

Comparison between a diagrammatic theory for the BCS-BEC crossover and quantum Monte Carlo results

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Predictions for the chemical potential and the excitation gap recently obtained by our diagrammatic theory for the Bardeen-Cooper-Schreiffer-Bose-Einstein Condensation crossover in the superfluid phase are compared with quantum Monte Carlo results at zero temperature now available in the literature. A remarkable agreement is found between the results obtained by the two approaches.

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The recent experimental realization of the Bardeen-Cooper-Schreiffer-Bose-Einstein Condensation (BCS-BEC) crossover with ultracold trapped Fermi atoms¹ has given impetus to theoretical investigations of this crossover. In a recent paper,² the t -matrix self-energy approach (originally conceived for the normal phase^{3,4}) was extended to the superfluid phase, aiming at improving the description of the BCS-BEC crossover by including pairing fluctuations on top of the BCS mean-field approach considered in Refs. 5 and 3 (see also Ref. 6).

In this theory, the effects of the collective Bogoliubov-Anderson mode is explicitly included in the fermionic self-energy, thus generalizing the theory due to Popov for a weakly interacting (dilute) superfluid Fermi gas.⁷ The theory is based on a judicious choice of the fermionic self-energy, such that it reproduces the fermionic mean-field BCS behavior plus pairing fluctuations in the weak-coupling limit as well as the Bogoliubov description for the composite bosons that form in the strong-coupling limit. In the intermediate-coupling region of interest about the unitarity limit, where no small parameter exists to control the many-body approximations, the theory is able to capture the essential physics of the problem, as the excellent agreement with a previously available quantum Monte Carlo (QMC) calculation⁸ at the unitarity point has already shown,⁹ and as more extensively demonstrated by the present comparison with more recent QMC data^{10,11} spanning the whole crossover region. Although the comparison with QMC data is here limited to the zero-temperature limit where they are available, the predictions of the theory of Ref. 2 extend as well to finite temperature and across the critical temperature.

The purpose of this Brief Report is to compare the theoretical predictions obtained from the theory of Ref. 2 with QMC data,^{10,11} which were published after completion of Ref. 2. A quantitative comparison between the results for the density profiles obtained from a local density version⁹ to the theory of Ref. 2 and the experimental data was already presented in Ref. 12.

Both our calculations and the QMC calculations of Refs. 10 and 11 are based on a model Hamiltonian describing a system of fermions mutually interacting via an attractive contact potential. This Hamiltonian proves appropriate to describe the BCS-BEC crossover with trapped Fermi gases for the case of a “broad” resonance.¹³ In the calculation of

physical quantities, the ultraviolet divergences introduced by the delta-function interaction are removed by taking the contact potential as an appropriate limit of a finite-range potential with given fermionic scattering length a_F (see Ref. 14). In this way, physical quantities are expressed in terms of the dimensionless parameter $(k_F a_F)^{-1}$, which drives the BCS-BEC crossover. For the homogeneous gas here considered, the Fermi wave vector is $k_F = (3\pi^2 n)^{1/3}$ where n is the particle density. Comparison will be made at zero temperature only, since finite-temperature QMC calculations for the BCS-BEC crossover are not yet available.

The overall agreement between the two alternative (diagrammatic and QMC) calculations turns out to be quite good, especially in the most interesting intermediate-coupling regime about $(k_F a_F)^{-1} = 0$.

Figure 1 shows the comparison for the chemical potential at zero temperature, as obtained by our calculation² and by the fixed-node quantum Monte Carlo (FNQMC) calculations of Ref. 11. As discussed in Ref. 2, on the weak-coupling side we find it appropriate to introduce a constant shift Σ_0 in the bare Green’s function entering the self-energy. This shift needs to be included only for coupling values $(k_F a_F)^{-1} \leq$

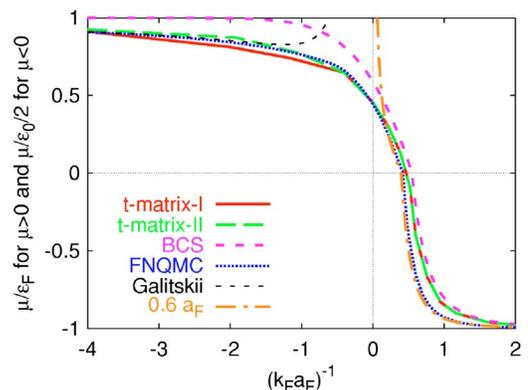


FIG. 1. (Color online) Chemical potential at zero temperature vs the coupling parameter $(k_F a_F)^{-1}$. The results of the present theory (t -matrix-I) and of its version without the inclusion of the self-energy shift Σ_0 (t -matrix-II) are compared with the BCS mean field (BCS), the fixed-node QMC data from Ref. 11 (FNQMC), the Galitskii’s expression for the dilute Fermi gas (Galitskii), and the asymptotic expression for strong coupling using the result $a_B = 0.6a_F$.

-0.5 , such that the self-energy can be considered to be approximately constant. The curve obtained by this procedure is reported in Fig. 1 with the label *t*-matrix-I and corresponds to the data reported in Fig. 6 of Ref. 2. For completeness, we also report in Fig. 1 the curve obtained without the inclusion of the self-energy shift Σ_0 (with the label *t*-matrix-II) [by definition, the two curves I and II coincide when $(k_F a_F)^{-1} \geq -0.5$]. Our results are in excellent agreement with the FN-QMC data in the range $-0.5 \leq (k_F a_F)^{-1} \leq 0.5$ spanning the crossover region.

For couplings $(k_F a_F)^{-1} \leq -0.5$, the FNQMC results are extremely close to both our curves, lying just in between them. In the weak-coupling region $(k_F a_F)^{-1} \leq -2$, our curves (as well as the FNQMC data) approach the asymptotic expression by Galitskii¹⁵ for the chemical potential of a dilute Fermi gas. The BCS mean field (also reported in Fig. 1) misses instead the Galitskii correction to the noninteracting chemical potential. More specifically, we have verified that our theory with the inclusion of the self-energy shift Σ_0 [*t*-matrix-I] recovers the complete Galitskii's expression $\mu/\epsilon_F = 1 + (4/3\pi)k_F a_F + (4/15\pi^2)(11 - 2 \ln 2)(k_F a_F)^2$ including the second-order correction in $k_F a_F$. The curve for the chemical potential obtained without the inclusion of the shift Σ_0 recovers instead only the leading order correction linear in $k_F a_F$. (It can also be shown that neglecting the shift Σ_0 introduces a spurious additional term $\frac{3}{2}[(4/3\pi)k_F a_F]^2$ to the second-order correction in the Galitskii's expression.)

On the strong-coupling side, for coupling values $(k_F a_F)^{-1} \geq 0.5$ our results deviate somewhat from the FN-QMC data. This discrepancy is due to the fact that in our approach the boson-boson scattering is treated at the level of the Born approximation, corresponding to the value $a_B = 2a_F$ of the bosonic scattering length a_B . The importance of including the correct value of the bosonic scattering length ($a_B = 0.6a_F$, as calculated in Ref. 16) in this region is clearly seen from the agreement between the FNQMC data and the asymptotic expression $\mu = -\epsilon_0/2 + \mu_B/2$, where ϵ_0 is the binding energy of the two-body problem and $\mu_B = 4\pi n_B a_B / m_B$, with $n_B = n/2$, $m_B = 2m$, and $a_B = 0.6a_F$. The asymptotic curve corresponding to the value $a_B = 2a_F$ almost coincides with our curve in this region. (This curve is not reported in Fig. 1 for overall clarity.) It is, finally, interesting to mention that the inclusion of the next-order correction to the bosonic chemical potential, corresponding to the expression $\mu_B = (4\pi n_B a_B / m_B) [1 + \frac{32}{3}(n_B a_B^3 / \pi)]^{1/3}$ obtained in Ref. 17, would worsen appreciably the comparison between the QMC data and the asymptotic curve in the coupling region $0.2 \leq (k_F a_F)^{-1} \leq 2$. The inclusion of this next-order term improves the comparison only in the truly asymptotic regime for $(k_F a_F)^{-1} \geq 2$ (not reported in the figure), where the next-order correction to the bosonic chemical potential is, however, already quite small. This finding could (at least partially) explain the absence of beyond-mean-field corrections on the bosonic side of the BCS-BEC crossover, recently reported in experiments with ultracold Fermi gases.¹⁸

Quite generally, any theory of the BCS-BEC crossover connects the equation for the chemical potential μ to the equation for the gap (order) parameter Δ in the superfluid phase. The latter quantity is not directly accessible to the

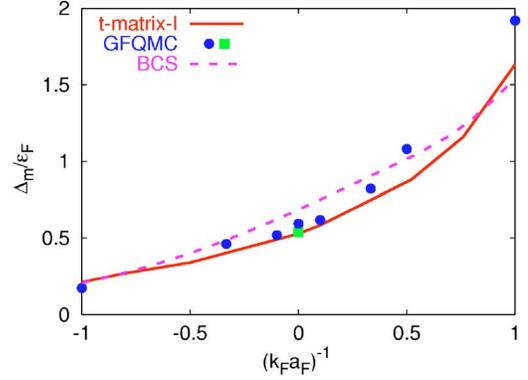


FIG. 2. (Color online) Excitation gap Δ_m at zero temperature vs the coupling parameter $(k_F a_F)^{-1}$. The results of the present theory (*t*-matrix-I) are compared with the Green's function QMC data of Refs. 8 and 10 (GFQMC) as well as with the BCS mean field (BCS).

QMC simulations of Refs. 10 and 11. In Ref. 10, however, the even-odd staggering of the ground-state energy for a system with a finite number of particles was exploited to calculate the single-particle excitation gap Δ_m . In a BCS-like framework (and for a sufficiently large number of particles) the gap Δ_m is expected to coincide with the gap (order) parameter Δ when μ is positive and with the quantity $(\Delta^2 + \mu^2)^{1/2}$ when μ is negative. For a given coupling, this gap occurs at the wave vector $|\mathbf{k}| = \sqrt{2\mu}$ for positive μ and at $\mathbf{k} = 0$ for negative μ . These BCS-like results are not expected to hold exactly away from a weak coupling. The calculations presented in Ref. 2, nevertheless, show that the identification of the single-particle excitation gap Δ_m with Δ for $\mu > 0$ and with $(\Delta^2 + \mu^2)^{1/2}$ for $\mu < 0$ works fairly well for all couplings of interest. In particular, in Fig. 14 of Ref. 2 this definition of the excitation gap Δ_m was compared with the results obtained from an accurate analysis of the single-particle spectral function $A(\mathbf{k}, \omega)$, showing that the two definitions are in good agreement with each other over a wide coupling range.

In Fig. 2 we compare Δ_m , as obtained from our results for Δ and μ , with the QMC data of Ref. 10. The BCS mean-field results are also reported for completeness. For the coupling value $(k_F a_F)^{-1} = 0$ a single QMC datum previously available from Ref. 8 is also reported in the figure (full square). Even for the excitation gap, our results appear to be in remarkable agreement with QMC data in the crossover region $-1 \leq (k_F a_F)^{-1} \leq 0.4$. At larger couplings, the QMC results start instead to deviate from our results, the discrepancy being mainly due to the finite range of the interaction potential used in the QMC calculations. In a strong coupling, both our excitation gap and that calculated from QMC simulations tend, in fact, to half the value of the binding energy ϵ_0 of the two-body problem. The binding energies for the contact potential and for the finite-range potential used in Ref. 10 are close to each other only in a narrow range about $(k_F a_F)^{-1} = 0$. At the coupling value $(k_F a_F)^{-1} = 1$, the binding energy for the finite-range potential of Ref. 10 is already larger by about 40% than the contact-potential binding energy. This difference is responsible for the discrepancy between our values and the QMC data of Ref. 10 on the strong-coupling side,

where the excitation gap is controlled by the binding energy of the two-body problem.

A further improvement of our diagrammatic theory would require us to include the corrections considered in Ref. 19 that reduce the value of the gap parameter on the weak-coupling side.

In conclusion, the theory of Ref. 2 for the BCS-BEC crossover in the broken-symmetry phase has been shown to compare rather well with recent QMC data at zero temperature. In particular, the agreement between the two ap-

proaches is extremely good in the intermediate-coupling (crossover) region that is the most interesting one, both theoretically and experimentally. This agreement suggests that the choice of the fermionic self-energy made in Ref. 2 captures the essential physics of the problem, as soon as the fermionic degrees of freedom get progressively quenched while forming composite bosons.

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- ¹M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, C. Chin, J. H. Denschlag, and R. Grimm, *Phys. Rev. Lett.* **92**, 120401 (2004); C. A. Regal, M. Greiner, and D. S. Jin, *ibid.* **92**, 040403 (2004); M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, A. J. Kerman, and W. Ketterle, *ibid.* **92**, 120403 (2004); T. Bourdel, L. Khaykovich, J. Cubizolles, J. Zhang, F. Chevy, M. Teichmann, L. Tarruell, S. J. J. M. F. Kokkelmans, and C. Salomon, *ibid.* **93**, 050401 (2004).
- ²P. Pieri, L. Pisani, and G. C. Strinati, *Phys. Rev. B* **70**, 094508 (2004).
- ³P. Nozières and S. Schmitt-Rink, *J. Low Temp. Phys.* **59**, 195 (1985).
- ⁴A. Perali, P. Pieri, G. C. Strinati, and C. Castellani, *Phys. Rev. B* **66**, 024510 (2002).
- ⁵A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter*, edited by A. Pekalski and R. Przystawa, Lecture Notes in Physics Vol. 115 (Springer-Verlag, Berlin, 1980), p. 13.
- ⁶For a general reference, see *Bose-Einstein Condensation*, edited by A. Griffin, D. W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, 1985).
- ⁷V. N. Popov, *Functional Integrals and Collective Excitations* (Cambridge University Press, Cambridge, 1987).
- ⁸J. Carlson, S.-Y. Chang, V. R. Pandharipande, and K. E. Schmidt, *Phys. Rev. Lett.* **91**, 050401 (2003).
- ⁹A. Perali, P. Pieri, L. Pisani, and G. C. Strinati, *Phys. Rev. Lett.* **92**, 220404 (2004).
- ¹⁰S. Y. Chang, V. R. Pandharipande, J. Carlson, and K. E. Schmidt, *Phys. Rev. A* **70**, 043602 (2004).
- ¹¹G. E. Astrakharchik, J. Boronat, J. Casulleras, and S. Giorgini, *Phys. Rev. Lett.* **93**, 200404 (2004).
- ¹²A. Perali, P. Pieri, and G. C. Strinati, *Phys. Rev. Lett.* **93**, 100404 (2004).
- ¹³For a “narrow” resonance, the use of a multichannel model is more appropriate [see S. Simonucci, P. Pieri, and G. C. Strinati, *Europhys. Lett.* **69**, 713 (2005)].
- ¹⁴P. Pieri and G. C. Strinati, *Phys. Rev. B* **61**, 15370 (2000).
- ¹⁵V. M. Galitskii, *Zh. Eksp. Teor. Fiz.* **34**, 151 (1958) [*Sov. Phys. JETP* **7**, 104 (1958)].
- ¹⁶D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, *Phys. Rev. Lett.* **93**, 090404 (2004).
- ¹⁷T. D. Lee and C. N. Yang, *Phys. Rev.* **105**, 1119 (1957).
- ¹⁸M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, C. Chin, J. H. Denschlag, and R. Grimm, *Phys. Rev. Lett.* **92**, 203201 (2004).
- ¹⁹L. P. Gor’kov and T. K. Melik-Barkhudarov, *Zh. Eksp. Teor. Fiz.* **40**, 1452 (1961) [*Sov. Phys. JETP* **13**, 1018 (1961)].