Renormalization of the BCS-BEC crossover by order-parameter fluctuations

Lorenz Bartosch and Peter Kopietz
Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

Alvaro Ferraz
International Center for Condensed Matter Physics, Universidade de Brasília, 70910-900 Brasília, DF, Brazil
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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-Bose-Einstein condensate (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.

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I. INTRODUCTION

The BCS-Bose-Einstein condensate (BEC) crossover in a two-component Fermi gas has attracted the attention of theorists for several decades.[1–5] 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., $1/k_F a_s \ll -1$, the paired state generated by the attractive interaction is a collection of spatially extended Cooper pairs (BCS limit), in the opposite limit $1/k_F a_s \gg 1$ 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 quasiparticle gap have been determined experimentally at the unitary point.[6–10] The unitary point has also been studied theoretically using Monte Carlo simulations[11,12] and various analytical methods based on field theoretical techniques[13–21] or the functional renormalization group (FRG).[22–25] While the experimental results seem to converge to the reliable large scale Monte Carlo results, the quantitative accuracy of field theoretical and FRG results still cannot compete with Monte Carlo calculations. On the other hand, numerical simulations do not give much insight into the nature of interaction processes which dominate the physics at the unitary point.

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 an 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.

The remainder of this work is organized as follows: in Sec. II we derive FRG flow equations for our model system of neutral fermions interacting via a short-range attractive interaction; we also discuss skeleton equations and Ward identities which we use to close our system of flow equations. In Sec. III we then present our numerical results and show plots of the renormalization group flow of the vertex correction factor γ, the wave function renormalization factor Z, the order parameter $\langle\chi\rangle$, the single-particle gap $\tilde{\Delta}$, and the chemical potential μ at the unitary point. Finally, in Sec. IV we discuss our results and close with some conclusions.

II. FRG FLOW EQUATIONS, SKELETON EQUATIONS, AND WARD IDENTITIES

We consider a system of neutral fermions with energy dispersion $\epsilon_{\boldsymbol{k}} = \boldsymbol{k}^2/(2m)$ and a short-range attractive two-body interaction $g_{\boldsymbol{p}}$ depending on the total momentum $\boldsymbol{p}$ of a fermion pair. After decoupling the interaction in the particle-particle channel using a complex Hubbard-Stratonovich field χ, 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[26]

$$S_0 = \sum_\sigma \int_K (-i\omega + \xi_{\boldsymbol{k}}) \bar{\psi}_{K\sigma}\psi_{K\sigma} + \int_P g_{\boldsymbol{p}}^{-1} \bar{\chi}_P \chi_P, \tag{1}$$

$$S_1 = \int_P \int_K [\bar{\psi}_{K+P\uparrow}\bar{\psi}_{-K\downarrow}\chi_P + \psi_{-K\downarrow}\psi_{K+P\uparrow}\bar{\chi}_P]. \tag{2}$$

Here, the energy $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$ is measured relative to the chemical potential μ, and the anticommuting fields $\psi_{K\sigma}$ and $\bar{\psi}_{K\sigma}$ represent fermions with energy momentum $K = (i\omega, \boldsymbol{k})$ and spin projection σ. The complex bosonic field χ_P is conjugate to the fluctuation of the superfluid order parameter with energy momentum $P = (i\bar{\omega}, \boldsymbol{p})$. It should be noted that while $i\omega$ denotes a fermionic Matsubara frequency, $i\bar{\omega}$ denotes a bosonic one. For convenience we choose our sign convention such that $g_{\boldsymbol{p}} > 0$ for attractive interactions.

To derive FRG flow equations for our model we introduce a cutoff Λ 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.[27,28] 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. 29. In contrast to a previous FRG calculation,[25] 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.[29] 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. This implies that we do not (re)generate vertices with more than two fermionic legs. Within these approximations, the FRG flow equations for the anomalous (Δ) and normal (Σ) fermionic self-energies in our cutoff scheme are

$$\partial_\Lambda \Delta(K) = \gamma \partial_\Lambda \langle \chi \rangle + \frac{\gamma^2}{2} \int_P [\dot{F}_P^{\ell\ell} - \dot{F}_P^{tt}] A(P-K), \tag{3}$$

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

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's 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 $\dot{F}_P^{ij}$ in Eqs. (3) and (4) are the bosonic single-scale propagators associated with longitudinal (upper index ℓ) or transverse (upper index t) fluctuations of the field χ. Choosing for simplicity a sharp momentum cutoff in the bosonic sector, the single-scale propagators are $\dot{F}_P^{ij} = -\delta(\Lambda - |\boldsymbol{p}|) F_P^{ij}$, where the bosonic propagators F_P^{ij} can be expressed in terms of the irreducible bosonic self-energies $\Pi^{ij}(P)$ (polarizations) as

$$\begin{bmatrix} F_P^{\ell\ell} & F_P^{\ell t} \\ F_P^{t\ell} & F_P^{tt} \end{bmatrix} = \frac{1}{N(P)} \begin{bmatrix} g_p^{-1} + \Pi^{tt}(P) & -\Pi^{\ell t}(P) \\ -\Pi^{t\ell}(P) & g_p^{-1} + \Pi^{\ell\ell}(P) \end{bmatrix} \tag{7}$$

with

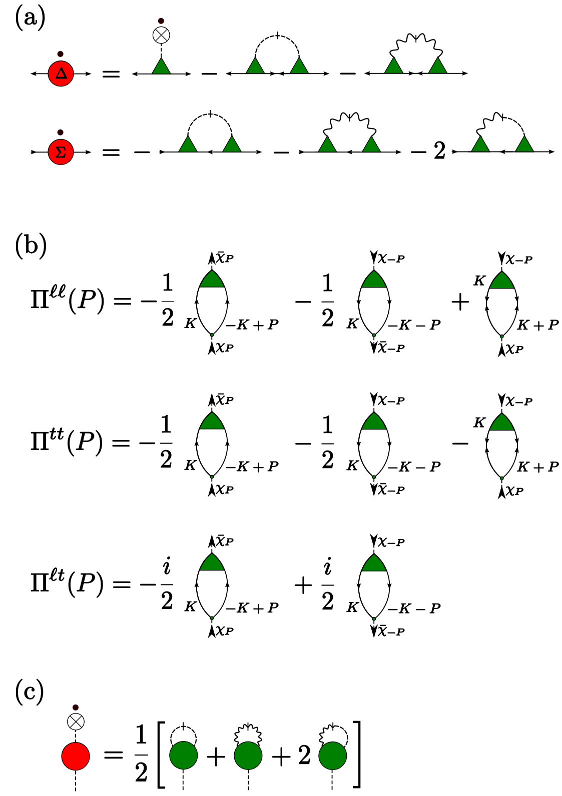

FIG. 1. (Color online) (a) Diagrammatic representation of our approximate FRG flow equations (3) and (4) for the fermionic self-energies $\Delta(K)$ and $\Sigma(K)$. (b) Exact skeleton equations for the bosonic self-energies $\Pi^{\ell\ell}(P), \Pi^{\ell t}(P), \Pi^{tt}(P)$. (c) Exact FRG flow equation for the order parameter $\langle \chi \rangle$. Solid arrows represent fermionic propagators, dashed arrows represent the complex boson fields χ and $\bar{\chi}$, dashed lines without arrow represent longitudinal components φ^ℓ of $\chi = (\varphi^\ell + i\varphi^t)/\sqrt{2}$, while wavy lines represent the transverse components φ^t.

$$N(P) = [g_p^{-1} + \Pi^{\ell\ell}(P)][g_p^{-1} + \Pi^{tt}(P)] + [\Pi^{\ell t}(P)]^2. \tag{8}$$

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 $\langle \chi \rangle$. Instead of explicitly writing down the FRG flow equations for $\Pi^{ij}(P)$, we shall use skeleton equations (which follow from Dyson-Schwinger equations[29]) to relate the bosonic self-energies to the fermionic ones.[30] 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 coupling $\gamma = \gamma_\Lambda$, these relations become

$$\Pi^{\ell\ell}(P) = -\frac{\gamma}{2} \int_K [B(K)B(-K+P) - A(K)A(K+P) + (P \to -P)], \tag{9a}$$

$$\Pi^{tt}(P) = -\frac{\gamma}{2} \int_K [B(K)B(-K+P) + A(K)A(K+P) + (P \to -P)], \tag{9b}$$

$$\Pi^{\ell t}(P) = -\frac{i\gamma}{2}\int_K [B(K)B(-K+P) - (P \to -P)]. \quad (9c)$$

To close our system of flow equations, we still need an equation for the vertex renormalization factor γ 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, $\Gamma^{\ell\ell\ell},\Gamma^{\ell\ell t},\Gamma^{\ell tt}$, as shown graphically in Fig. 1(c). The crucial point is now that from the requirement that the FRG flow preserves the gapless nature of the Bogoliubov-Anderson (BA) mode[31] we can easily obtain an expression for $\partial_\Lambda\langle\chi\rangle$ 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

$$g_0^{-1} + \Pi^{tt}(0) = 0. \quad (10)$$

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 Λ we simply require that Eq. (10) remains valid during the entire RG flow. With $\Pi^{tt}(0)$ given by Eq. (9b), 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 (4) 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 γ

$$\Delta(0) = \gamma\langle\chi\rangle. \quad (11)$$

Equations (3)–(8), (9a)–(9c), (10), and (11) form a closed system of integrodifferential equations for the fermionic self-energies $\Delta(K)$ and $\Sigma(K)$, the vertex renormalization factor γ, 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, Δ_0 is the single-particle gap in the BCS approximation.

The numerical analysis of the system of coupled integro-differential equations (3)–(8), (9a)–(9c), (10), and (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 $\Delta(K)\to\Delta$ and $\Sigma(K)\to\Sigma-(Z^{-1}-1)i\omega$, where

$$Z = \frac{1}{1 - \left.\frac{\partial\Sigma(i\omega,0)}{\partial(i\omega)}\right|_{\omega=0}} \quad (12)$$

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

$$\tilde{A}(K) = -\tilde{\Delta}/(\omega^2 + \tilde{E}_{\boldsymbol{k}}^2), \quad (13)$$

$$\tilde{B}(K) = -(i\omega + \tilde{\xi}_{\boldsymbol{k}})/(\omega^2 + \tilde{E}_{\boldsymbol{k}}^2) \quad (14)$$

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

$$\Lambda\partial_\Lambda\tilde{\mu} = \eta\tilde{\mu} - \gamma(\Lambda/k_{F,0})^D\epsilon_{F,0} \times \int \frac{d\bar{\omega}}{2\pi}[\tilde{F}_P^{\ell\ell} + \tilde{F}_P^{tt} - 2i\tilde{F}_P^{\ell t}]\tilde{B}(P), \quad (15)$$

$$\Lambda\partial_\Lambda \ln\gamma = -(\gamma/\tilde{\Delta})(\Lambda/k_{F,0})^D\epsilon_{F,0}\int \frac{d\bar{\omega}}{2\pi}[\tilde{F}_P^{\ell\ell} - \tilde{F}_P^{tt}]\tilde{A}(P). \quad (16)$$

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

$$\eta = \gamma(\Lambda/k_{F,0})^D\epsilon_{F,0}\int \frac{d\bar{\omega}}{2\pi}[\tilde{F}_P^{\ell\ell} + \tilde{F}_P^{tt} - 2i\tilde{F}_P^{\ell t}] \times \frac{\tilde{E}_\Lambda^2 - \bar{\omega}^2 + 2i\bar{\omega}\tilde{\xi}_\Lambda}{(\bar{\omega}^2 + \tilde{E}_\Lambda^2)^2}. \quad (17)$$

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

$$\tilde{\Delta} = Z\gamma\langle\chi\rangle \quad (18)$$

imposed by the Ward identity (11). The dimensionless interaction terms $\tilde{F}_P^{ij}$ appearing above are defined by $\tilde{F}_P^{ij}=Z^2\gamma\nu_0F_P^{ij}$, and $\epsilon_{F,0}$, $k_{F,0}$, and ν_0 denote the Fermi energy, the Fermi wave vector and the density of states at the Fermi energy (per spin projection) of a noninteracting 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 $g_{\boldsymbol{p}}\to g_0$. In dimensions $D\geq 2$ this gives rise to an ultraviolet divergence in the BCS gap equation which also appears in the polarizations $\tilde{\Pi}^{ii}(P)=\Pi^{ii}(P)/(Z^2\gamma\nu_0)$. For $D>2$ we may absorb this divergence into the bare coupling by introducing the dressed coupling g via $(Z^2\gamma g)^{-1}=(Z^2\gamma g_0)^{-1}-V^{-1}\Sigma_{\boldsymbol{k}}(2\tilde{\epsilon}_{\boldsymbol{k}})^{-1}$ so that the constraint (10) that the BA mode remains gapless turns into

$$\frac{1}{Z^2\gamma g} = \frac{1}{V}\sum_{\boldsymbol{k}}\left[\frac{1}{2\tilde{E}_{\boldsymbol{k}}} - \frac{1}{2\tilde{\epsilon}_{\boldsymbol{k}}}\right]. \quad (19)$$

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.

III. RESULTS

Together with the rescaled Ward identity (18) and the gapless condition (19), the flow equations (15)–(17) form a

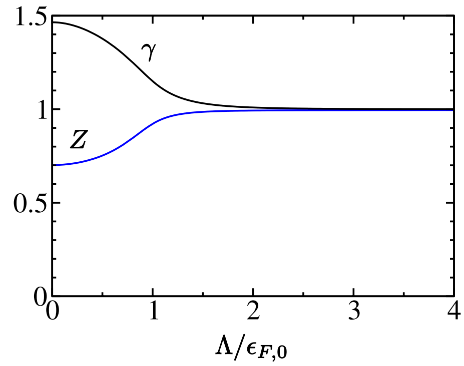

FIG. 2. (Color online) Renormalization group flow, the three-legged vertex γ, and the wave function renormalization factor Z at the unitary point ($k_F a_s = \infty$) in three dimensions.

closed system of RG equations for the five parameters $\langle \chi \rangle$, $\tilde{\Delta}$, $\tilde{\mu} = Z(\mu - \Sigma)$, η, and γ which can be solved numerically without further approximation. All bosonic polarizations can be expressed in terms of these parameters via skeleton equations. For every value of the cutoff Λ this requires the numerical evaluation of a three-dimensional integral. The renormalization group flow of the three-legged vertex γ 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 renormalized single-particle gap $\tilde{\Delta}$, and the chemical potential μ in units of the Fermi energy ϵ_F of a noninteracting system having exactly the same density as our flowing system.

Note that ϵ_F is determined by the true density ρ of the system which we calculate via the normal component of the one-particle Green's function for a given value of the cutoff Λ

$$\rho = \frac{Z}{V} \sum_k \left[1 - \frac{\tilde{\xi}_k}{\tilde{E}_k} \right]. \tag{20}$$

The flowing Fermi energy ϵ_F can now be obtained from

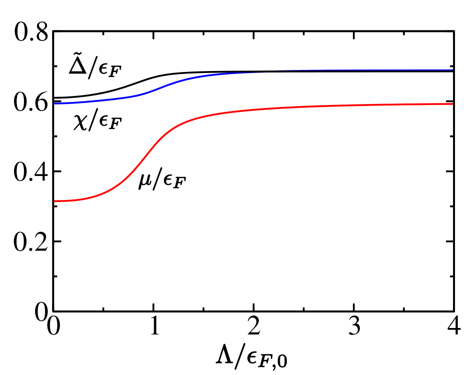

FIG. 3. (Color online) Renormalization group flow, the order parameter $\langle \chi \rangle$, the renormalized single-particle gap $\tilde{\Delta}$, and the chemical potential μ at the unitary point in $D=3$. Here, ϵ_F is the Fermi energy of a noninteracting system which has the same density as our interacting system.

$$\frac{\epsilon_F}{\epsilon_{F,0}} = \left(\frac{\rho}{\rho_0} \right)^{2/D}, \tag{21}$$

where $\epsilon_{F,0}$ and ρ_0 are the mean-field values at the beginning of the flow. At the end of the flow we find the following renormalized quantities:

$$\mu/\epsilon_F = 0.32, \quad \tilde{\Delta}/\epsilon_F = 0.61, \quad \langle \chi \rangle / \epsilon_F = 0.59. \tag{22}$$

At the unitary point we may calculate the ground-state energy per particle from $\varepsilon_0 = D\mu/(D+2) = 0.19$. The above numbers should be compared with the mean-field results $\mu/\epsilon_F = 0.59$ and $\tilde{\Delta}/\epsilon_F = \langle \chi \rangle / \epsilon_F = 0.69$.

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.*[19] 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.*[23] while the FRG result for $\tilde{\Delta}/\epsilon_F$ by Krippa[22] is only 3% smaller than the mean-field result. In contrast to our approach, the FRG calculations of Refs. 22 and 23 are based on a truncated gradient expansion and do not distinguish between the quasiparticle gap and the order parameter, which are conceptually different quantities.

IV. CONCLUSIONS

In summary, using a 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 in three dimensions and obtained reasonable agreement with experiments and other calculations. While we have concentrated on the physically most interesting unitary point where results can be most easily compared with those of others, the formalism developed here is valid for arbitrary interactions so that fluctuation corrections can in principle be calculated for the whole BCS-BEC crossover regime. In contrast to the truncated derivative expansion of FRG flow equation for the BCS-BEC crossover used in Refs. 23 and 24, our strategy is based on a truncation of the vertex expansion of the partially bosonized theory using Dyson-Schwinger equations and Ward identities. In our approach the FRG flow equations allow for different renormalizations of the quasiparticle gap and the order parameter which are however tied together by the remarkably simple Ward identity $\tilde{\Delta} = Z\gamma \langle \chi \rangle$, see Eq. (18). 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 demonstrates that Eliashberg-type approximations are not quantitatively accurate close to the unitary point.

ACKNOWLEDGMENTS

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