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 BCS-BEC crossover in the superfluid phase are compared with novel 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 BCS-BEC crossover with ultracold trapped Fermi atoms has given impetus to theoretical investigations of this crossover. In a recent paper, the t-matrix self-energy approach (originally conceived for the normal phase) 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. 2 and 3.

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. 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 which 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 QMC calculation at the unitarity point \((k_Fa_F)^{-1} = 0\) has already shown, and as more extensively demonstrated by the present comparison with more recent QMC data spanning the whole crossover region. The theory of Ref. 2 is completely \textit{ab initio} and it contains no adjustable parameter. 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.

Purpose of this Brief Report is to compare the theoretical predictions obtained from the theory of Ref. 2 with novel Quantum Monte Carlo (QMC) data, which were published after completion of Ref. 2. A quantitative comparison between the results for the density profiles obtained from a local density version to the theory of Ref. 2 and the experimental data was already presented in Ref. 11.

Both our calculations and the QMC calculations of Refs. 8 and 9,10 are based on a model Hamiltonian describing a system of fermions mutually interacting via an attractive contact potential. In Ref. 12 this Hamiltonian was proved appropriate to describe the BCS-BEC crossover with trapped Fermi gases. In this model, the only dimensionless parameter representing the effective coupling strength is the (inverse of the) product \(k_Fa_F\) between the Fermi wave vector \(k_F\) and the fermionic scattering length \(a_F\). For the homogeneous gas here considered, \(k_F = (3\pi^2n)^{1/3}\) 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 \((k_Fa_F)^{-1} = 0\). Figure 1 shows the comparison for the chemical potential at zero temperature, as obtained by our calculations and by the Fixed Node QMC (FNQMC) calculations of Ref. 10. As discussed in Ref. 2, on the weak-coupling side we find...
it appropriate to introduce a constant shift $\Sigma_0$ in the
bare Green’s function entering the self-energy. This shift
needs to be included only for coupling values $(k_Fa_F)^{-1} \leq
-0.5$, such that the self-energy can be considered to be
approximatively 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 ob-
tained without the inclusion of the self-energy shift $\Sigma_0
$ (with the label t-matrix-II) (by definition, the two curves
I and II coincide when $(k_Fa_F)^{-1} \geq -0.5$). Our results
are in excellent agreement with the FNMQMC data in the
range $-0.5 \lesssim (k_Fa_F)^{-1} \lesssim 0.5$ spanning the crossover
region.

For couplings $(k_Fa_F)^{-1} \leq -0.5$, the FNQMC results
are extremely close to both our curves, lying just in be-
tween them. In the weak-coupling region $(k_Fa_F)^{-1} \lesssim
-2$, our curves (as well as the FNQMC data) approach the
asymptotic expression by Galitskii\cite{gal} for the
chemical potential of a dilute Fermi gas. The BCS mean
field (also reported in Fig. 1) misses instead the Gal-
tskii correction to the non-interacting chemical poten-
tial. More specifically, we have verified that our the-
ory with the inclusion of the self-energy shift $\Sigma_0
$ [t-
matrix-I] recovers the complete Galitskii’s expression
$\mu/\epsilon_F = 1 + \frac{1}{2}(k_Fa_F) + \frac{4}{15}(11 - 2\ln 2)(k_Fa_F)^2$
including the second-order correction in $k_Fa_F$. The curve for the
chemical potential obtained without the inclusion of the
shift $\Sigma_0$ recovers instead only the leading order correc-
tion linear in $k_Fa_F$. [It can also be shown that neglect-
ing the shift $\Sigma_0$ introduces a spurious additional term
$\frac{4}{15}(k_Fa_F)^2$ to the second-order correction in the Galit-
skii’s expression.]

On the strong-coupling side, for coupling values $(k_Fa_F)^{-1} \gtrsim
0.5$ our results deviate somewhat from the
FNQMC 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
$a_F$. The importance of including the correct value of the
bosonic scattering length $(a_B = 0.6a_F$, as calculated in
Ref. [13] 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 $\epsilon_0$ is the binding energy of
the 2-body problem and $\mu_B = 4\pi n_B a_B^2/m_B$, with $n_B = n/2,$
$m_B = 2m$, and $a_B = 0.6a_F$. The asymptotic curve cor-
responding 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 $\mu_B = \frac{4m_B a_B^2}{m} \left[1 + \frac{2}{15}(n_B a_B^3/\pi)\right]^{1/3}$
obtained in Ref. [13] would worsen appreciably the comparison be-
tween the QMC data and the asymptotic curve in the
coupling region $0.2 \lesssim (k_Fa_F)^{-1} \lesssim 2$. The inclusion of this
next-order term improves the comparison only in the
truly asymptotic regime for $(k_Fa_F)^{-1} \gtrsim 2$ (not re-
ported 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 ex-
periments with ultracold Fermi gases.\cite{ultra}

Quite generally, any theory of the BCS-BEC crossover
connects the equation for the chemical potential $\mu$ to the
equation for the gap (order) parameter $\Delta$ in the super-
fluid phase. The latter quantity is not directly accessible
to the QMC simulations of Refs. [6] and [10]. In Ref. [4],
however, the even-odd staggering of the ground-state en-
ergy for a system with a finite number of particles was
exploited to calculate the single-particle excitation gap
$\Delta_m$. In a BCS-like framework (and for a sufficiently
large number of particles) the gap $\Delta_m$ is expected to
coincide with the gap (order) parameter $\Delta$ when $\mu$
is positive and with the quantity $(\Delta^2 + \mu^2)^{1/2}$
when $\mu$ is negative. For a given coupling, this gap occurs at the
wave vector $|k| = \sqrt{2\mu}$ for positive $\mu$ and at $k = 0$ for
negative $\mu$. These BCS-like results are not expected to
hold exactly away from weak coupling. The calculations
presented in Ref. [6] nevertheless, show that the identifi-
cation of the single-particle excitation gap $\Delta_m$ with $\Delta$
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. [4] this definition of the excitation gap $\Delta_m$ was com-
pared with the results obtained from an accurate analysis
of the single-particle spectral function $A(k, \omega)$, showing
that the two definitions are in good agreement with each
other over a wide coupling range.

In Fig. 2 we compare $\Delta_m$, as obtained from our results
for $\Delta$ and $\mu$, with the QMC data of Ref. [6]. The BCS
mean field results are also reported for completeness. For
the coupling value $(k_Fa_F)^{-1} = 0$ a single QMC datum
previously available from Ref. [6] is also reported in the fig-
ure (full square). Even for the excitation gap, our results appear to be in remarkable agreement with QMC data in the crossover region $-1 \lesssim (k_F a_F)^{-1} \lesssim 0.4$. At larger couplings, the QMC results start instead to deviate from our results, the discrepancy mainly due to the finite range of the interaction potential used in the QMC calculations. In strong coupling, both our excitation gap and that calculated from QMC simulations tend, in fact, to half the value of the binding energy $\epsilon_0$ of the two-body problem. The binding energies for the contact potential and for the finite-range potential used in Ref. 8 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. 8 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. 8 on the strong-coupling side, where the excitation gap is controlled by the binding energy of the two-body problem.

In conclusion, the theory of Ref. 2 for the BCS-BEC crossover in the broken-symmetry phase has been shown to compare extremely well with recent QMC data at zero temperature, especially in the intermediate-coupling (crossover) region which 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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