Renormalization of the BCS-BEC crossover by order parameter fluctuations

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We use the functional renormalization group approach with partial bosonization in the particle-particle channel to study the effect of order parameter fluctuations on the BCS-BEC crossover of superfluid fermions in three dimensions. Our approach is based on a new truncation of the vertex expansion where the renormalization group flow of bosonic two-point functions is closed by means of Dyson-Schwinger equations and the superfluid order parameter is related to the single particle gap via a Ward identity. We explicitly calculate the chemical potential, the single-particle gap, and the superfluid order parameter at the unitary point and compare our results with experiments and previous calculations.

The BCS-BEC crossover in a two-component Fermi gas has attracted the attention of theorists for several decades\textsuperscript{[1,2,3,4,5]}\cite{1}. It is generally accepted that the nature of the superfluid state exhibits a smooth crossover as a function of the dimensionless parameter $1/k_F a_s$, where $k_F$ is the Fermi momentum and $a_s$ is the s-wave scattering length in vacuum. While for a small negative scattering length, i.e., $1/k_F a_s < -1$, the paired state generated by the attractive interaction is a collection of spatially extended Cooper pairs (BCS limit), in the opposite limit $1/k_F a_s > 1$ the superfluid state can be viewed as a Bose-Einstein condensate of tightly bound fermion pairs (BEC limit). Of particular interest is the unitary point $1/k_F a_s = 0$ where the scattering length diverges and $k_F$ sets the only length scale of the system. In this regime quantitative calculations are difficult because there is no small parameter to justify approximations.

In the past few years several observables such as the chemical potential and the quasi-particle gap have been determined experimentally at the unitary point\textsuperscript{[6,7,8,9]}\cite{6}, but there is still some uncertainty in the precise numerical values of these quantities. The unitary point has also been studied theoretically using Monte Carlo simulations\textsuperscript{[10]} and various analytical methods based on field theoretical techniques\textsuperscript{[11,12,13,14,15,16,17]} or the functional renormalization group (FRG)\textsuperscript{[18,19,20,21]}\cite{18}, but also in this case the theoretical results have not converged yet. In such a situation it is desirable to study this problem using new approximation strategies which are complementary to previous calculations. In this work we shall therefore develop a novel FRG approach for the BCS-BEC crossover which is based on a suitable truncation of the vertex expansion using skeleton equations and Ward identities. For fixed density we explicitly calculate the chemical potential, the single-particle gap, and the superfluid order-parameter at the unitary point in three dimensions, and compare our results with experiments and with previous calculations.

We consider a system of neutral fermions with energy dispersion $\varepsilon_k = k^2/(2m)$ and a short-range attractive two-body interaction $g_p$ depending on the total momentum $p$ of a fermion pair. After decoupling the interaction in the particle-particle channel using a complex Hubbard-Stratonovich field $\chi$, the Euclidean action of our model can be written as $S = S_0 + S_1$, with Gaussian part $S_0$ and interaction $S_1$ given by\textsuperscript{[22]}

\begin{align}
S_0 &= \sum_\sigma \int_K (-i\omega + \xi_k) \bar{\psi}_{K\sigma} \psi_{K\sigma} + \int_p g_p^{-1} \bar{\chi}_p \chi_p, \quad (1) \\
S_1 &= \int_p \int_K \left[ \bar{\psi}_{K+P\uparrow} \bar{\psi}_{-K\downarrow} \chi_P + \bar{\psi}_{-K\uparrow} \psi_{K+P\downarrow} \chi_P \right]. \quad (2)
\end{align}

Here, the energy $\xi_k = \varepsilon_k - \mu$ is measured relative to the chemical potential $\mu$, and the anti-commuting fields $\psi_{K\sigma}$ and $\bar{\psi}_{K\sigma}$ represent fermions with energy-momentum $K = (i\omega, k)$ and spin projection $\sigma$. The complex bosonic field $\chi$ is conjugate to the fluctuation of the superfluid order parameter with energy-momentum $P = (i\omega, p)$. For convenience we choose our sign convention such that $g_p > 0$ for attractive interactions.

To derive FRG flow equations for our model we introduce a cutoff $\Lambda$ into the Gaussian propagators appearing in Eq. (1) and consider the evolution of the generating functional of the irreducible vertices as the cutoff is reduced\textsuperscript{[23,24]}\cite{23}. The physical vertices are then recovered for $\Lambda \to 0$. The FRG equations for the irreducible vertices of the above mixed boson-fermion theory follow as a special case of the general FRG flow equations derived in Ref.\textsuperscript{[25]}. In contrast to a previous FRG calculation\textsuperscript{[21]}, we use here a scheme where the cutoff is introduced only in the bosonic part of the Gaussian propagator. The advantage of our boson cutoff scheme is that the initial condition for the fermionic self-energy is simply given by the self-consistent Hartree-Fock approximation (i.e. the BCS approximation), while the initial vertices in the
bosonic sector are given by closed fermion loops with an arbitrary number of bosonic external legs \[25\]. In particular, at the initial scale the bosonic two-point functions are given by the ladder approximation. In order to obtain numerically tractable FRG equations, we have to make further approximations: first of all, we neglect the momentum-frequency dependence of the vertices with one boson and two fermion legs, replacing these vertices by a momentum- and frequency-independent coupling \(\gamma = \gamma_\Lambda\). Moreover, we completely ignore vertices with two fermion legs and more than one boson leg. Within these approximations, the FRG flow equations for the anomalous (\(\Delta\)) and normal (\(\Sigma\)) fermionic self-energies in our cutoff scheme are

\[
\partial_\Lambda \Delta(K) = \gamma \partial_\Lambda(\chi) + \frac{\gamma^2}{2} \int_p [F^\ell P - \dot{F}^\ell P] A(P - K), \tag{3}
\]

\[
\partial_\Lambda \Sigma(K) = -\frac{\gamma^2}{2} \int_p [\dot{F}^{\ell P} + F^{\ell P} - 2i\dot{F}^{\ell i} F^{\ell i P}] B(P - K), \tag{4}
\]

which are shown graphically in Fig. 1(a). Here, \(A(K)\) and \(B(K)\) are the anomalous and normal component of the fermionic single-particle Green function, which are related to the self-energies by

\[
A(K) = -\frac{\Delta(K)}{D(K)}, \tag{5}
\]

\[
B(K) = \frac{G^{-1}(-K)}{D(K)}, \tag{6}
\]

where \(G^{-1}(K) = i\omega - \xi_k - \Sigma(K)\) and \(D(K) = G^{-1}(K)G^{-1}(-K) + |\Delta(K)|^2\). The functions \(\dot{F}^{\ell P}\) in Eqs. (3) and (4) are the bosonic single-scale propagators associated with longitudinal (upper index \(\ell\)) or transverse (upper index \(t\)) fluctuations of the field \(\chi\). Choosing for simplicity a sharp momentum cutoff in the bosonic sector, the single-scale propagators are \(\dot{F}^{\ell P} = -\delta(A - |p|)F^{\ell P}\), where the bosonic propagators \(F^{\ell P}\) can be expressed in terms of the irreducible bosonic self-energies \(\Pi^{ij}(P)\) (polarizations) as

\[
\begin{bmatrix}
F^{\ell P} & F^{\ell i P} \\
F^{\ell i P} & F^{\ell i i P}
\end{bmatrix}
= \frac{1}{N(P)}
\begin{bmatrix}
g_p^{-1} + \Pi^{ij}(P) & -\Pi^{ij}(P) \\
-\Pi^{ij}(P) & g_p^{-1} + \Pi^{ij}(P)
\end{bmatrix}, \tag{7}
\]

with

\[
N(P) = [g_p^{-1} + \Pi^{ij}(P)][g_p^{-1} + \Pi^{ij}(P)] + |\Pi^{ij}(P)|^2. \tag{8}
\]

In order to determine the fermionic self-energies from Eqs. (3) and (4) we need additional equations for the polarizations \(\Pi^{ij}(P)\) and for the flowing order parameter \(\chi\). Instead of explicitly writing down the FRG flow equations for \(\Pi^{ij}(P)\), we shall use skeleton equations (which follow from Dyson-Schwinger equations \[23\]) to relate the bosonic self-energies to the fermionic ones \[23\]. Graphically, the exact skeleton equations for the irreducible bosonic self-energies \(\Pi^{ij}(P)\) are shown in Fig. 1(b). Within our truncation where the three-legged boson-fermion vertex is approximated by a flowing cou-
pling $\gamma = \gamma_\Lambda$, these relations become

$$ \Pi^{\ell\ell}(P) = -\frac{\gamma}{2} \int_K \left[ B(K) B(-K + P) - A(K) A(K + P) \right] + (P \rightarrow -P) ,$$

(9a)

$$ \Pi^{tt}(P) = -\frac{\gamma}{2} \int_K \left[ B(K) B(-K + P) + A(K) A(K + P) \right] + (P \rightarrow -P) ,$$

(9b)

$$ \Pi^{\ell t}(P) = -\frac{i\gamma}{2} \int_K \left[ B(K) B(-K + P) \right] - (P \rightarrow -P) .$$

(9c)

To close our system of flow equations, we still need an equation for the vertex renormalization factor $\gamma$ and the flowing order parameter $\langle \chi \rangle$ appearing in Eq. (3). In our boson cutoff scheme, the flow of $\langle \chi \rangle$ is driven by the irreducible vertices with three bosonic legs, $\Gamma^{\ell\ell\ell}, \Gamma^{\ell\ell t}, \Gamma^{tt\ell},$ as shown graphically in Fig. (1c). The crucial point is now that from the requirement that the FRG flow preserves the gapless nature of the Bogoliubov-Anderson (BA) mode [26] we can easily obtain an expression for $\partial_\Lambda \gamma$ without explicitly considering the RG flow of the bosonic three-legged vertices. Therefore we note that the condition for the vanishing of the gap of the BA mode is

$$ g_0^{-1} + \Pi^{\ell\ell}(0) = 0 .$$

(10)

This condition is obviously satisfied at the initial RG scale $\Lambda = \Lambda_0$ because the ladder approximation with self-consistent Hartree-Fock propagators is conserving. To make sure that the BA mode remains gapless for any value of $\Lambda$ we simply require that Eq. (10) remains valid during the entire RG flow. With $\Pi^{\ell\ell}(0)$ given by Eq. (10b), this is an implicit relation between $\partial_\Lambda \Delta(K)$ and $\partial_\Lambda \Sigma(K)$. By demanding that this relation is consistent with Eqs. (3) and (1) we can uniquely fix the RG flow of the order parameter $\langle \chi \rangle$. Finally, using the $U(1)$-gauge symmetry of the action given in Eqs. (1) and (2) we can derive a Ward identity which relates the ratio of the anomalous self-energy and the superfluid order parameter to the vertex renormalization factor $\gamma$,

$$ \Delta(0) = \gamma \langle \chi \rangle .$$

(11)

Eqs. (3)–(11) form a closed system of integro-differential equations for the fermionic self-energies $\Delta(K), \Sigma(K)$, the vertex renormalization factor $\gamma$ and the order parameter $\langle \chi \rangle$, which should be solved with the initial conditions $\Delta(K)_{\Lambda_0} = \langle \chi \rangle_{\Lambda_0} = \Delta_0$ and $\Sigma(K)_{\Lambda_0} = 0.$ Here, $\Delta_0$ is the single-particle gap in the BCS approximation.

The numerical analysis of the system of coupled integro-differential equations (3)–(11) is beyond the scope of this work. Here, we further simplify these equations by neglecting the momentum-dependence of the fermionic self-energies and keeping only the linear frequency correction to the normal self-energy, replacing $\Delta(K) \rightarrow \Delta$ and $\Sigma(K) \rightarrow \Sigma - (Z^{-1} - 1)i\omega$, where

$$ Z = \frac{1}{1 - \frac{\partial \Sigma(\omega, 0)}{\partial \omega} \bigg|_{\omega = 0} (\omega^2 + \tilde{E}_k^2)^2} .$$

(12)

is the inverse flowing wave function renormalization factor. The flowing single-particle propagators are then given by $A(K) = Z \tilde{A}(K)$ and $B(K) = Z \tilde{B}(K)$, where

$$ \tilde{A}(K) = -\tilde{\Delta}/(\omega^2 + \tilde{E}_k^2) ,$$

(13)

$$ \tilde{B}(K) = -(i\omega + \tilde{\xi}_k)/(\omega^2 + \tilde{E}_k^2) ,$$

(14)

with $\tilde{E}_k = [\tilde{\xi}_k^2 + \tilde{\Delta}^2]^{1/2}, \tilde{\xi}_k = \tilde{\epsilon}_k - \tilde{\mu}, \tilde{\epsilon}_k = Z \epsilon_k, \tilde{\mu} = Z(\mu - \Sigma),$ and $\tilde{\Delta} = Z\Delta$. It should be noted that $\Delta$ can be identified with the physical single particle gap which can be measured, e.g., in tunnelling experiments. With these approximations, our system of flow equations reduces in $D$ dimensions to

$$ \Lambda \delta_\Lambda \tilde{\mu} = \eta \tilde{\mu} - \gamma (\Lambda/k_{F,0}) D \epsilon_{F,0} ,$$

$$ \times \int \frac{d\omega}{2\pi} \left[ \tilde{F}_{P}^{\ell\ell} + \tilde{F}_{P}^{tt} - 2i\tilde{F}_{P}^{\ell t} \right] \tilde{B}(P) ,$$

(15)

$$ \Lambda \delta_\Lambda \ln \gamma = -\left(\gamma/\tilde{\Delta}\right) (\Lambda/k_{F,0}) D \epsilon_{F,0} ,$$

$$ \times \int \frac{d\omega}{2\pi} \left[ \tilde{F}_{P}^{\ell\ell} - \tilde{F}_{P}^{tt} \right] \tilde{A}(P) .$$

(16)

The wave function renormalization factor is determined by $\Lambda \delta_\Lambda Z = \eta Z$, with the flowing anomalous dimension

$$ \eta = \gamma (\Lambda/k_{F,0}) D \epsilon_{F,0} \int \frac{d\omega}{2\pi} \left[ \tilde{F}_{P}^{\ell\ell} + \tilde{F}_{P}^{tt} - 2i\tilde{F}_{P}^{\ell t} \right]$$

$$ \times \frac{\tilde{E}_k^2 - \omega^2 + 2i\omega \tilde{\xi}_k}{(\omega^2 + \tilde{E}_k^2)^2} .$$

(17)

Due to the sharp momentum cutoff we may set $P = (i\omega, \Lambda)$. The FRG flow is further constrained by the condition (10) that the BA mode is gapless and by the relation

$$ \tilde{\Delta} = Z \gamma \langle \chi \rangle .$$

(18)

imposed by the Ward identity (11). The dimensionless interaction terms $\tilde{F}_{P}^{ij}$ appearing above are defined by $\tilde{F}_{P}^{ij} = Z^2 \gamma_{0E} F_{P}^{ij}$, and $\epsilon_{F,0}, k_{F,0},$ and $\gamma_{0}$ denote the Fermi energy, the Fermi wave vector and the density of states at the Fermi energy (per spin projection) of a non-interacting system which has exactly the same density as our interacting system at the initial scale $\Lambda = \Lambda_0$.

For convenience, we work with a momentum-independent bare coupling $g_0 \rightarrow g$. In dimensions $D \geq 2$ this gives rise to an ultraviolet divergence in the BCS gap equation which also appears in the polarizations $\Pi^{ii}(P) = \Pi^{ii}(P)/(Z^2 \gamma_0)$. For $D > 2$ we may absorb this divergence into the bare coupling by introducing the dressed coupling $g$ via $(Z^2 \gamma g)^{-1} \rightarrow (Z^2 \gamma g_0)^{-1} - \epsilon_0$.
$V^{-1} \sum_k (2\tilde{\epsilon}_k)^{-1}$, so that the constraint (10) that the BA mode remains gapless turns into

$$\frac{1}{Z^2 \gamma g} = \frac{1}{V} \sum_k \left[ \frac{1}{2E_k} - \frac{1}{2\tilde{\epsilon}_k} \right].$$

(19)

In $D = 3$ the dressed coupling is related to the s-wave scattering length $a_s$ via $g = -4\pi a_s/m$. It is intriguing to note that we can derive exactly the same equation by means of a skeleton equation for the order parameter. This means that the gaplessness of the BA mode is in fact a natural consequence of our truncation scheme. Together with the rescaled Ward identity (18), the gapless condition (19), the flow equations (15)–(17) form a closed system of RG equations for the five parameters $\langle \chi \rangle$, $\Lambda$, $\tilde{\mu} = Z(\mu - \Sigma)$, $\eta$ and $\gamma$ which can be solved numerically without further approximation. All bosonic polarizations can be expressed in terms of these parameters via skeleton approximations. For every value of the cutoff $\Lambda$ this requires the numerical evaluation of a three-dimensional integral. The RG flow of the three-legged vertex $\gamma$ and the wave function renormalization factor $Z$ at the unitary point in three dimensions is shown in Fig. 2. Moreover, in Fig. 3 we present our results for the order parameter $\langle \chi \rangle$, the single-particle gap $\Delta$, and the chemical potential $\mu$ at the unitary point in $D = 3$. Here, $\epsilon_F$ is the Fermi energy of a noninteracting system which has the same density as our interacting system.

Our value $\mu / \epsilon_F = 0.32$ is smaller than the Monte Carlo results 0.44 (Ref. 11) and 0.42 (Ref. 12), but it is quite close to the value 0.36 obtained by Haussmann et al. 16 and agrees perfectly with the experiment by Bartenstein et al. 6. Our value for the renormalized single-particle gap is within the error bars of the Monte Carlo simulations 11, 12, and agrees with the FRG calculation by Diehl et al. 19, while the FRG result for $\Delta / \epsilon_F$ by Krippa 18 is only 3% smaller than the mean-field result. In contrast to our approach, the FRG calculations of Refs. 18, 19 are based on a truncated gradient expansion and do not distinguish between the quasi-particle gap and the order parameter, which are conceptually different quantities.

In summary, using a new truncation strategy of the FRG flow equations for the BCS-BEC crossover we have calculated the chemical potential, the single-particle gap, and the order parameter at the unitary point in three dimensions and obtained reasonable agreement with experiments and other calculations. In contrast to the truncated derivative expansion of FRG flow equation for the BCS-BEC crossover used in Refs. 19, 20, our strategy is based on a truncation of the vertex expansion of the partially bosonized theory using Dyson-Schwinger equations and Ward identities. Moreover, by introducing a momentum cutoff only in the bosonic sector, we can directly calculate fluctuation corrections to the mean-field approximation, which serves as the initial condition for the FRG flow. The strong vertex correction of almost 50% shown in Fig. 2 shows that Eliashberg type approximations are not quantitatively accurate close to the unitary point.

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