Reliable equation of state for composite bosons in the 2D BCS-BEC crossover

L. Salasnich

Received: date / Accepted: date

Abstract We briefly discuss recent experiments on the BCS-BEC crossover with ultracold alkali-metal atoms both in three-dimensional configurations and two-dimensional ones. Then we analyze the quantum-field-theory formalism used to describe an attractive D-dimensional Fermi gas taking into account Gaussian fluctuations. Finally, we apply this formalism to obtain a reliable equation of state of the 2D system at low temperatures in the BEC regime of the crossover by performing a meaningful dimensional regularization of the divergent zero-point energy of collective bosonic excitations.

Keywords BCS-BEC crossover · Ultracold atoms · Dimensional regularization

1 BCS-BEC crossover with ultracold atoms

In 2004 the 3D BCS-BEC crossover has been observed with ultracold gases made of fermionic $^{40}$K and $^{6}$Li alkali-metal atoms [1,2,3,4]. As schematically shown in Fig. 1, this crossover is obtained by changing with a Feshbach resonance the s-wave scattering length $a_F$ of the inter-atomic potential. There are three characteristic regimes which depend on the value of the scattering length $a_F$ [5]:

- $a_F \to 0^-$, that is the BCS regime of weakly-interacting Cooper pairs;
- $a_F \to \pm \infty$, that is unitarity limit of strongly-interacting Cooper pairs;
- $a_F \to 0^+$, that is the BEC regime of bosonic dimers.

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 ($a_F = \pm \infty$), and it has been shown that the system is metastable [1,2,3,4]. The detection of quantized vortices under rotation [6] has clarified that this dilute gas of ultracold atoms is superfluid. Usually the BCS-BEC crossover is analyzed in terms of

$$y = \frac{1}{k_F a_F}$$

(1)

the inverse scaled interaction strength, where $k_F = (3\pi^2 n_0)^{1/3}$ is the Fermi wave number and $n$ the total fermionic 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 BCS-BEC crossover has been achieved [7] with a quasi-2D Fermi gas of $^6$Li atoms with widely tunable s-wave interaction, measuring the pressure $P$ vs the gas parameter $a_B n_B^{1/2}$, with $a_B = a_F/(2^{1/2} e^{3/4})$ the bosonic scattering length between
molecules (see below and [8]) and $n_B = n/2$ the bosonic density. In Fig. 2 we plot the pressure $P$ of the system as a function of the gas parameter.

Fig. 2 shows a good agreement between the experimental data [7] and our theoretical curves only in the deep weak-coupling regime $k_B T / \mu < 0.01$ and assuming a very small scaled temperature $k_B T / \mu_{id}$. In the next two sections we shall discuss some details of our beyond-mean-field theory [8][9].

### 2 Theory for a $D$-dimensional Fermi superfluid

To study the attractive $D$-dimensional Fermi liquid we adopt the path integral formalism [10]. The partition function $Z$ 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

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

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

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

is the Euclidean action functional with Lagrangian density

$$\mathcal{L} = \bar{\psi}_s \left[ \hbar \partial_r - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + g \bar{\psi}_s \psi_s \bar{\psi}_s \psi_s$$

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

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:

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

where

$$S_c(\psi_s, \bar{\psi}_s; \Delta, \bar{\Delta}) = \int_0^{\beta \hbar} dt \int_{L^D} d^D r \mathcal{L}_c(\psi_s, \bar{\psi}_s; \Delta, \bar{\Delta})$$

and the (exact) effective Euclidean Lagrangian density

$$\mathcal{L}_c(\psi_s, \bar{\psi}_s; \Delta, \bar{\Delta})$$

reads

$$\mathcal{L}_c = \bar{\psi}_s \left[ \hbar \partial_r - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi_s + \Delta \bar{\psi}_s \psi_s + \bar{\Delta} \bar{\psi}_s \psi_s - \frac{1}{2} \frac{\Delta^2}{g}.$$ (7)

We want to investigate the effect of fluctuations of the gap field $\Delta(r, t)$ around its mean-field value $\Delta_0$, which may be taken to be real. For this reason we set

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

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

In particular, we are interested in the grand potential $\Omega$, given by

$$\Omega = \frac{1}{\beta} \ln (Z) \simeq \frac{1}{\beta} \ln (Z_{mf} Z_g) = \Omega_{mf} + \Omega_g,$$ (9)

where

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

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.

To make a long story short, one finds that in the gas of paired fermions there are two kinds of elementary excitations [10][11][12]: fermionic single-particle excitations with energy

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

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

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

where $\lambda$ 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 $\lambda$ and $\epsilon_s$ depend on the chemical potential $\mu$ [12].

Moreover, at the Gaussian level, the total grand potential reads [10][12]

$$\Omega = \Omega_{mf} + \Omega_g,$$  \hspace{1cm} (14)

where

$$\Omega_{mf} = -\frac{A^2}{g} L^D + \Omega_F^{(0)} + \Omega_F^{(T)}$$  \hspace{1cm} (15)

is the mean-field grand potential with

$$\Omega_F^{(0)} = -\sum_k \left( E_{sp}(k) - \frac{\hbar^2 k^2}{2m} + \mu \right)$$  \hspace{1cm} (16)

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

$$\Omega_F^{(T)} = \frac{2}{\beta} \sum_k \ln (1 + e^{-\beta E_{sp}(k)})$$  \hspace{1cm} (17)

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

The grand-potential of Gaussian fluctuations reads

$$\Omega_g = \Omega_{g,B}^{(0)} + \Omega_{g,B}^{(T)},$$  \hspace{1cm} (18)

where

$$\Omega_{g,B}^{(0)} = \frac{1}{\beta} \sum_q E_{col}(q)$$  \hspace{1cm} (19)

is the zero-point energy of bosonic collective excitations and

$$\Omega_{g,B}^{(T)} = \frac{1}{\beta} \sum_q \ln (1 - e^{-\beta E_{col}(q)})$$  \hspace{1cm} (20)

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 [12][8].

3 Results of the two-dimensional Fermi superfluid

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

$$\epsilon_b = \frac{4}{\epsilon_1} \frac{\hbar^2}{ma_F^2},$$  \hspace{1cm} (21)

where $\gamma = 0.577...$ is the Euler-Mascheroni constant [13]. 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 [14]

$$\frac{1}{g} = \frac{2L^2}{\beta} \sum_k \frac{n_{k+e\epsilon_b}}{2m} + \frac{1}{2}\epsilon_b.$$  \hspace{1cm} (22)

In the 2D BCS-BEC crossover, at zero temperature ($T = 0$) the mean-field grand potential $\Omega_{mf}$ can be written as [12][14]

$$\Omega_{mf} = \frac{mL^2}{2\pi\hbar^2} (\mu + \frac{1}{2}\epsilon_b)^2$$  \hspace{1cm} (23)

with $\epsilon_b > 0$. Using

$$n = -\frac{1}{\beta L^2} \frac{\partial \Omega_{mf}}{\partial \mu}$$  \hspace{1cm} (24)

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

$$\mu = \frac{\pi \hbar^2}{m} n - \frac{1}{2}\epsilon_b.$$  \hspace{1cm} (25)

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

Performing dimensional regularization of Gaussian fluctuations, we have recently found [8] that the zero-temperature total grand potential is

$$\Omega = \Omega_{mf} + \Omega_g = -\frac{mL^2}{\pi\hbar^2} (\mu + \frac{1}{2}\epsilon_b)^2 \ln \left( \frac{\epsilon_b}{2(\mu + \frac{1}{2}\epsilon_b)} \right)$$  \hspace{1cm} (26)

in the deep BEC regime. Introducing $\mu_B = 2(\mu + \epsilon_b/2)$ as the chemical potential of composite bosons with mass $m_B = 2m$ and density $n_B = n/2$, the zero-temperature total grand potential can be rewritten as

$$\Omega = -\frac{m_B L^2}{8\pi \hbar^2} \mu_B^2 \ln \left( \frac{\epsilon_B}{\mu_B} \right),$$  \hspace{1cm} (27)

that is exactly the Popov equation of state of 2D weakly-interacting bosons [15] provided that we identify the parameter

$$\epsilon_0 = \frac{4}{\epsilon_1^{3/2}} \frac{\hbar^2}{m_B a_B^2}$$  \hspace{1cm} (28)

of the Popov theory of bosons with scattering length $a_B$ [15] with the binding energy

$$\epsilon_b = \frac{4}{\epsilon_1^{3/2}} \frac{\hbar^2}{m a_F^2}$$  \hspace{1cm} (29)

of paired fermions with scattering length $a_F$ [13]. Thus, we find [8]

$$a_B = \frac{1}{2\pi^2\epsilon_0} a_F.$$

The value $a_B/a_F = 1/(2^{1/2}\epsilon_0^{1/4}) \approx 0.551$ is in full agreement with other theoretical predictions: $a_B/a_F = 0.56$ obtained from four-body scattering theory [17].
\( a_B/a_F = 0.55(4) \) obtained by Monte Carlo calculations \[13\], and \( a_B/a_F = 0.56 \) obtained very recently by using Gaussian fluctuations with convergence-factor regularization \[19\].

At finite temperature \( (T \neq 0) \) the pressure \( P \) is immediately obtained using the thermodynamic formula \( P = -\Omega/L^2 \). Taking into account that the main thermal contribution is due to collective bosonic excitations, we obtain \[10\] from Eqs. (20) and (27) the finite-temperature pressure

\[
P = \frac{m_B}{8\pi h^2 \mu_B^2} \left[ \ln \left( \frac{\epsilon_0}{\mu_B} \right) + 4\zeta(3) \left( \frac{k_B T}{\mu_B} \right)^3 \right], \tag{31}
\]

and also, by using \( n_B = \left( \frac{\partial^2 P}{\partial n_B^2} \right)_{T,\Omega} \), the bosonic density

\[
n_B = \frac{m_B}{4\pi h^2 \mu_B} \left[ \ln \left( \frac{\epsilon_0}{\mu_B e^{1/2}} \right) - 2\zeta(3) \left( \frac{k_B T}{\mu_B} \right)^3 \right] \tag{32}
\]

where \( \zeta(x) \) is the Riemann zeta function and \( \zeta(3) = 1.20205 \). Eqs. 31 and 32 give, at fixed \( k_B T/\mu_B \), a parametric formula for the pressure \( P \) as a function of the density \( n_B \) where \( \mu_B \) is the dummy parameter (see Fig. 2). Thus, we have a reliable equation of state for composite bosons in the 2D BEC-BEC crossover at low temperatures, i.e. when the system is well below the Berezinsky-Kosterlitz-Thouless critical temperature of the superfluid-normal transition \[10\].

### 4 Conclusions

We have shown that the \( D \)-dimensional superfluid Fermi gas in the BCS-BEC crossover has a divergent zero-point energy due to fermionic single-particle excitations (mean-field) and bosonic collective excitations (Gaussian fluctuations). However, the regularization of the divergent zero-point energy gives remarkable analytical results for composite bosons in two dimensions \[5\]: a reliable 2D equation of state and an analytical formula connecting the scattering length \( a_B \) between composite bosons and the scattering \( a_F \) between fermionic atoms. Finally, we notice that also in three-dimensions one can regularize the divergent zero-point energy due to fermionic and bosonic excitations \[20-22\]. In particular, by performing a cutoff regularization and renormalization of Gaussian fluctuations, we have found very recently \[23\] that \( a_B = (2/3)a_F \) for composite bosons in the 3D BCS-BEC crossover.

### Acknowledgements

This work was partially supported by MIUR through the PRIN Project “Collective Quantum Phenomena: from Strongly-Correlated Systems to Quantum Simulators”.

### References

1. C.A. Regal, et al., Phys. Rev. Lett. 92, 040403 (2004).
2. M.W. Zwierlein, et al., Phys. Rev. Lett. 92, 120403 (2004).
3. M. Bartenstein et al., Phys. Rev. Lett. 92, 120401 (2004).
4. J. Kinast, et al., Phys. Rev. Lett. 92, 150402 (2004).
5. M.M. Scherer, S. Floerchinger, and H. Ges, Phil. Trans. Roy. Soc. Lond. A 368, 2779 (2011).
6. M.W. Zwierlein, et al., Science 311, 492 (2006); M.W. Zwierlein, et al., Nature 442, 54 (2006).
7. V. Makhulov, K. Martiyanov, and A. Turlapov, Phys. Rev. Lett. 112, 045301 (2014).
8. L. Salasnich and F. Toigo, Phys. Rev. A 91, 011604(R) (2015).
9. L. Salasnich and F. Toigo, in preparation.
10. N. Nagaosa, Quantum Field Theory in Condensed Matter Physics (Springer, 1999).
11. L. Salasnich, Phys. Rev. A 82, 063619 (2010).
12. L. Salasnich, P.A. Marchetti, and F. Toigo, Phys. Rev. A 88, 053612 (2013).
13. C. Mora and Y. Castin, Phys. Rev. A 67, 053615 (2003).
14. M. Randeria, J-M. Duan, and L-Y. Shieh, Phys. Rev. Lett. 62, 981 (1989).
15. V.N. Popov, Theor. Math. Phys. A 11, 565 (1972).
16. C. Mora and Y. Castin, Phys. Rev. Lett. 102, 180404 (2009).
17. D.S. Petrov, M.A. Baranov, and G.V. Shlyapnikov, Phys. Rev. A 67, 031601(R) (2003).
18. G. Bertaina and S. Giorgini, Phys. Rev. Lett. 106, 110403 (2011).
19. L. He, H. Lv, G. Cao, H. Hu, and X.-J. Liu, Phys. Rev. A 92, 023620 (2015).
20. P. Pieri and G. Strinati, Phys. Rev. B 61, 15370 (2000).
21. H.Hu, X.-J. Liu, and P. Drummond, EPL 74, 574 (2006).
22. R.B. Diener, R. Sensarma, and M. Randeria, Phys. Rev. A 77, 023626 (2008).
23. L. Salasnich and G. Bighin, Phys. Rev. A 91, 033610 (2015).