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
In 2004 the 3D BCS-BEC crossover has been observed with ultracold gases made of fermionic $^{40}\text{K}$ and $^{6}\text{Li}$ 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

\[
y = \frac{1}{k_F a_F}
\]  \(\text{(1)}\)

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.

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**$^4$.


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 $\mu$ reads

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

(2)

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

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

(3)

is the Euclidean action functional with Lagrangian density

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

(4)

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

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 $\Delta(r, \tau)$ so that:

$$Z = \int D[\psi_s, \bar{\psi}_s] D[\Delta, \bar{\Delta}] \exp \left\{ -\frac{S_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta})}{\hbar} \right\} ,$$  \hspace{1cm} (5)

where

$$S_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta}) = \int_0^{\hbar \beta} d\tau \int_{L^D} d^D r \mathcal{L}_e(\psi_s, \bar{\psi}_s, \Delta, \bar{\Delta})$$  \hspace{1cm} (6)

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

$$\mathcal{L}_e = \bar{\psi}_s \left[ \hbar \partial_{\tau} - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + \bar{\Delta} \psi \downarrow \psi \uparrow + \Delta \bar{\psi} \uparrow \bar{\psi} \downarrow - \frac{|\Delta|^2}{g} .$$  \hspace{1cm} (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 $\Delta_0$ which may be taken to be real. For this reason we set

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

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

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

where

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

is the mean-field partition function and

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

is the partition function of Gaussian pairing fluctuations.
One finds that in the gas of paired fermions there are two kinds of elementary excitations: fermionic single-particle excitations with energy

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

(12)

where \( \Delta_0 \) is the pairing gap, and bosonic collective excitations with energy

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

(13)

where \( \lambda \) is the first correction to the familiar low-momentum phonon dispersion \( E_{col}(q) \sim c_s \hbar q \) and \( c_s \) is the sound velocity. Notice that both \( \lambda \) and \( c_s \) depend on the chemical potential \( \mu \).
Moreover, at the Gaussian level, the total grand potential reads

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

where

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

is the mean-field grand potential with

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

the grand potential of the order parameter $\Delta_0$,

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

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

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

the finite-temperature grand potential of the fermionic single-particle excitations.
The grand-potential of bosonic Gaussian fluctuations reads

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

(19)

where

$$\Omega_{g,B}^{(0)} = \frac{1}{2} \sum_q E_{col}(q)$$

(20)

is the zero-point energy of bosonic collective excitations and

$$\Omega_{g,B}^{(T)} = \frac{1}{\beta} \sum_q \ln (1 - e^{-\beta E_{col}(q)})$$

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

\[
\frac{m}{4\pi \hbar^2 a_F} = \frac{1}{g} - \frac{1}{L^3} \sum_{|k|<\Lambda} \frac{m}{\hbar^2 k^2},
\]

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

\[
\frac{m}{4\pi \hbar^2 a_F} = \frac{1}{g} + \frac{m}{2\pi^2 \hbar^2 \Lambda}.
\]

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

\textsuperscript{6}A.J. Leggett, Quantum Liquids (Oxford Univ. Press, 2006).
In the deep BEC regime of the crossover, where the fermionic scattering length $a_F$ becomes positive and the chemical potential $\mu$ becomes negative, taking into account the result

\[ \Lambda = \frac{\pi}{2 a_F} \]  

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

\[ \Omega_{g, B}^{(0)} = \frac{1}{2} \sum_{|q|<\Lambda} E_{col}(q) \]  

we have recently found\(^7\) that the zero-temperature grand potential becomes

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

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

The total number $N$ of fermions must be calculated as follows

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

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

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

To obtain this formula we have used

$$\mu = -\frac{\hbar^2}{2ma_F^2} + \frac{1}{4} \frac{ma_F^2}{\hbar^2} \Delta_0^2 , \quad (29)$$

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

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

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\(^8\)S.N. Klimin, J.T. Devreese, and J. Tempere, NJP 14, 103044 (2012).
Taking into account Eq. (28), we get

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

(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

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

(32)

This analytical result\(^9\) is in good agreement with numerical beyond-mean-field theoretical predictions.\(^{10}\)

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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, the binding energy $\epsilon_b > 0$ of two fermions can be written in terms of the positive 2D fermionic scattering length $a_F$ as

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

where $\gamma = 0.577...$ 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

$$-\frac{1}{g} = \frac{1}{2L^2} \sum_k \frac{1}{\frac{\hbar^2 k^2}{2m} + \frac{1}{2} \epsilon_b}.$$
In the **2D BCS-BEC crossover**, at zero temperature \((T = 0)\) the mean-field grand potential \(\Omega_{mf}\) can be written as\(^{13}\) \((\varepsilon_b > 0)\)

\[
\Omega_{mf} = -\frac{mL^2}{2\pi\hbar^2}(\mu + \frac{1}{2}\varepsilon_b)^2 .
\] (35)

Using

\[
n = -\frac{1}{L^2} \frac{\partial \Omega_{mf}}{\partial \mu}
\] (36)

one immediately finds the chemical potential \(\mu\) as a function of the number density \(n = N/L^2\), i.e.

\[
\mu = \frac{\pi\hbar^2}{m} n - \frac{1}{2}\varepsilon_b .
\] (37)

In the BCS regime, where \(\varepsilon_b \ll \varepsilon_F\) with \(\varepsilon_F = \pi\hbar^2 n/m\), one finds \(\mu \simeq \varepsilon_F > 0\) while in the BEC regime, where \(\varepsilon_b \gg \varepsilon_F\) one has \(\mu \simeq -\varepsilon_b/2 < 0\).

\(^{13}\)M. Randeria, J-M. Duan, and L-Y. Shieh, PRL 62, 981 (1989).
Performing dimensional regularization of Gaussian fluctuations, we have recently found\textsuperscript{14} that the zero-temperature total grand potential is

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

(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

\[ a_B = \frac{1}{2^{1/2}e^{1/4}} a_F. \]  

(39)

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

\textsuperscript{14}LS and F. Toigo, PRA 91, 011604(R) (2015).

\textsuperscript{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\textsuperscript{16} and in two dimensions\textsuperscript{17}.

\textsuperscript{17}LS and Toigo, Phys. Rev. A \textbf{91}, 011604(R) (2015).