$$

of Eq. (23) when $g \to -\infty$ and performing cutoff regularization and renormalization of zero-point Gaussian fluctuations

$$\Omega^{(0)}_{g,B} = \frac{1}{2} \sum_{|\mathbf{q}|<\Lambda} E_{col}(q) \tag{25}$$

we have recently found[7] that the zero-temperature grand potential becomes

$$\Omega = -L^3 \frac{(1+\alpha)}{256\pi} \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\Delta_0^4}{|\mu|^{3/2}} \, , \tag{26}$$

with $\alpha = 2$ due to zero-point Gaussian fluctuations.

[7] LS and G. Bighin, Phys. Rev. A **91**, 033610 (2015).

Results of the 3D model at T=0 (III)

The total number N of fermions must be[8] calculated as follows

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{L^3,\Delta_0} - \left(\frac{\partial\Omega}{\partial\Delta_0}\right)_{L^3,\mu} \frac{\partial\Delta_0}{\partial\mu} , \tag{27}$$

and the number density $n = N/L^3$ reads

$$n = \frac{(1+\alpha)}{16\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{\Delta_0^2}{|\mu|^{1/2}} . \tag{28}$$

To obtain this formula we have used

$$\mu = -\frac{\hbar^2}{2m{a_F}^2} + \frac{1}{4}\frac{m{a_F}^2}{\hbar^2}\Delta_0^2 , \tag{29}$$

derived (in the BEC regime, $a_F \to 0^+$) from the gap equation

$$\left(\frac{\partial\Omega_{mf}}{\partial\Delta_0}\right)_{L^3,\mu} = 0 . \tag{30}$$

[8] S.N. Klimin, J.T. Devreese, and J. Tempere, NJP **14**, 103044 (2012).

Results of the 3D model at T=0 (IV)

Taking into account Eq. (28), we get

$$\mu = -\frac{\hbar^2}{2m{a_F}^2} + \frac{\pi\hbar^2}{m}\frac{a_F}{(1+\alpha)}n \, , \qquad (31)$$

where the second term is half of the chemical potential $\mu_B = 4\pi\hbar^2 a_B n_B/m_B$ of composite bosons of mass $m_B = 2m$, density $n_B = n/2$, and boson-boson scattering length

$$\boxed{a_B = \frac{2}{(1+\alpha)} a_F = \frac{2}{3} a_F \; .} \qquad (32)$$

This analytical result[9] is in good agreement with numerical beyond-mean-field theoretical predictions.[10]

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[9]LS and G. Bighin, Phys. Rev. A **91**, 033610 (2015).

[10]P. Pieri and G. Strinati, PRB **61**, 15370 (2000); D.S. Petrov, C. Salomon, and G.V. Shlyapnikov, PRL **93**, 090404 (2004); H.Hu, X.-J. Liu, and P. Drummond, EPL **74**, 574 (2006); R.B. Diener, R. Sensarma, and M. Randeria, PRA **77**, 023626 (2008).

Results of the 2D model at T=0 (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[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

$$\epsilon_b = \frac{4}{e^{2\gamma}} \frac{\hbar^2}{m {a_F}^2} \, , \tag{33}$$

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[12]

$$-\frac{1}{\mathbf{g}} = \frac{1}{2L^2} \sum_{\mathbf{k}} \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2}\epsilon_b} \, . \tag{34}$$

[11] C. Mora and Y. Castin, 2003, PRA **67**, 053615.

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

Results of the 2D model at T=0 (II)

In the **2D BCS-BEC crossover**, at zero temperature ($T = 0$) the mean-field grand potential Ω_{mf} can be written as[13] ($\epsilon_b > 0$)

$$\Omega_{mf} = -\frac{mL^2}{2\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_b)^2 \ . \tag{35}$$

Using

$$n = -\frac{1}{L^2}\frac{\partial\Omega_{mf}}{\partial\mu} \tag{36}$$

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

$$\mu = \frac{\pi\hbar^2}{m}n - \frac{1}{2}\epsilon_b \ . \tag{37}$$

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

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

Results of the 2D model at T=0 (III)

Performing dimensional regularization of Gaussian fluctuations, we have recently found[14] that the zero-temperature total grand potential is

$$\Omega = \Omega_{mf} + \Omega_g = -\frac{mL^2}{64\pi\hbar^2}(\mu + \frac{1}{2}\epsilon_b)^2 \ \ln\left(\frac{\epsilon_b}{2(\mu + \frac{1}{2}\epsilon_b)}\right) . \quad (38)$$

in the deep BEC regime. This is exactly Popov's equation of state of two-dimensional repulsive composite bosons with chemical potential $\mu_B = 2(\mu + \epsilon_b/2)$ and mass $m_B = 2m$. In this way we have identified the two-dimensional scattering length a_B of composite bosons as

$$\boxed{a_B = \frac{1}{2^{1/2}e^{1/4}} \ a_F \ .} \quad (39)$$

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

[14] LS and F. Toigo, PRA **91**, 011604(R) (2015).
[15] G. Bertaina and S. Giorgini, PRL **106**, 110403 (2011).

Conclusions

- The D-dimensional superfluid Fermi gas in the BCS-BEC crossover has a divergent zero-point energy.
- This divergent zero-point energy is due to both fermionic single-particle excitations and bosonic collective excitations.
- The regularization of zero-point energy gives remarkable analytical results for composite bosons in three dimensions[16] and in two dimensions[17].

[16] LS and Bighin, Phys. Rev. A **91**, 033610 (2015).
[17] LS and Toigo, Phys. Rev. A **91**, 011604(R) (2015).