PHYSICAL REVIEW A **75**, 023610 (2007)

Thermodynamics of the BCS-BEC crossover

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(Received 11 August 2006; revised manuscript received 8 November 2006; published 8 February 2007)

We present a self-consistent theory for the thermodynamics of the BCS-BEC crossover in the normal and superfluid phase which is both conserving and gapless. It is based on the variational many-body formalism developed by Luttinger and Ward and by DeDominicis and Martin. Truncating the exact functional for the entropy to that obtained within a ladder approximation, the resulting self-consistent integral equations for the normal and anomalous Green functions are solved numerically for arbitrary coupling. The critical temperature, the equation of state, and the entropy are determined as a function of the dimensionless parameter $1/k_Fa$, which controls the crossover from the BCS regime of extended pairs to the BEC regime of tightly bound molecules. The tightly bound pairs turn out to be described by a Popov-type approximation for a dilute, repulsive Bose gas. Even though our approximation does not capture the critical behavior near the continuous superfluid transition, our results provide a consistent picture for the complete crossover thermodynamics which compares well with recent numerical and field-theoretic approaches at the unitarity point.

DOI: 10.1103/PhysRevA.75.023610 PACS number(s): 03.75.Ss, 03.75.Hh, 74.20.Fg

I. INTRODUCTION

The problem of a two-component attractive Fermi gas near a resonance of the *s*-wave scattering length describing the effective interaction is one of the basic many-body problems which has been brought into focus by the recent realization of molecular condensates in ultracold Fermi gases [1–3] and the subsequent exploration of the crossover from a Bose-Einstein condensate (BEC) to a BCS-like state of weakly bound fermion pairs [4]. Clear signatures for the existence of paired fermion superfluidity with cold atoms have been provided by spectroscopic measurements of the gap [5] and the observation of a vortex lattice on the BCS side of the transition [6]. The ability of tuning the interaction in cold Fermi gases through Feshbach resonances relies on the resonant coupling of the scattering state near zero energy of two colliding atoms with a bound state in a closed channel [7]. A particularly challenging problem arises right at the Feshbach resonance, where the two-particle scattering length is infinite [8,9]. Precisely at this point and for broad Feshbach resonances, where the range $r^\star$ of the effective interaction is much smaller than the mean interparticle spacing [10–13], the full many-body problem has the Fermi energy ε_F as the only energy scale. As pointed out by Ho [14], the thermodynamics of the unitary Fermi gas is then a function only of the dimensionless temperature $\theta=T/T_F$. More generally, as emphasized recently by Nikolić and Sachdev [15], the universality also extends to the behavior away from the Feshbach resonance, as long as the broad resonance condition $k_Fr^\star \ll 1$ is obeyed. Thus, for instance, the critical temperature T_c/T_F for the transition to superfluidity is a universal function of the inverse coupling constant $1/k_Fa$.

A quantitative theoretical understanding of the many-body problem near a Feshbach resonance has been developed recently through numerical calculations. In particular, at zero temperature and for a homogeneous system, fixed-node Green function Monte Carlo calculations provide quantitative results for the gap parameter [16], the equation of state [17], and also the momentum distribution, the condensate fraction, and the pair size [18] of the ground state for arbitrary values of $1/k_Fa$. As expected in the case of an *s*-wave resonance [19], these quantities all evolve continuously as the coupling is varied from the BCS to the BEC limit. An important ingredient in these results is their account for the repulsive interaction between strongly bound dimers in the BEC limit with scattering length $a_{dd}\approx 0.60a>0$ [20]. This interaction is missing in the early qualitative descriptions of the $T=0$ BCS-BEC crossover problem by Eagles [21] and Leggett [22], which are based on using the standard BCS ground state as a variational ansatz for *arbitrary* coupling [23]. Beyond a purely numerical approach, the BCS-BEC crossover problem has recently become amenable also to analytical methods via an $\epsilon=4-d$ expansion [24]. It is based on the observation [25] that at the unitarity point in $d=4$ (i.e., the point where a two-particle bound state appears) the two-component Fermi gas is in fact an ideal Bose gas, because a zero-range interaction in $d=4$ can bind a state only at infinitely strong attraction. In two dimensions, in turn, binding appears at arbitrary small couplings and the unitary Fermi gas in $d\leq 2$ coincides with a noninteracting one [25]. Within a field-theoretic description, the physically interesting three-dimensional (3D) problem can thus be approached by extrapolating expansions from the upper and lower critical dimensions $d=4$ and $d=2$, respectively [26]. At finite temperature, numerical calculations are available for the thermodynamics at the unitarity point. They are based on an auxiliary field quantum Monte Carlo method for the continuum problem [27] and on a diagrammatic determinant Monte Carlo method for the negative-U Hubbard model [28]. Field-theoretic results at finite temperature, which open the possibility for controlled and systematic expansions for the crossover thermodynamics, have been obtained very recently by Nishida [26] within an expansion around both the upper and lower critical dimensions and by Nikolic and Sachdev [15] within a $1/N$ expansion for a $2N$-component Fermi gas.

Our aim in the following is to present a self-consistent many-body theory for the thermodynamics of resonantly interacting fermions at arbitrary temperatures and detuning, which directly addresses the physically relevant case of a three-dimensional, two-component Fermi gas. The theory is based on a conserving, so-called Φ-derivable approach to the many-body problem, in which the exact one- or two-particle Green functions serve as an infinite set of variational parameters. It is an extension of earlier work by one of us [29–31] and employs a combination of the Luttinger-Ward and De Dominicis–Martin approach for obtaining the grand canonical potential and the entropy, respectively. The condition of gaplessness is enforced by a modified coupling constant, thus accounting for the proper low-energy behavior in terms of a Bogoliubov-Anderson mode. We provide quantitative results for the critical temperature, the equation of state, and the entropy near the Feshbach resonance as a function of both T/T_F and $1/k_F a$. In spite of the fact that the critical behavior at the continuous superfluid transition is not captured correctly in our approach, which gives rise to a weak first-order transition, the results provide a quantitative and consistent picture of the crossover which obeys thermodynamic relations at the percent level. Our variational method is complementary both to purely numerical and to field-theoretic approaches to the problem. The results can be used, e.g., to predict the final temperature reached after an adiabatic ramp across the Feshbach resonance starting deeply in the BEC regime [32] or to determine the size of the atom cloud in a harmonic trap near unitarity as a function of temperature.

The paper is organized as follows: in Sec. II we introduce our model and the basic many-body formalism necessary for deriving a set of self-consistent equations for the Green and vertex functions which are the variational parameters of the theory. The complete thermodynamics is then determined by integrals of the momentum- and frequency-dependent Green functions. It is shown that with a modified coupling constant, the theory can be formulated in a way consistent with Ward identities, which guarantees a gapless Bogoliubov-Anderson mode for arbitrary strength of the coupling. In Sec. III we discuss the numerical solution, providing quantitative results for the critical temperature, the pressure, internal energy, and the entropy of the BCS-BEC crossover in both the normal and superfluid phases. They are compared with both experimental and theoretical results based on numerical and field-theoretic approaches. Finally in Sec. IV we give a brief summary and indicate open problems.

II. MANY-BODY THEORY OF RESONANTLY INTERACTING FERMIONS

In order to describe interacting fermions near a Feshbach resonance, it is in general necessary to include the resonant, closed-channel bound state explicitly—e.g., within a Bose-Fermi-resonance model [33,34]. As has been shown, for instance, by Diener and Ho [11], however, the situation can be simplified in the case of broad Feshbach resonances, where the effective range $r^\star$ of the resonant interaction is much smaller than both the background scattering length a_{bg} and the Fermi wavelength λ_F. In this limit, which is in fact appropriate for the existing experimental studies of the BCS-BEC crossover problem in ^{6}Li [5] and ^{40}K [1], the problem can be reduced to a single-channel Hamiltonian with an instantaneous interaction [10–13]. The associated effective two-body interaction is thus described by a pseudopotential $V(\mathbf{r}) \sim \delta(\mathbf{r})$ (appropriately renormalized; see below) with a strength proportional to the scattering length

$$a = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right). \tag{2.1}$$

Here a_{bg} is the off-resonant background scattering length in the absence of the coupling to the closed channel while ΔB and B_0 describe the width and position of the resonance which may be tuned by an external magnetic field B. The interacting Fermi system is thus described by the standard Hamiltonian

$$\hat{H} = \int d^d r \sum_\sigma \frac{\hbar^2}{2m}[\nabla \psi_\sigma^\dagger(\mathbf{r})][\nabla \psi_\sigma(\mathbf{r})] + \frac{1}{2}\int d^d r \int d^d r' \times \sum_{\sigma\sigma'} V(\mathbf{r}-\mathbf{r}')\psi_\sigma^\dagger(\mathbf{r})\psi_{\sigma'}^\dagger(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}), \tag{2.2}$$

where $\psi_\sigma(\mathbf{r})$ and $\psi_\sigma^\dagger(\mathbf{r})$ are the usual fermion field operators. The formal spin index σ labels two internal degrees of freedom, which in practice are two different hyperfine states. In the approximation, where the effective range of the resonant interaction is taken to zero, the interaction potential can formally be replaced by a δ potential between fermions of opposite spin:

$$V(\mathbf{r}-\mathbf{r}') = g_0\delta(\mathbf{r}-\mathbf{r}'). \tag{2.3}$$

Its strength g_0 needs to be renormalized for dimensions $d \geq 2$ by introducing the scattering amplitude g via

$$\frac{1}{g} = \frac{1}{g_0} + \int \frac{d^d k}{(2\pi)^d}\frac{m}{\hbar^2 \mathbf{k}^2}. \tag{2.4}$$

For dimensions $d \geq 2$ the integral diverges at high momenta. Since the scattering amplitude g is kept constant, the bare interaction parameter g_0 must be taken to zero in the limit where the cutoff diverges. The associated limiting process $g_0 \to -0$ accounts for the replacement of the bare potential (2.3) by a pseudopotential with the proper scattering length. While the formulas are derived for arbitrary space dimensions d, eventually we consider fermions for $d=3$. In this case the scattering amplitude g is simply connected to the s-wave scattering length a given in Eq. (2.1) by $g = 4\pi\hbar^2 a/m$.

In the following, we consider a homogeneous situation described by a grand canonical distribution at fixed temperature and chemical potential. The thermodynamic properties thus follow from the grand partition function

$$Z = \mathrm{Tr}\{\exp(-\beta[\hat{H} - \mu\hat{N}])\} \tag{2.5}$$

and the associated grand potential

$$\Omega = \Omega(T,\mu) = -\beta^{-1}\ln Z, \tag{2.6}$$

which is directly related to the pressure p via $\Omega = -pV$. Within our simplified model, where the range of the interaction is set to zero, the Fermi system is described by three parameters: the temperature T, the chemical potential μ, and the s-wave scattering length a. Apart from an overall scale, the thermodynamics thus depends only on two dimensionless ratios. It is convenient to replace the chemical potential μ by the fermion density $n=k_F^3/3\pi^2$, which defines the Fermi wave number k_F and the Fermi energy $\varepsilon_F=\hbar^2k_F^2/2m$ as characteristic length and energy scales. The equilibrium state is then uniquely determined by only two parameters: the dimensionless temperature $\theta=T/\varepsilon_F$ (we choose units for the temperature in which $k_B=1$) and the dimensionless interaction strength $v=1/k_Fa$. In the special case $B=B_0$ of an infinite scattering length (the so-called unitarity limit), the parameter v drops out and the resulting thermodynamic quantities are universal functions of θ [14].

A. Luttinger-Ward formalism

The BCS-BEC crossover is controlled by two physical phenomena. The first one is connected with the formation of pairs due to the attractive interaction. The second one is the transition to superfluidity below a certain critical temperature T_c. In the BCS limit, the formation of pairs and the superfluid transition are simultaneous. The transition is driven by the thermal breakup of pairs—i.e., by excitations which may be described by a purely fermionic theory. With increasing strength of the interaction, however, there is an increasingly wide range of temperatures where bound pairs coexist with unpaired fermions. In the BEC limit, pair formation, as a chemical equilibrium between bound and dissociated atoms, occurs at a temperature scale much higher than the superfluid transition. The latter is driven by collective excitations of a then purely bosonic system. A proper description of the crossover thus requires one to account for both bosonic and fermionic excitations simultaneously.

Following the formalism developed by Luttinger and Ward [35] for nonsuperfluid interacting Fermi systems, the grand thermodynamic potential (2.6) can be expressed as a unique functional of the Green function

$$G_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}',\tau-\tau') = \begin{pmatrix} \delta_{\sigma\sigma'}\mathcal{G}(\mathbf{r}-\mathbf{r}',\tau-\tau') & \varepsilon_{\sigma\sigma'}\mathcal{F}(\mathbf{r}-\mathbf{r}',\tau-\tau') \\ -\varepsilon_{\sigma\sigma'}\mathcal{F}^*(\mathbf{r}'-\mathbf{r},\tau-\tau') & -\delta_{\sigma\sigma'}\mathcal{G}(\mathbf{r}'-\mathbf{r},\tau'-\tau) \end{pmatrix} \tag{2.7}$$

in the form

$$\Omega[G]=\beta^{-1}\left(-\tfrac{1}{2}\,\mathrm{Tr}\{-\ln G+[G_0^{-1}G-1]\}-\Phi[G]\right). \tag{2.8}$$

The trace Tr is defined with respect to the formal index $X=(\mathbf{r},\tau,\sigma,\alpha)$ which combines the space variable $\mathbf{r}$, the imaginary time τ, the spin index σ, and the Nambu index α. The interaction between the fermions is described by the functional $\Phi[G]$, which can be expressed in terms of a perturbation series of irreducible Feynman Diagrams where the propagator lines are dressed and identified by the matrix Green function G of Eq. (2.7).

While the formalism of Luttinger and Ward was originally derived for normal quantum liquids, it is well suited also to describe superfluid systems. Indeed the nondiagonal elements of the matrix Green function G represent the order parameter of the superfluid transition. The minimization of the grand potential $\Omega[G]$ as a functional of the Green function G thus incorporates the standard thermodynamic criterion that the order parameter be found by minimizing the thermodynamic potential. The stationarity condition

$$\delta\Omega[G]/\delta G=0 \tag{2.9}$$

uniquely determines the full matrix Green function G of the interacting system and hence the order parameter. It is important to note that the thermodynamic potential $\Omega[G]$ depends on the exact Green function G. The formalism of Luttinger and Ward thus leads via Eq. (2.9) to a self-consistent theory for the matrix Green function G. Since the Green functions contain information about the full dynamical behavior via the imaginary time dependence of the Matsubara formalism, the Luttinger-Ward approach not only provides results for the equilibrium thermodynamic quantities but also determines spectral functions and transport properties. In our present work, however, dynamical properties will not be discussed.

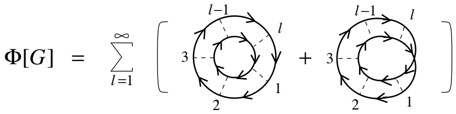


FIG. 1. The functional $\Phi[G]$ in self-consistent ladder approximation. The propagator lines are dressed lines identified by the matrix Green function G.

The functional $\Phi[G]$ is defined by an infinite perturbation series of irreducible Feynman diagrams, and an exact expression for $\Phi[G]$ is clearly beyond what can be done analytically. An approximation which properly describes the formation of pairs is a ladder approximation [36]. In Fig. 1, the related diagrams of $\Phi[G]$ are shown. The ladder approximation is self-consistent because the propagator lines are dressed lines which are identified by the matrix Green function G. In the weak-coupling BCS regime the ladder approximation becomes exact. For very strong attractive interactions, well above the pairing threshold, the fermion system is a Bose liquid of dilute atom pairs. In this limit the ladder approximation describes the formation of pairs (two-particle problem) exactly, however the interaction between the pairs (four-particle problem) only approximately [20,37]. In particular the resulting dimer-dimer scattering length is given by the Born approximation $a_{dd}^{(B)}=2a$.

B. De Dominicis–Martin formalism

An extension of the Luttinger-Ward formalism was given by De Dominicis and Martin [38]. They introduce up to four external fields, which couple to products of one-, two-, three-, and four-field operators and perform the Legendre transformations to the corresponding conjugate variables—the Green functions. For fermion systems only two external fields are relevant which couple to even products of fermion field operators. The related two conjugate variables of the

Legendre transformation are the one-particle Green function G and the two-particle Green function G_2. Within our approach below, the second Legendre transformation is performed explicitly. A more convenient conjugate variable is then the vertex function Γ which is related to G_2 by Eq. (2.15) below. Thus, De Dominicis and Martin obtain a thermodynamic potential which is a functional of both G and Γ. More precisely, it turns out that the relevant functional is the entropy $S=F^{(2)}$ where

$$\begin{aligned} F^{(2)}[G,\Gamma] = {} & \tfrac{1}{2}\,\mathrm{Tr}\{-\ln G + [(-i\hbar\,\omega_n)G - 1]\} \\ & + \tfrac{1}{2}\,\mathrm{Tr}\Big\{\ln\Big[1-\tfrac{1}{2}\bar{\Gamma}\Big] + \tfrac{1}{2}\bar{\Gamma} + \tfrac{1}{2}\Big[\tfrac{1}{2}\bar{\Gamma}\Big]^2 - (1/4\,!)[\bar{\Gamma}]^2\Big\} \\ & + \mathcal{K}^{(2)}[G,\Gamma] \end{aligned} \qquad (2.10)$$

[see (61) in the second paper of Ref. [38] and identify $G_1=G$, $C_2=-\Gamma$, and $\bar{C}_2=-\bar{\Gamma}$ therein]. $\bar{\Gamma}$ is defined in Eq. (2.14) below.

The formalism of De Dominicis and Martin is ideally adapted to describe the BCS-BEC crossover because it explicitly deals with the one-particle Green function G, which represent the properties of the single fermions, and the vertex function Γ, which describes the eventually purely bosonic properties of the fermion pairs (both condensed or noncondensed). In particular, a full implementation of their formalism is needed to correctly account for four-particle correlation, which is necessary to obtain the exact result $a_{dd}=0.60a$ for the dimer-dimer scattering length in the BEC limit.

As in standard thermodynamics, the entropy (2.10) is maximized under the constraint that all conserved quantities be kept constant. For the interacting fermion system defined by the Hamiltonian (2.2) the conserved quantities are the internal energy $U=\langle\hat{H}\rangle$ and the particle number $N=-\frac{1}{2}\,\mathrm{Tr}\{G\}$. Evaluating the thermal average of the Hamiltonian (2.2) we find that U can be expressed in terms of G and Γ [see Eqs. (2.15) and (2.24) below].

Consequently, the entropy $F^{(2)}[G,\Gamma]=S[G,\Gamma]$, the internal energy $U[G,\Gamma]$, and the particle number $N[G]$ are functionals depending on G and Γ. In order to find the maximum of the entropy under the constraint of given average values of the particle number and the internal energy, De Dominicis and Martin [38] consider the functional

$$W[G,\Gamma] = F^{(2)}[G,\Gamma] - \lambda_U U[G,\Gamma] - \lambda_N N[G], \qquad (2.11)$$

where λ_U and λ_N are two Lagrange parameters for the two constraints. Alternatively and equivalently, we consider the functional

$$\Omega[G,\Gamma] = U[G,\Gamma] - TS[G,\Gamma] - \mu N[G], \qquad (2.12)$$

which is the grand thermodynamic potential where the temperature T and the chemical potential μ are the Lagrange parameters. Both functionals (2.11) and (2.12) must be stationary under small variations of G and Γ. In this way, we obtain the stationarity criteria

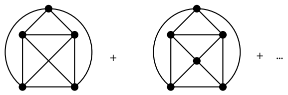
$\mathcal{K}^{(2)}[G,\Gamma] =$ 

FIG. 2. The functional $\mathcal{K}^{(2)}[G,\Gamma]$ is the sum of all two-line irreducible diagrams. The propagator lines and the vertices (solid circles) are dressed and identified with G and Γ, respectively.

$$\delta\Omega[G,\Gamma]/\delta G = 0 \quad \text{and} \quad \delta\Omega[G,\Gamma]/\delta\Gamma = 0, \qquad (2.13)$$

which uniquely determine the one-particle Green function G and the vertex function Γ.

In order to simplify the second trace in the entropy functional (2.10) it is convenient to define a modified vertex function $\bar{\Gamma}$ by

$$\bar{\Gamma}_{X_1X_2X_3X_4} = G^{1/2}_{X_1Y_1}G^{1/2}_{X_2Y_2}\Gamma_{Y_1Y_2Y_3Y_4}G^{1/2}_{Y_3X_3}G^{1/2}_{Y_4X_4}, \qquad (2.14)$$

where the four external propagator lines are amputated only halfway [see (46) in the second paper of [38]]. For a proper definition of the second trace and the related matrix products the four indices of the modified vertex function must be grouped into pairs according to $\bar{\Gamma}=\bar{\Gamma}_{(X_1X_2)(X_3X_4)}$. The last term in Eq. (2.10), the functional $\mathcal{K}^{(2)}[G,\Gamma]$ (depicted in Fig. 2), is defined by an infinite perturbation series of two-line irreducible Feynman diagrams, where the propagator lines and the vertices are dressed and identified by the one-particle Green function G and by the vertex function Γ, respectively.

In order to understand the physical meaning of the various contributions to the thermodynamic potential, we note that the Luttinger-Ward formalism and the De Dominicis–Martin formalism are related to each other by a Legendre transformation, in which the bare two-particle interaction as an external field is transformed into the two-particle Green function G_2. This Legendre transformation may be interpreted as a renormalization procedure. Since the two-particle Green function G_2 is expressed in terms of the vertex function Γ by

$$\begin{aligned} G_{2,X_1X_2X_3X_4} = {} & G_{X_1X_3}G_{X_2X_4} - G_{X_1X_4}G_{X_2X_3} - G_{X_1X_2}G_{X_3X_4} \\ & - G_{X_1Y_1}G_{X_2Y_2}\Gamma_{Y_1Y_2Y_3Y_4}G_{Y_3X_3}G_{Y_4X_4}, \end{aligned} \qquad (2.15)$$

the bare two-particle interaction is replaced by the vertex function Γ as the renormalized interaction, which is the many-particle generalization of the scattering amplitude g.

We may compare the functionals (2.8) and (2.10) directly with each other. The first trace in Eq. (2.10) is identified by the trace in Eq. (2.8), which describe the contribution of single particles to the grand canonical potential and entropy, respectively. The second trace and the functional $\mathcal{K}^{(2)}[G,\Gamma]$ in Eq. (2.10) which represent the interaction terms are related to the functional $\Phi[G]$ in Eq. (2.8). By close inspection [see (62) in Ref. [38]] we find that the second trace in Eq. (2.10) represents the inverted perturbation series of ladder diagrams. It includes both particle-particle and particle-hole ladders, which describe the scattering and formation of pairs, and it also includes bubble diagrams, which describe the screening of the interaction.

These three types of diagrams and mixtures of them arise because the vertices are symmetrized so that each of them can be expressed as a sum of three unsymmetrized vertices. As a result, the self-consistent ladder approximation of the functional $\Phi[G]$ shown in Fig. 1 can be reformulated within the formalism of De Dominicis and Martin in the following way: the second trace is approximated by keeping only the particle-particle ladders and the complicated functional $\mathcal{K}^{(2)}[G,\Gamma]$ is set equal to zero. This neglects the screening of the interaction due to particle-hole excitations (see Sec. III A below) and also the coupling between collective excitations and bound pairs.

In the following subsections we employ the formalism of De Dominicis and Martin to construct explicit expressions for $S[G,\Gamma]$, $U[G,\Gamma]$, and $N[G]$. From Eq. (2.12) we obtain the functional $\Omega[G,\Gamma]$. The stationarity criteria (2.13) imply two self-consistent equations for the Green function G and the vertex function Γ. Solving the second equation with respect to Γ and inserting the resulting vertex function into $\Omega[G,\Gamma]$ we recover the functional $\Omega[G]$ of the Luttinger-Ward formalism together with the stationarity condition (2.9). This fact explicitly demonstrates the equivalence of the Luttinger-Ward and De Dominics–Martin formalism for our approximation scheme [see Eqs. (2.41)–(2.43) below] once the appropriate stationarity conditions have been taken into account.

C. Thermodynamic potentials

The formalism of Luttinger and Ward [35] allows one to calculate directly the grand thermodynamic potential Ω. The functional $\Phi[G]$ has been evaluated explicitly in Ref. [31]. Inserting this result into Eq. (2.8) we obtain

$$\begin{aligned}\Omega[G] = -L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{&-\ln[G(\mathbf{k},\omega_n)] \\ &+ [G_0(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n) - 1]\} + L^d g_0|\mathcal{F}(\mathbf{0},0)|^2 \\ &+ \frac{1}{2}L^d \int \frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n} \mathrm{Tr}\{\ln[1 + g_0\chi(\mathbf{K},\Omega_n)]\}.\end{aligned} \tag{2.16}$$

In this formula the matrix Green function is defined by

$$G(\mathbf{k},\omega_n) = (G_{\alpha\alpha'}(\mathbf{k},\omega_n)) = \begin{pmatrix} \mathcal{G}(\mathbf{k},\omega_n) & \mathcal{F}(\mathbf{k},\omega_n) \\ \mathcal{F}(\mathbf{k},\omega_n)^* & -\mathcal{G}(\mathbf{k},\omega_n)^* \end{pmatrix}. \tag{2.17}$$

Knowledge of the matrix Green functions determines the matrix pair propagator via

$$\begin{aligned}\chi(\mathbf{K},\Omega_n) &= (\chi_{\alpha\alpha'}(\mathbf{K},\Omega_n)) \\ &= \left(\int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} G_{\alpha\alpha'}(\mathbf{K}-\mathbf{k},\Omega_n-\omega_n) \right.\\ &\qquad \left. \times G_{\alpha\alpha'}(\mathbf{k},\omega_n)\right).\end{aligned} \tag{2.18}$$

In order to distinguish between fermionic and bosonic functions the fermionic wave vectors and Matsubara frequencies are denoted by small letters, while the bosonic wave vectors and Matsubara frequencies are denoted by capital letters. In the second term of Eq. (2.16) the anomalous Green function is identified by $\mathcal{F}(\mathbf{0},0)=\mathcal{F}(\mathbf{r}=\mathbf{0},\tau=0)$. The formulas are derived for an arbitrary dimension of space d. The volume is assumed to be a cube with edge length L and periodic boundary conditions, where the limit $L\to\infty$ is taken.

The strength of the attractive interaction is included by the bare interaction parameter g_0. The kinetic energy of the atoms, $\varepsilon_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$, and the chemical potential μ are implicitly included via the free matrix Green function $G_0(\mathbf{k},\omega_n)$, which is related to the free normal Green function

$$\mathcal{G}_0(\mathbf{k},\omega_n) = 1/[-i\hbar\,\omega_n + \varepsilon_{\mathbf{k}} - \mu] \tag{2.19}$$

and the free anomalous Green function

$$\mathcal{F}_0(\mathbf{k},\omega_n) = 0 \tag{2.20}$$

by a formula which is analogous to Eq. (2.17). The temperature T is included explicitly by the factors $1/\beta$ and implicitly by the Matsubara frequencies ω_n and Ω_n.

As evident from Eq. (2.16), the formalism of Luttinger and Ward, though including the exact single-particle Green function, still contains the bare coupling constant g_0. In the De Dominicis–Martin formalism the bare coupling is renormalized and replaced by the exact vertex function Γ via a second Legendre transformation. The corresponding functional $S[G,\Gamma]=F^2[G,\Gamma]$ is just the dimensionless entropy as given in Eq. (2.10).

As discussed above we restrict the second trace in Eq. (2.10) to the particle-particle ladders and by the nature of our interaction potential (2.3) to s-wave scattering. Furthermore, we omit the two-line irreducible Feynman diagrams by setting $\mathcal{K}^{(2)}[G,\Gamma]=0$. This approximation covers the essential features of the crossover problem: namely, the formation of pairs and their condensation. Within our ladder approximation, the De Dominicis–Martin formalism thus leads to an expression for the entropy of the form

$$\begin{aligned}S[G,\Gamma] = \beta L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{&-\ln[G(\mathbf{k},\omega_n)] \\ &+ [-i\hbar\,\omega_n G(\mathbf{k},\omega_n) - 1]\} \\ &+ \frac{1}{2}\beta L^d \int \frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n} \mathrm{Tr}\{\ln[1 - \chi(\mathbf{K},\Omega_n)\Gamma(\mathbf{K},\Omega_n)] \\ &+ \chi(\mathbf{K},\Omega_n)\Gamma(\mathbf{K},\Omega_n)\}.\end{aligned} \tag{2.21}$$

The first term is clear. It is directly obtained from the first trace in Eq. (2.10). However, the second term resulting from the second trace in Eq. (2.10) needs further explanation. From Eq. (2.14) and the definition of the pair propagator (2.18) we infer

$$\bar{\Gamma}(\mathbf{K},\Omega_n) = \chi(\mathbf{K},\Omega_n)^{1/2}\Gamma(\mathbf{K},\Omega_n)\chi(\mathbf{K},\Omega_n)^{1/2} = \chi(\mathbf{K},\Omega_n)\Gamma(\mathbf{K},\Omega_n) = \Gamma(\mathbf{K},\Omega_n)\chi(\mathbf{K},\Omega_n). \tag{2.22}$$

The reduction to particle-particle ladders implies that the Nambu indices are pairwise identical. In this way, the four Nambu indices of the vertex function Γ reduce to two Nambu indices. As a result, the vertex function $\Gamma(\mathbf{K},\Omega_n) = (\Gamma_{\alpha\alpha'}(\mathbf{K},\Omega_n))$ is a 2×2 matrix in the Nambu space similar to the matrix Green function (2.17). For the formalism of Luttinger and Ward the reduction of the vertex is described in detail in Ref. [31] and also in Ref. [29]. Since the second trace of Eq. (2.10) is reduced to the particle-particle ladders and the structure of the vertex function is simplified considerably due to s-wave scattering, the prefactors of the terms in the second trace of Eq. (2.21) are changed. The factor of $\frac{1}{2}$ in front of $\bar{\Gamma}$ disappears. Furthermore, the quadratic terms in the second trace cancel.

Another important quantity to consider is the internal energy U. With the help of the δ potential (2.3) we find, for the expectation value of the Hamiltonian (2.2),

$$U = \int d^d r \sum_{\sigma} \frac{\hbar^2}{2m}\langle[\nabla\psi_\sigma^\dagger(\mathbf{r})][\nabla\psi_\sigma(\mathbf{r})]\rangle + \frac{1}{2}\int d^d r \sum_{\sigma\sigma'} g_0 \langle \psi_\sigma^\dagger(\mathbf{r})\psi_{\sigma'}^\dagger(\mathbf{r})\psi_{\sigma'}(\mathbf{r})\psi_\sigma(\mathbf{r})\rangle. \tag{2.23}$$

The second term contains an average of four fermion field operators which can be expressed in terms of the two-particle Green function G_2. Following the formalism of De Dominicis and Martin [38] and using Eq. (2.15) the two-particle Green function can be expressed by four terms. The first three terms represent the three possibilities to factorize the two-particle Green function into products of two one-particle Green functions according to the Wick theorem. These terms provide the Hartree energy, the Fock energy, and the Bogoliubov energy. The fourth term is the connected part of the two-particle Green function and provides the correlation energy. Taking all terms together we obtain the internal energy

$$U[G,\Gamma] = -2L^d \int \frac{d^d k}{(2\pi)^d}\varepsilon_{\mathbf{k}}\mathcal{G}(\mathbf{k},\tau=-0) + L^d g_0 |\mathcal{F}(\mathbf{0},0)|^2 + \frac{1}{2}L^d \int \frac{d^d K}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n} g_0 \mathrm{Tr}\{\chi(\mathbf{K},\Omega_n) - \chi(\mathbf{K},\Omega_n)\Gamma(\mathbf{K},\Omega_n)\chi(\mathbf{K},\Omega_n)\}. \tag{2.24}$$

Finally, the particle number N is defined by the average

$$N = \langle \hat{N}\rangle = \int d^d r \sum_{\sigma} \langle \psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r})\rangle, \tag{2.25}$$

which can be expressed in terms of the normal Green function in the standard form

$$N[G] = -2L^d \int \frac{d^d k}{(2\pi)^d}\mathcal{G}(\mathbf{k},\tau=-0). \tag{2.26}$$

The entropy (2.21), the internal energy (2.24), and the particle number (2.26) are the basic functionals of the formalism of De Dominicis and Martin. The entropy $S[G,\Gamma]$ is maximized under the constraints that the internal energy $U[G,\Gamma]$ and the particle number $N[G]$ be constant. In order to do this, the grand thermodynamic potential $\Omega[G,\Gamma]$ is defined by Eq. (2.12) where the temperature T and the chemical potential μ are Lagrange parameters. The self-consistent equations for the Green function G and the vertex function Γ are obtained from the stationarity conditions (2.13). Formally, the formalism of De Dominicis and Martin yields a different expression for the grand thermodynamic potential Ω than the formalism of Luttinger and Ward does by Eq. (2.16). However, it can be shown that the results are identical if and only if G and Γ satisfy the self-consistent equations (see the end of Sec. II E).

The functionals (2.21), (2.24), and (2.26) do not depend explicitly on the thermodynamic parameters T and μ. While the temperature appears explicitly via the factor $\beta=1/T$ and the Matsubara frequency $\omega_n \sim \Omega_n \sim T$, a proper rescaling of the functions $G\to\beta G$, $\chi\to\beta\chi$, and $\Gamma\to\Gamma$ implies that all factors β and T cancel in all three functionals. The temperature T and the chemical potential μ enter only as Lagrange parameters via the constraints. This fact is a general property of the formalism of De Dominicis and Martin. The fermion mass m, the kinetic energy $\varepsilon_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$, and the interaction parameter g_0, which determine the microscopic properties of the interacting fermion system, are present only in the internal energy functional (2.24).

An alternative expression for the entropy is obtained from the grand thermodynamic potential of Luttinger and Ward Eq. (2.16), according to the standard thermodynamic relation

$$S = -\partial\Omega/\partial T. \tag{2.27}$$

Taking the partial derivative we obtain an expression which formally differs from Eq. (2.21). However, provided that G and Γ satisfy the self-consistent equations, the results for the entropy will be identical. Therefore, both the Luttinger-Ward and the De Dominicis–Martin formalism exactly obey all the standard thermodynamic relations provided the Green functions obey the stationarity conditions (2.9) and (2.13). The equivalence of the different formal expressions in thermal equilibrium is very important for the consistency of our theory and the compatibility of the self-consistent ladder approximation for all thermodynamic quantities. Apart from the entropy, we can also determine the pressure $p=-\Omega/L^d$ as a functional of the Green function G using Eq. (2.16) or (2.12). The dimensionless thermodynamic quantities $\Omega/N\varepsilon_F$, $U/N\varepsilon_F$, and S/N will be calculated numerically in Sec. III and discussed in the following sections.

D. Self-consistent equations for the Green and vertex functions

The self-consistent equations for the Green functions follow directly from the stationarity condition (2.9). Inserting the general functional of the Luttinger-Ward formalism (2.8) into this condition we obtain the Dyson equation

$$G^{-1}_{\alpha\alpha'}(\mathbf{k},\omega_n) = G^{-1}_{0,\alpha\alpha'}(\mathbf{k},\omega_n) - \Sigma_{\alpha\alpha'}(\mathbf{k},\omega_n). \tag{2.28}$$

The self-energy Σ is identified by the functional derivative

$$\Sigma_{\alpha\alpha'}(\mathbf{k},\omega_n) = -\frac{1}{\beta L^d}\frac{\delta\Phi[G]}{\delta G_{\alpha'\alpha}(\mathbf{k},\omega_n)}. \tag{2.29}$$

The functional $\Phi[G]$ is defined by a perturbation series. The related Feynman diagrams are shown in Fig. 1 for the self-consistent ladder approximation. Inserting the grand thermodynamic potential (2.16) into the constraint (2.9), we obtain an explicit expression for the self-energy which is

$$\Sigma_{\alpha\alpha'}(\mathbf{r},\tau) = \Sigma_{1,\alpha\alpha'}\delta(\mathbf{r})\delta_F(\tau/\hbar) + G_{\alpha'\alpha}(-\mathbf{r},-\tau)\Gamma_{\alpha\alpha'}(\mathbf{r},\tau). \tag{2.30}$$

In the first term $\delta_F(\tau/\hbar)$ is the fermionic delta function which is antiperiodic. The order parameter of the superfluid transition

$$\Delta = g_0\mathcal{F}(\mathbf{0},0) \tag{2.31}$$

is represented by the nondiagonal elements of the matrix

$$\Sigma_1 = \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix}. \tag{2.32}$$

In the second term of Eq. (2.30), Γ is the matrix vertex function, which is related to the matrix pair propagator χ by

$$\Gamma^{-1}_{\alpha\alpha'}(\mathbf{K},\Omega_n) = g_0^{-1}\delta_{\alpha\alpha'} + \chi_{\alpha\alpha'}(\mathbf{K},\Omega_n). \tag{2.33}$$

Eventually, χ is represented in terms of the matrix Green function by Eq. (2.18). Equation (2.33) is just the Bethe-Salpeter equation in ladder approximation. It is responsible for the fact that the binding of fermion pairs is described appropriately. Taken together, we have now a set of self-consistent equations for the matrix Green function G and the matrix vertex function Γ which have to be solved numerically.

Alternatively we can derive the self-consistent equations by inserting the functional (2.12) of the formalism of De Dominicis and Martin into the related stationarity conditions (2.13). We obtain the Dyson equation (2.28) from the first condition and the Bethe-Salpeter equation (2.33) from the second condition. In this way we prove that both the Luttinger-Ward formalism and the De Dominicis–Martin formalism are equivalent within our approximation.

Unfortunately, in the present form, the matrix pair propagator χ defined in Eq. (2.18) is divergent. While the sum over the Matsubara frequencies is finite, the integral over the wave vector is ultraviolet divergent for dimensions $d \geq 2$. For this reason a renormalization is necessary. We define the regularized pair propagator by

$$M_{\alpha\alpha'}(\mathbf{K},\Omega_n) = \int \frac{d^dk}{(2\pi)^d}\left[\frac{1}{\beta}\sum_{\omega_n} G_{\alpha\alpha'}(\mathbf{K}-\mathbf{k},\Omega_n-\omega_n) \times G_{\alpha\alpha'}(\mathbf{k},\omega_n) - \frac{m}{\hbar^2\mathbf{k}^2}\delta_{\alpha\alpha'}\right]. \tag{2.34}$$

Inserting this formula into Eq. (2.33) we obtain the renormalized Bethe-Salpeter equation

$$\Gamma^{-1}_{\alpha\alpha'}(\mathbf{K},\Omega_n) = g^{-1}\delta_{\alpha\alpha'} + M_{\alpha\alpha'}(\mathbf{K},\Omega_n). \tag{2.35}$$

The bare interaction strength g_0 is renormalized according to Eq. (2.4) and replaced by the scattering amplitude g. For $d=3$ dimensions g is expressed in terms of the s-wave scattering length a by $g=4\pi\hbar^2 a/m$.

The zero range of the interaction between the fermions implies that

$$\mathcal{F}(\mathbf{0},0) = \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n}\mathcal{F}(\mathbf{k},\omega_n) \tag{2.36}$$

is infinite. For this reason the order-parameter formula (2.31) must be renormalized, too. Replacing the bare interaction strength g_0 by the scattering amplitude g according to Eq. (2.4), we obtain the renormalized formula

$$\Delta = g\int \frac{d^dk}{(2\pi)^d}\left[\mathcal{F}(\mathbf{k},\tau=0) + \Delta\frac{m}{\hbar^2\mathbf{k}^2}\right]. \tag{2.37}$$

Here, the integral over the wave vector is finite.

E. Reformulation in terms of mean-field Green functions

In the mean-field approximation the self-energy $\Sigma(\mathbf{k},\omega_n)$ is replaced by Σ_1 defined in Eq. (2.32). Since Σ_1 depends neither on wave vector nor on frequency, the approximation $\Sigma \approx \Sigma_1$ just describes the formation of a pair condensate within a BCS-type mean-field theory where the destruction of superfluidity is driven by the breakup of pairs. This is the correct description in the weak-coupling limit; however, for strong coupling the superfluid transition is driven by finite momentum pairs whose contribution is contained in the second term of the self-energy (2.30). Inserting the mean-field self-energy into the Dyson equation (2.28) we obtain

$$G_1(\mathbf{k},\omega_n)^{-1} = G_0(\mathbf{k},\omega_n)^{-1} - \Sigma_1 = \begin{pmatrix} -i\omega_n + (\varepsilon_{\mathbf{k}}-\mu) & -\Delta \\ -\Delta^* & -i\omega_n - (\varepsilon_{\mathbf{k}}-\mu) \end{pmatrix}, \tag{2.38}$$

where G_1 is the matrix Green function in mean-field approximation.

If we consider the self-consistent equations and the formulas for the thermodynamic potentials, we realize that the spectrum $\varepsilon_{\mathbf{k}}$ of the fermionic atoms and the chemical potential μ enter the formulas only implicitly via the free matrix Green function G_0. We can transform the formulas so that G_0 is replaced in favor of the mean-field matrix Green function G_1. As a result we obtain the Dyson equation

$$G^{-1}_{\alpha\alpha'}(\mathbf{k},\omega_n) = G^{-1}_{1,\alpha\alpha'}(\mathbf{k},\omega_n) - \tilde{\Sigma}_{\alpha\alpha'}(\mathbf{k},\omega_n), \tag{2.39}$$

where

$$\tilde{\Sigma}_{\alpha\alpha'}(\mathbf{r},\tau) = G_{\alpha'\alpha}(-\mathbf{r},-\tau)\Gamma_{\alpha\alpha'}(\mathbf{r},\tau) \tag{2.40}$$

is the second term of the self-energy (2.30). The other self-consistent equations remain unchanged. The grand thermodynamic potential (2.16) is transformed into

$$\Omega = -L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{\beta} \sum_{\omega_n} \mathrm{Tr}\{-\ln[G(\mathbf{k},\omega_n)] + [G_1(\mathbf{k},\omega_n)^{-1} G(\mathbf{k},\omega_n) - 1]\} - L^d \frac{|\Delta|^2}{g_0} + \frac{1}{2} L^d \int \frac{d^dK}{(2\pi)^d} \frac{1}{\beta} \sum_{\Omega_n} \mathrm{Tr}\{-\ln[\Gamma(\mathbf{K},\Omega_n)/g_0]\}. \tag{2.41}$$

For a combination of the internal energy (2.24) and the particle number (2.26) we obtain the formula

$$U - \mu N = -L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{\beta} \sum_{\omega_n} \mathrm{Tr}\{[G_1(\mathbf{k},\omega_n)^{-1} + i\hbar\,\omega_n] \times G(\mathbf{k},\omega_n)\} - L^d \frac{|\Delta|^2}{g_0} - \frac{1}{2} L^d \int \frac{d^dK}{(2\pi)^d} \times \frac{1}{\beta} \sum_{\Omega_n} \mathrm{Tr}\{[\Gamma(\mathbf{K},\Omega_n)/g_0 - 1]\}. \tag{2.42}$$

The entropy (2.21) depends neither on G_0 nor on G_1. We transform the formula into

$$S = \beta L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{\beta} \sum_{\omega_n} \mathrm{Tr}\{-\ln[G(\mathbf{k},\omega_n)] + [-i\hbar\,\omega_n G(\mathbf{k},\omega_n) - 1]\} - \frac{1}{2} \beta L^d \int \frac{d^dK}{(2\pi)^d} \times \frac{1}{\beta} \sum_{\Omega_n} \mathrm{Tr}\{-\ln[\Gamma(\mathbf{K},\Omega_n)/g_0] + [\Gamma(\mathbf{K},\Omega_n)/g_0 - 1]\}. \tag{2.43}$$

In the above three formulas we have simplified the terms involving the vertex function Γ by using the Bethe-Salpeter equation (2.33). The grand thermodynamic potential (2.41) was derived using the formalism of Luttinger and Ward [35] while the other two quantities (2.42) and (2.43) were derived using the formalism of De Dominicis and Martin [38]. It is now not hard to see that the above expressions obey the thermodynamic relation

$$\Omega = U - TS - \mu N, \tag{2.44}$$

which explicitly shows that both formalisms are indeed equivalent, yielding the same results for all thermodynamic potentials in the self-consistent ladder approximation provided G and Γ satisfy the appropriate stationarity equations.

F. Mean-field approximation

If we insert G_1 for the matrix Green function G and neglect all terms containing the vertex function Γ, we obtain the thermodynamic potentials in mean-field approximation. In particular the mean-field grand thermodynamic potential is given by

$$\Omega_1 = -L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{\beta} \sum_{\omega_n} \mathrm{Tr}\{-\ln[G_1(\mathbf{k},\omega_n)]\} - L^d \frac{|\Delta|^2}{g_0}, \tag{2.45}$$

while the mean-field formula for the combination of the internal energy and the particle number is

$$U_1 - \mu N_1 = -L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{\beta} \sum_{\omega_n} \mathrm{Tr}\{[G_1(\mathbf{k},\omega_n)^{-1} + i\hbar\,\omega_n] \times G_1(\mathbf{k},\omega_n)\} - L^d \frac{|\Delta|^2}{g_0} \tag{2.46}$$

and the mean-field entropy is

$$S_1 = \beta L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{\beta} \sum_{\omega_n} \mathrm{Tr}\{-\ln[G_1(\mathbf{k},\omega_n)] + [-i\hbar\,\omega_n G_1(\mathbf{k},\omega_n) - 1]\}. \tag{2.47}$$

In order to obtain finite results, we must define the sums over the Matsubara frequencies as described in Appendix A. The sums can be evaluated explicitly. This yields

$$\Omega_1 = E_0 - \frac{1}{\beta} 2L^d \int \frac{d^dk}{(2\pi)^d} \ln[1 + \exp(-\beta(E_{\mathbf{k}} - \mu)], \tag{2.48}$$

$$U_1 - \mu N_1 = E_0 + 2L^d \int \frac{d^dk}{(2\pi)^d} (E_{\mathbf{k}} - \mu) n_{\mathbf{k}}, \tag{2.49}$$

$$S_1 = -2L^d \int \frac{d^dk}{(2\pi)^d} \{(1 - n_{\mathbf{k}})\ln(1 - n_{\mathbf{k}}) + n_{\mathbf{k}} \ln n_{\mathbf{k}}\}, \tag{2.50}$$

which are the well-known results of a BCS variational ansatz for arbitrary coupling where

$$E_0 = -2L^d \int \frac{d^dk}{(2\pi)^d} \frac{1}{2} [(E_{\mathbf{k}} - \mu) - (\varepsilon_{\mathbf{k}} - \mu)] - L^d \frac{|\Delta|^2}{g_0} \tag{2.51}$$

is an energy constant which after renormalization $g_0 \to g$ [see Eq. (2.57)] reduces to the BCS condensation energy. Here $E_{\mathbf{k}}$ is the spectrum of the quasiparticles, defined by

$$(E_{\mathbf{k}} - \mu) = [(\varepsilon_{\mathbf{k}} - \mu)^2 + |\Delta|^2]^{1/2}, \tag{2.52}$$

and $n_{\mathbf{k}}$ denotes the Fermi distribution function of the quasiparticles:

$$n_{\mathbf{k}} = 1/\{\exp[\beta(E_{\mathbf{k}} - \mu)] + 1\}. \tag{2.53}$$

We find that the regularization of the Matsubara-frequency sums described in Appendix A affects only the energy constant E_0. The regularization has been chosen such that for zero interaction the results for the ideal Fermi gas are obtained which implies $E_0 = 0$. The other terms in Eqs. (2.48)–(2.50) are not affected by the regularization.

G. Beyond the mean-field approximation

In the mean-field approximation, the formation and condensation of fermion pairs occur at the same temperature. This is the well-known BCS scenario, which is perfectly captured by the exact solution of the reduced BCS Hamiltonian. Formally, this solution can easily be extended to arbitrary coupling strengths [23]. At zero temperature, it provides a smooth crossover from the BCS ground state of highly overlapping pairs to a perfect Bose-Einstein condensate at infinite coupling, similar to the variational ansatz of Eagles [21] and Leggett [22]. At finite temperature, however, superfluidity in this model is destroyed by fermionic excitations: namely, the breakup of pairs. The critical temperature is therefore of the same order as the pairing gap at zero temperature, consistent with the well-known BCS relation $2\Delta_0/T_c=3.52$ in weak coupling. Clearly, such a picture is appropriate for weak coupling, where the transition to superfluidity is driven by the gain in *potential* energy associated with pair formation. By contrast, for sufficiently strong interactions, the superfluid to normal transition is instead driven by a gain in *kinetic* energy, associated with the condensation of preformed pairs rather than their thermal breakup. The critical temperature is then of the order of the degeneracy temperature of the gas and thus is completely unrelated to the pair binding energy. For a proper description of the BCS-BEC crossover at finite temperature and arbitrary coupling, we therefore need to go beyond the mean-field approximation, including excitations, which drive the superfluid order parameter to zero without destroying the bound pairs altogether. On a formal level, this is accomplished by the nontrivial wave-vector- and frequency-dependent term $G\Gamma$ in the exact fermion self-energy, as given in Eq. (2.30).

For the numerical calculation we decompose the thermodynamic potentials into a mean-field part and a correction term according to $\Omega=\Omega_1+\Delta\Omega$, $S=S_1+\Delta S$, etc. The mean-field contributions have been derived in the previous subsection. While in these contributions the Matsubara-frequency sums have been performed explicitly, the integrals over the wave vector remain and must be evaluated numerically. By subtracting the mean-field formulas (2.45)–(2.47) from the general formulas (2.41)–(2.43) we obtain the correction for the grand thermodynamic potential,

$$\begin{aligned}\Delta\Omega = &-L^d\int\frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n}\mathrm{Tr}\{-\ln[G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n)]\\ &+[G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n)-1]\}+\frac{1}{2}L^d\int\frac{d^dK}{(2\pi)^d}\\ &\times\frac{1}{\beta}\sum_{\Omega_n}\mathrm{Tr}\{-\ln[\Gamma(\mathbf{K},\Omega_n)/g_0]\},\end{aligned}\qquad(2.54)$$

the correction for the combination of the internal energy and the particle number,

$$\begin{aligned}\Delta U-\mu\Delta N = &-L^d\int\frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n}\mathrm{Tr}\{[G_1(\mathbf{k},\omega_n)^{-1}+i\hbar\,\omega_n]\\ &\times[G(\mathbf{k},\omega_n)-G_1(\mathbf{k},\omega_n)]\}\\ &-\frac{1}{2}L^d\int\frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n}\mathrm{Tr}\{[\Gamma(\mathbf{K},\Omega_n)/g_0-1]\},\end{aligned}\qquad(2.55)$$

and the correction for the entropy,

$$\begin{aligned}\Delta S = &\,\beta L^d\int\frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n}\mathrm{Tr}\{-\ln[G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n)]\\ &+(-i\hbar\,\omega_n)[G(\mathbf{k},\omega_n)-G_1(\mathbf{k},\omega_n)]\}\\ &-\frac{1}{2}\beta L^d\int\frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n}\mathrm{Tr}\{-\ln[\Gamma(\mathbf{K},\Omega_n)/g_0]\\ &+[\Gamma(\mathbf{K},\Omega_n)/g_0-1]\}.\end{aligned}\qquad(2.56)$$

In formulas (2.54)–(2.56) the sums over the fermionic Matsubara frequencies ω_n converge so that the regularization of Appendix A is not needed. However, the sums over the bosonic Matsubara frequencies Ω_n are not well defined and must be regularized. Thus, for a numerical evaluation the formulas (2.54)–(2.56) must be transformed further, which will be done in the next subsection.

H. Renormalization of the thermodynamic potentials

Since the interaction has zero range, the interaction strength g_0 must be renormalized and replaced by the scattering amplitude g according to Eq. (2.4). In a first step we renormalize the mean-field formulas of the thermodynamic potentials. In Eqs. (2.48)–(2.50) the interaction strength g_0 does not occur explicitly. The integrals are thus finite, and no renormalization is needed for these formulas. However, the condensation energy (2.51) contains two infinite terms—a divergent integral and the last term with the infinite factor $1/g_0$—which compensate each other. By renormalizing the interaction strength we obtain

$$E_0=-2L^d\int\frac{d^dk}{(2\pi)^d}\frac{1}{2}\left[(E_{\mathbf{k}}-\mu)-(\varepsilon_{\mathbf{k}}-\mu)-\frac{|\Delta|^2}{2\varepsilon_{\mathbf{k}}}\right]-L^d\frac{|\Delta|^2}{g},\qquad(2.57)$$

where both the integral and the last term are now separately finite. Note that the wave vector integrals in Eqs. (2.48)–(2.50) and in Eq. (2.57) are finite in any spatial dimension d with $2<d<4$.

In a second step we renormalize the correction formulas. In the correction of the grand thermodynamic potential (2.54) we decompose $\ln[\Gamma(\mathbf{K},\Omega_n)/g_0]=\ln[\Gamma(\mathbf{K},\Omega_n)/g]+\ln[g/g_0]$. The separated term $\ln[g/g_0]$ can be neglected because it does not depend on the Matsubara frequencies Ω_n. Following the arguments of Appendix A the Matsubara-frequency sum of this term is zero. Thus, for the correction of the grand thermodynamic potential we obtain the renormalized formula

$$\Delta\Omega = -L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{-\ln[G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n)] + [G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n) - 1]\} + \frac{1}{2}L^d \int \frac{d^dK}{(2\pi)^d}\frac{1}{\beta} \times \sum_{\Omega_n} \mathrm{Tr}\{-\ln[\Gamma(\mathbf{K},\Omega_n)/g]\}. \tag{2.58}$$

Both terms of this formula are now finite. However, Eq. (A4) is needed to evaluate the second term.

In correction (2.55) the second term must be renormalized. This can be achieved by the following sequence of equations:

$$\begin{aligned}
&-L^d \int \frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n} \mathrm{Tr}\{[\Gamma(\mathbf{K},\Omega_n)/g_0 - 1]\} \\
&= L^d \int \frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n} \mathrm{Tr}\{\Gamma(\mathbf{K},\Omega_n)\chi(\mathbf{K},\Omega_n)\} \\
&= L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{\tilde{\Sigma}(\mathbf{k},\omega_n)G(\mathbf{k},\omega_n)\} \\
&= L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{G_1(\mathbf{k},\omega_n)^{-1}[G(\mathbf{k},\omega_n) - G_1(\mathbf{k},\omega_n)]\}.
\end{aligned} \tag{2.59}$$

First, by using the Bethe-Salpeter equation (2.33) we write the integrand as a product of the matrix vertex function Γ and the matrix pair propagator χ. Second, we express χ in terms of the matrix Green function G by Eq. (2.18), interchange the orders of the integrals and sums, and combine Γ with one of the G into the self-energy $\tilde{\Sigma}$ by Eq. (2.40). Finally, we replace $\tilde{\Sigma}$ in favor of G and G_1 by using the Dyson equation (2.39). The bosonic integral and sum are transformed into a fermionic integral and sum. Hence, the second term of Eq. (2.55) can be combined with the first term. As a result we finally obtain

$$\Delta U - \mu\Delta N = -\frac{1}{2}L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{[G_1(\mathbf{k},\omega_n)^{-1} + 2i\hbar\,\omega_n] \times [G(\mathbf{k},\omega_n) - G_1(\mathbf{k},\omega_n)]\}. \tag{2.60}$$

By considering Eq. (2.38) we explicitly prove

$$G_1(\mathbf{k},\omega_n)^{-1} + 2i\hbar\,\omega_n = G_1(\mathbf{k},-\omega_n)^{-1}. \tag{2.61}$$

Consequently, for the correction of the combination of the internal energy and the particle number we obtain the compact formula

$$\Delta U - \mu\Delta N = -\frac{1}{2}L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{G_1(\mathbf{k},-\omega_n)^{-1} \times [G(\mathbf{k},\omega_n) - G_1(\mathbf{k},\omega_n)]\}, \tag{2.62}$$

which is essential for a stable numerical evaluation of the correction term. The Matsubara-frequency sum is evaluated by using Eq. (A3). The wave vector integral is finite.

The correction of the entropy (2.56) is renormalized in an analogous way. Alternatively, we use the thermodynamic relation (2.44). As a result we obtain

$$\begin{aligned}
\Delta S = {}& \beta L^d \int \frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{-\ln[G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n)] + [G_1(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n) - 1]\} - \frac{1}{2}\beta L^d \int \frac{d^dk}{(2\pi)^d} \\
&\times \frac{1}{\beta}\sum_{\omega_n} \mathrm{Tr}\{G_1(\mathbf{k},-\omega_n)^{-1}[G(\mathbf{k},\omega_n) - G_1(\mathbf{k},\omega_n)]\} \\
&- \frac{1}{2}\beta L^d \int \frac{d^dK}{(2\pi)^d}\frac{1}{\beta}\sum_{\Omega_n} \mathrm{Tr}\{-\ln[\Gamma(\mathbf{K},\Omega_n)/g]\}.
\end{aligned} \tag{2.63}$$

The final results are the mean-field formulas (2.48)–(2.50) together with Eq. (2.57) and the correction formulas (2.58), (2.62), and (2.63). In these formulas each term by itself is finite. Eventually, the thermodynamic potentials are obtained by adding the terms together according to $\Omega = \Omega_1 + \Delta\Omega$, $S = S_1 + \Delta S$, etc.

I. Symmetry breaking and Thouless criterion

The interacting fermion system is invariant under the symmetry transformation

$$\psi_\sigma(\mathbf{r}) \to e^{i\lambda}\psi_\sigma(\mathbf{r}), \quad \psi_\sigma^\dagger(\mathbf{r}) \to e^{-i\lambda}\psi_\sigma^\dagger(\mathbf{r}), \tag{2.64}$$

which is related to a global change of phase of the fermion fields by λ. The superfluid phase breaks this symmetry since the order parameter Δ is transformed as $\Delta \to e^{2i\lambda}\Delta$. Clearly, however, the thermodynamic potentials must remain invariant under a global change of the phase in both the normal and superfluid states. In the superfluid, the free energy increase associated with a *slowly varying* phase $\lambda(\mathbf{r})$ vanishes like $(\nabla\lambda)^2$. By Goldstone' s theorem, this implies the existence of modes whose energy vanishes in the long-wavelength limit. For a neutral superfluid, this is the well-known Bogoliubov-Anderson mode. It has a sound like dispersion $\omega(k) = ck$ and is physically related to fluctuations of the phase of the order parameter.

In technical terms, the existence of zero-energy collective modes can be derived from Ward identities related to the symmetry transformation. By considering the grand thermodynamic potential $\Omega[G]$, in Ref. [31] the Ward identity

$$\sum_{YY'} \Gamma^{-1}_{XX',Y'Y}\delta_\lambda \Sigma_{YY'} = 0 \tag{2.65}$$

has been derived [see (2.57) in Ref. [31]]. Here $\delta_\lambda \Sigma_{XX'}$ is the variation of the self-energy under the transformation (2.64) with an infinitesimal phase change $\delta\lambda$. This quantity may be interpreted as the generalized order parameter of the system. On the other hand, $\Gamma^{-1}_{XX',YY'}$ is the inverse vertex function. For a shorthand notation the indices X, X' and Y, Y' are used, which represent a combination $X = (\mathbf{r}, \tau, \sigma, \alpha)$ of the space variable $\mathbf{r}$, the imaginary time τ, the spin index σ, and the

Nambu index α. According to Eq. (2.65) the inverse vertex function Γ^{-1} may be interpreted as a linear operator which acts on the order parameter $\delta_\lambda\Sigma$. In the superfluid state the order parameter is nonzero so that the inverse vertex function must have a zero eigenvalue, which is related to a zero-energy collective mode. For superfluid fermion systems this fact is known as the Thouless criterion [39].

The Ward identity (2.65) has been derived for the exact theory. However, our present crossover theory is an approximation, based on a certain truncation of the exact functional which enters either into the Luttinger-Ward or the De Dominicis–Martin formalism. In general, such a truncated functional will not obey the Ward identity. Indeed, we find that our inverse vertex function $\Gamma^{-1}_{\alpha\alpha'}(\mathbf{K},\Omega_n)$ obeys instead the equation

$$\sum_{\alpha'} \Gamma^{-1}_{\alpha\alpha'}(\mathbf{K}=\mathbf{0},\Omega_n=0)\Delta_{\alpha'} = \mathcal{O}(|\Delta|^3), \tag{2.66}$$

where $(\Delta_\alpha)=(\Delta,\Delta^*)$ [see (3.56) in Ref. [31]]. Taking the longitudinal part, this equation correctly describes the smooth evolution from a Ginzburg-Landau-type description of weak-coupling BCS superfluids to a Gross-Pitaevskii-like theory of a dilute, repulsive Bose gas [31]. The transverse part, however, also gives a finite value on the right-hand side of Eq. (2.66) in the limit $\mathbf{K}=\mathbf{0}$ and $\Omega_n=0$, thus violating the Ward identity by terms of order $|\Delta|^3$. As a result, the Thouless criterion is violated and there is no proper Bogoliubov-Anderson mode in our approach without a further modification (see below).

Unfortunately, the violation of the Goldstone theorem for continuous symmetries is a general property of conserving approximations based on the Luttinger-Ward formalism. This problem has been known for a long time for superfluid Bose systems [40] and is sometimes referred to as the "conserving-gapless dichotomy" [41,42] in the literature. For the exact theory, a Ward identity holds for the inverse matrix boson Green function G_B, which reads

$$\sum_{\alpha'} G^{-1}_{B,\alpha\alpha'}(\mathbf{K}=\mathbf{0},\Omega_n=0)\Psi_{B,\alpha'} = 0. \tag{2.67}$$

In the superfluid state the inverse matrix boson Green function has a vanishing eigenvalue. For superfluid boson systems this is known as the Hugenholtz-Pines theorem [43]. Conserving approximations, however, violate the Hugenholtz-Pines theorem. For example, this is true already for the lowest approximation, the well-known Hartree-Fock-Bogoliubov theory.

In our fermion system for strong attractive interactions $v=1/k_Fa \gg 1$, the fermions are bound into pairs. These pairs form a Bose system with an effective repulsive interaction which, for a dilute system, is described by the exact scattering length $a_{dd}\approx 0.60a$ of the four-particle problem associated with dimer-dimer scattering. In the strong-coupling limit, therefore, our crossover theory for interacting fermions must converge to an effective theory of repulsively interacting bosons, where both theories are based on the Luttinger-Ward formalism. From the analytical arguments in Refs. [29,31] and also from our numerical calculations, we find that the crossover theory converges to the Hartree-Fock-Bogoliubov theory quickly for interactions $v=1/k_Fa>2$. The boson order parameter Ψ_B and the matrix boson Green function $G_B(\mathbf{K},\Omega_n)$ can be identified with the order parameter Δ and the vertex function $\Gamma(\mathbf{K},\Omega_n)$ according to [29,31]

$$\Psi_B = \pm i[8\pi\varepsilon_b^2 a^3]^{-1/2}\Delta, \tag{2.68}$$

$$G_B(\mathbf{K},\Omega_n) = -[8\pi\varepsilon_b^2 a^3]^{-1}\Gamma(\mathbf{K},\Omega_n). \tag{2.69}$$

The validity of these relations requires both strong coupling, but also low frequencies and momenta. Indeed, it is only at low energies where the composite particles behave like bosons. At higher frequencies or momenta, the composite nature of the pairs becomes visible. This becomes evident, for instance, in the different behavior $G_B\sim\Omega_n^{-1}$ of a Bose Green function at large frequencies compared to that of the vertex function, which behaves like $\Gamma\sim\Omega_n^{-1/2}$ as a result of the two-particle continuum associated with broken fermion pairs. Clearly, at large coupling constants $v\gg 1$, this continuum moves up to very large frequencies of the order of the binding energy $\epsilon_b\sim v^2$.

We conclude that the violation of the Thouless criterion in our crossover theory is related to the violation of the Hugenholtz-Pines theorem in the Hartree-Fock-Bogoliubov theory for bosons to which our Luttinger-Ward formulation of the fermionic many-body problem converges at large coupling. In the following section, it will be shown that this problem may be solved by an appropriate modification of the coupling constant. In this manner, a self-consistent formulation of the many-body problem is possible which obeys Goldstone's theorem and thus provides a correct description of both fermionic and collective, bosonic excitations along the BCS-BEC crossover.

J. Modified coupling and gapless Bogoliubov-Anderson mode

In the following, our aim is to modify the theory in a way which is consistent with the Thouless criterion, giving rise to a gapless Goldstone mode in the whole regime of coupling strengths. If we require the Thouless criterion

$$\sum_{\alpha'} \Gamma^{-1}_{\alpha\alpha'}(\mathbf{K}=\mathbf{0},\Omega_n=0)\Delta_{\alpha'} = 0, \tag{2.70}$$

a further equation will be added to the self-consistent equations for the Green and vertex functions in Sec. II D. However, then another equation must be discarded or a further parameter must be introduced. We find that the Bethe-Salpeter equation (2.35) and the order-parameter equation (2.37) cannot be satisfied together if Eq. (2.70) is required. For this reason we modify the theory by introducing a modified scattering amplitude g_{mod}, which is determined by the modified order-parameter equation

$$\Delta = g_{\text{mod}} \int \frac{d^dk}{(2\pi)^d}\left[\mathcal{F}(\mathbf{k},\tau=0) + \Delta\frac{m}{\hbar^2\mathbf{k}^2}\right]. \tag{2.71}$$

We have solved the self-consistent equations together with the Thouless criterion (2.70) and the modified order-parameter equation (2.71). The numerical effort is much less for the modified theory than for the original theory. Since the scattering amplitude g is related to the scattering length a, we obtain a modified dimensionless interaction strength $v_{\mathrm{mod}}=1/k_F a_{\mathrm{mod}}$. We find a difference $\delta v_{\mathrm{mod}}=v_{\mathrm{mod}}-v$ in the range between 0.0 and −0.1.

In order to obtain a consistent theory, we must check that the modification is compatible with the Luttinger-Ward formalism. We must find a modified grand thermodynamic potential $\Omega_{\mathrm{mod}}[G]$, so that the condition for stationarity (2.9) yields the self-consistent equations with the modified order-parameter equation (2.71). For this purpose we consider the second term of Eq. (2.16) which reads

$$\Omega_0[G]=L^d g_0|\mathcal{F}(\mathbf{0},0)|^2=L^d|\Delta|^2/g_0. \tag{2.72}$$

We replace this term by the modified term

$$\Omega_{0,\mathrm{mod}}[G]=L^d|\Delta|^2/\tilde{g}_{0,\mathrm{mod}}(|\Delta|), \tag{2.73}$$

where

$$\Delta=g_{0,\mathrm{mod}}(|\Delta|)\mathcal{F}(\mathbf{0},0) \tag{2.74}$$

is the modified order-parameter equation. The modified interaction strengths $\tilde{g}_{0,\mathrm{mod}}=\tilde{g}_{0,\mathrm{mod}}(|\Delta|)$ and $g_{0,\mathrm{mod}}=g_{0,\mathrm{mod}}(|\Delta|)$ depend on the order parameter $|\Delta|$, are not equal, and differ from the bare interaction strength g_0. In order to apply the stationarity condition (2.9) we must consider the variation of Eq. (2.73) with respect to G. Since the modified parameter $\tilde{g}_{0,\mathrm{mod}}(|\Delta|)$ depends implicitly on G via Eq. (2.74), the chain rule of differential calculus must be applied. Eventually, the variation of Eq. (2.73) must have the form

$$\begin{aligned}\delta\Omega_{0,\mathrm{mod}}[G]&=L^d\int\frac{d^dk}{(2\pi)^d}\frac{1}{\beta}\sum_{\omega_n}\mathrm{Tr}\{\Sigma_1\delta G(\mathbf{k},\omega_n)\}\\&=L^d[\Delta\,\delta\mathcal{F}(\mathbf{0},0)^*+\Delta^*\delta\mathcal{F}(\mathbf{0},0)].\end{aligned} \tag{2.75}$$

By comparing the resulting terms with Eq. (2.75), we obtain the differential equation

$$\frac{\partial}{\partial|\Delta|}\frac{|\Delta|^2}{\tilde{g}_{0,\mathrm{mod}}(|\Delta|)}=2|\Delta|\frac{\partial}{\partial|\Delta|}\frac{|\Delta|}{g_{0,\mathrm{mod}}(|\Delta|)}. \tag{2.76}$$

On the other hand, Eq. (2.66) implies that the Thouless criterion holds without modification if $|\Delta|=0$. Thus, we find

$$\tilde{g}_{0,\mathrm{mod}}=g_{0,\mathrm{mod}}=g_0 \quad \text{for} \quad |\Delta|=0, \tag{2.77}$$

which is an initial condition for Eq. (2.76). Equation (2.76) can be integrated together with Eq. (2.77). We obtain

$$\frac{1}{\tilde{g}_{0,\mathrm{mod}}(|\Delta|)}=\frac{2}{g_{0,\mathrm{mod}}(|\Delta|)}-\frac{1}{|\Delta|^2}\int_0^{|\Delta|}\frac{2|\Delta'|d|\Delta'|}{g_{0,\mathrm{mod}}(|\Delta'|)}. \tag{2.78}$$

The thermodynamic state of the interacting fermion system in the superfluid state is therefore determined by three parameters. We may choose the order parameter $|\Delta|$, the chemical potential μ, and the interaction strength g_0 for these parameters. Hence, the modified interaction strengths $g_{0,\mathrm{mod}}=g_{0,\mathrm{mod}}(|\Delta|,\mu,g_0)$ and $\tilde{g}_{0,\mathrm{mod}}=\tilde{g}_{0,\mathrm{mod}}(|\Delta|,\mu,g_0)$ are functions of these parameters. While $g_{0,\mathrm{mod}}(|\Delta|,\mu,g_0)$ is uniquely determined by Eq. (2.74) and the other self-consistent equations, $\tilde{g}_{0,\mathrm{mod}}(|\Delta|,\mu,g_0)$ depends on the path in the parameter space when the integral (2.78) is calculated. Since g_0 and μ are external parameters of the theory, for a correct formulation of the modification these parameters must be kept constant.

The modification is compatible also with the De Dominicis–Martin formalism. In this case the internal energy $U[G,\Gamma]$ includes the term (2.72) which must be modified according to Eq. (2.73). The modification of the coupling constant g_0 described by Eqs. (2.76)–(2.78) is derived in an analogous way.

Equations (2.72)–(2.78) describe the modification of the crossover theory in terms of the bare interaction parameters g_0, $g_{0,\mathrm{mod}}$, and $\tilde{g}_{0,\mathrm{mod}}$. A renormalized version of the modification is obtained if we replace the bare parameters by the renormalized scattering amplitudes g, g_{mod}, and $\tilde{g}_{\mathrm{mod}}$ according to Eq. (2.4). Equations (2.76)–(2.78) are valid also for the renormalized scattering amplitudes without changes. From Eq. (2.78) we obtain

$$\frac{1}{\tilde{g}_{\mathrm{mod}}(|\Delta|)}=\frac{2}{g_{\mathrm{mod}}(|\Delta|)}-\frac{1}{|\Delta|^2}\int_0^{|\Delta|}\frac{2|\Delta'|d|\Delta'|}{g_{\mathrm{mod}}(|\Delta'|)}. \tag{2.79}$$

The renormalized modified order-parameter equation is defined by Eq. (2.71). In order to obtain the modified formulas of the renormalized thermodynamic potentials in Sec. II H only a single change is needed. We must replace the energy constant (2.57) by

$$\begin{aligned}E_{0,\mathrm{mod}}=&-2L^d\int\frac{d^dk}{(2\pi)^d}\frac{1}{2}\left[(E_{\mathbf{k}}-\mu)-(\varepsilon_{\mathbf{k}}-\mu)-\frac{|\Delta|}{2\varepsilon_{\mathbf{k}}}\right]\\&+L^d|\Delta|^2(\tilde{g}_{\mathrm{mod}}^{-1}-2g^{-1}).\end{aligned} \tag{2.80}$$

The other formulas (2.58), (2.62), and (2.63) remain unchanged. Since the renormalized scattering amplitude g is related to the dimensionless interaction parameter $v=1/k_F a$, we can transform Eq. (2.79) into a dimensionless form. For $\delta v_{\mathrm{mod}}=v_{\mathrm{mod}}-v$ and $\delta\tilde{v}_{\mathrm{mod}}=\tilde{v}_{\mathrm{mod}}-v$ we obtain

$$\begin{aligned}\delta\tilde{v}_{\mathrm{mod}}(|\Delta|/\varepsilon_F,v)=&\,2\delta v_{\mathrm{mod}}(|\Delta|/\varepsilon_F,v)-(|\Delta|/\varepsilon_F)^{-2}\\&\times\int_0^{|\Delta|/\varepsilon_F}\delta v_{\mathrm{mod}}(X,v)2XdX.\end{aligned} \tag{2.81}$$

While δv_{mod} is obtained directly from Eq. (2.71) by solving the self-consistent equations, $\delta\tilde{v}_{\mathrm{mod}}$ is obtained by evaluating the integral in Eq. (2.81) numerically. As a result we obtain modifications which are restricted to the interval

$$-0.1\lesssim\delta v_{\mathrm{mod}}<\delta\tilde{v}_{\mathrm{mod}}<0 \quad \text{for} \quad |\Delta|>0. \tag{2.82}$$

In Fig. 3 the modifications δv_{mod} and $\delta\tilde{v}_{\mathrm{mod}}$ are shown as a red solid curve and blue dashed curve, respectively, for $T=0$ and $|\Delta|=|\Delta_0|$. Clearly, the modifications are largest in the crossover region close to the unitarity point. At finite temperature for increasing T the order parameter $|\Delta|$ and the modifications δv_{mod} and $\delta\tilde{v}_{\mathrm{mod}}$ decrease together. Eventually, for $|\Delta|=0$ the modifications are $\delta v_{\mathrm{mod}}=\delta\tilde{v}_{\mathrm{mod}}=0$.

In the previous subsection we have argued that for strong attractive interactions the fermions are bound into pairs. Our

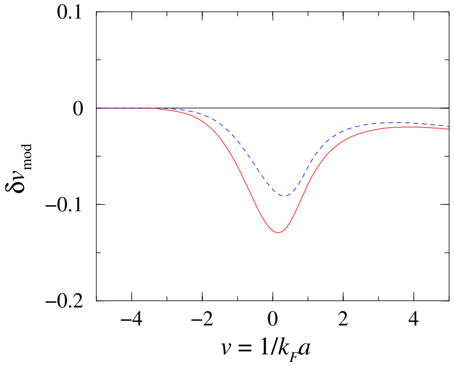


FIG. 3. (Color online) Modifications of the dimensionless interaction parameter: the red solid curve shows $\delta v_{\rm mod}$ and the blue dashed curve depicts $\delta\tilde{v}_{\rm mod}$ as a function of v for $T=0$ and $|\Delta|=|\Delta_0|$.

crossover theory for the interacting fermion system then converges to a Luttinger-Ward-type theory for interacting bosons. Since the modified version of our theory obeys the Ward identity, its strong-coupling limit necessarily leads to a description of dilute, repulsive bosons which has the correct linear spectrum of excitations at low energies. It turns out that the limiting theory here is the Luttinger-Ward version of the so-called Shohno theory [44,45] which is equivalent to the more well-known Popov approximation. While we have not been able to derive the Shohno-Popov theory analytically from the Luttinger-Ward functional of the original fermionic model, we find a quick convergence numerically in all thermodynamic quantities for dimensionless couplings $v>2$. Considering the entropy, in particular, the Shohno-Popov theory gives rise to the standard expression

$$S = L^d \int \frac{d^dK}{(2\pi)^d}\{(1+n_{\mathbf{K}}^B)\ln(1+n_{\mathbf{K}}^B) - n_{\mathbf{K}}^B \ln n_{\mathbf{K}}^B\} \quad (2.83)$$

for the entropy of a noninteracting gas of bosonic quasiparticles with the standard distribution function

$$n_{\mathbf{K}}^B = 1/[\exp(\beta[E_{\mathbf{K}}^B - \mu_B]) - 1]. \quad (2.84)$$

The corresponding spectrum of excitation energies

$$E_{\mathbf{K}}^B - \mu_B = [(\hbar^2\mathbf{K}^2/2m_B)^2 + (\hbar^2\mathbf{K}^2/2m_B)2g_B|\Psi_B|^2]^{1/2} \quad (2.85)$$

has the well-known form of a Bogoliubov spectrum with a temperature-dependent condensate density $n_{B,0}=|\Psi_B|^2$ and a positive Bose-Bose scattering amplitude g_B. Within our approximation, we have $g_B=2g$; i.e., the exact dimer-dimer scattering length $a_{dd}\approx 0.60a$ is replaced by its Born approximation result $a_{dd}^{(B)}=2a$ [46]. The effective mass and chemical potential take their obvious values $m_B=2m$ and $\mu_B=2\mu+\varepsilon_b$ where $\varepsilon_b=\hbar^2/ma^2$ is the two-particle binding energy on the BEC side of the crossover, where $a>0$. The order parameter Ψ_B is given by Eq. (2.68). Other thermodynamic quantities are obtained using more complicated expressions, which are not presented here in detail [47]. As will be shown explicitly in the following sections, the numerical results for the critical temperature or the entropy converge quickly to that of the Shohno-Popov theory for coupling strengths $v>2$.

III. NUMERICAL RESULTS

Following the detailed discussion of the formalism used to describe the thermodynamics of attractively interacting fermions at arbitrary coupling and temperature, we now present numerical results which cover both the normal and superfluid regimes. These results require a solution of the self-consistent equations determining the Green function G and the vertex function Γ, which are scalars above and two-by-two matrices below the critical temperature. An iteration procedure is performed where a numerical Fourier transformation is needed to transform the functions back and forth. Since the Green function G, the vertex function Γ, and the related functions $\tilde{\Sigma}$ and M are singular at small values of $\mathbf{r}$ and τ and also exhibit significant variation over several orders of magnitude, the numerical Fourier transformation is quite challenging. In practice, the variables need to be discretized on logarithmic scales. Standard procedures like the fast Fourier transformation are therefore not applicable. The basic principles of our special numerical Fourier transformation are described in Appendix B.

A. Critical temperature

The crucial quantity which determines the overall structure of the phase diagram is of course the critical temperature T_c for the transition to a superfluid. This temperature is known analytically only in the extreme BCS and BEC limits. In the BCS limit $k_F|a|\to 0$, where the average distance between the fermions is much larger than the magnitude of the scattering length, the standard solution of the gap equation for an attractive pseudopotential gives a critical temperature

$$T_c^{(BCS)} = \frac{8e^{\gamma_E}}{\pi e^2}\varepsilon_F \exp(-\pi/2k_F|a|), \quad (3.1)$$

with $\gamma_E=0.5772\ldots$ Euler's constant. $T_c^{(BCS)}$ is exponentially small on the characteristic scale of the Fermi energy. Since typical Fermi temperatures in cold gases are of the order of micro-kelvins, the BCS regime is in practice hardly attainable in these systems.

The leading-order corrections to the BCS result in an expansion in the small parameter $k_F|a|\ll 1$ were determined a long time ago by Gorkov and Melik-Barkhudarov [48]. They arise from induced interactions, where one fermion sees the polarization in the Fermi gas due to a second fermion. The density-induced interaction changes the dimensionless coupling constant $N(0)g=2k_Fa/\pi$ of the BCS theory to [49]

$$g \to g + g^2 N(0)\frac{1+2\ln 2}{3}, \quad (3.2)$$

where $N(0)=mk_F/2\pi^2\hbar^2$ is the standard density of states per spin at the Fermi energy. Since the additional contribution to the two-body scattering amplitude $g<0$ is positive, the induced interactions weaken the attractive interaction between two fermions in vacuum and lead to a reduction of the tran-

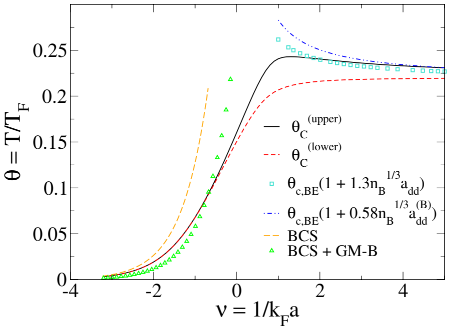


FIG. 4. (Color online) $\theta_c^{(lower)}$ (red dashed line) and $\theta_c^{(upper)}$ (solid black line, identified as T_c) compared with the Shohno result (blue dot-dashed line) with $a_{dd}^{(B)}=2a$ and the exact (QMC) result (light-blue squares) with $\Delta T_c/T_{BEC}=cn_B^{1/3}a_{dd}$and $c=1.31$ and $a_{dd}=0.60a$. The yellow dashed line and green triangles show the BCS result without and with Gorkov and Melik-Barkhudarov corrections.

sition temperature by a factor $(4e)^{-1/3}\approx 0.45$. The nonanalytic dependence of the BCS-transition temperature on the dimensionless coupling constant $k_F a$ thus gives rise to a finite change in the prefactor in Eq. (3.1) from the BCS value 0.61 to 0.28, even though the contribution of induced interactions is of order $k_F a$ compared to the bare interaction.

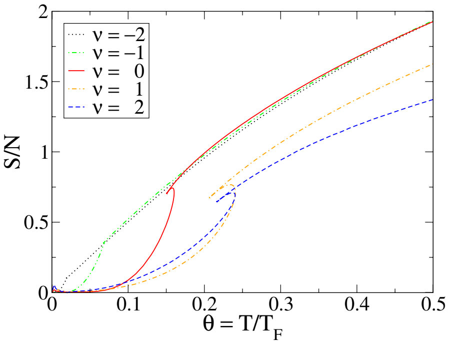


FIG. 5. (Color online) $S(T)$ at various interaction strengths v.

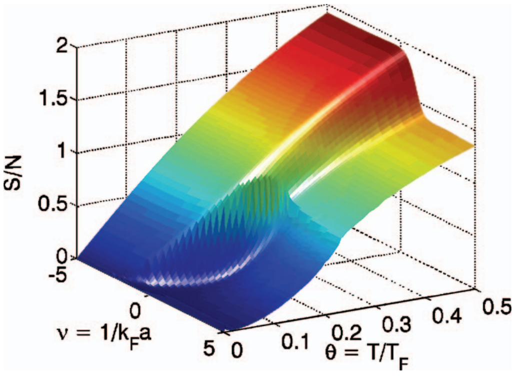


FIG. 6. (Color) Entropy as a function of θ and v obtained using Eqs. (2.50) and (2.63).

On the BEC side, the zeroth-order result for the critical temperature is obtained from the value

$$T_c^{(BEC)} = 3.31\frac{\hbar^2 n_B^{2/3}}{m_B} = 0.218\varepsilon_F, \tag{3.3}$$

obtained for an ideal Bose gas with density $n_B=n/2$ and mass $m_B=2m$. The leading corrections to this result arise from the residual interactions between the strongly bound bosonic dimers. As shown by Petrov *et al.* [20,50], these interactions can be described by a positive dimer-dimer scattering length $a_{dd}\approx 0.60a$. With the quite plausible assumption that the total potential energy in a dilute gas of dimers is the sum of its *two-body* interactions, the scattering length of the four-fermion problem determines the corresponding interaction constant in the theory of a weakly interacting Bose gas in the regime of a small gas parameter $n_B^{1/3}a_{dd}\ll 1$, where Bogoliubov theory is applicable. The exact dependence of the critical temperature of the dilute, repulsive Bose gas on the interaction strength has been calculated only in recent years. To lowest order in the interaction, the shift is positive and linear in the scattering length [51],

$$T_c/T_c^{(BEC)} = 1 + cn_B^{1/3}a_{dd} + \cdots, \tag{3.4}$$

with a numerical constant $c\approx 1.31$ [52,53]. As a result, the evolution of the critical temperature in the homogeneous case as a function of the dimensionless coupling constant $v=1/k_F a$ necessarily exhibits a maximum, since the asymptotic ideal Bose gas result is approached from above. Such a maximum was found in the early calculations of T_c along the BCS-BEC crossover by Nozières and Schmitt-Rink [54] and by Randeria [55]. The precise height and location of this maximum, however, have not been determined so far in a quantitatively reliable manner. Given that our present theory exhibits a first-order transition, there is a range of multivaluedness of the thermodynamic potentials as a function of temperature. This regime is bounded in Fig. 4 by the upper and lower T_c curves, respectively. The lower T_c curve (shown as the red dashed line) which is monotonic in v coincides with the T_c curve previously calculated [30] by implementing the Thouless criterion coming from the normal fluid side. In a situation where a true first-order transition is expected, we would need to perform a Maxwell construction to obtain the proper transition line. As was discussed above, however, the first-order transition is an artifact of the ap-

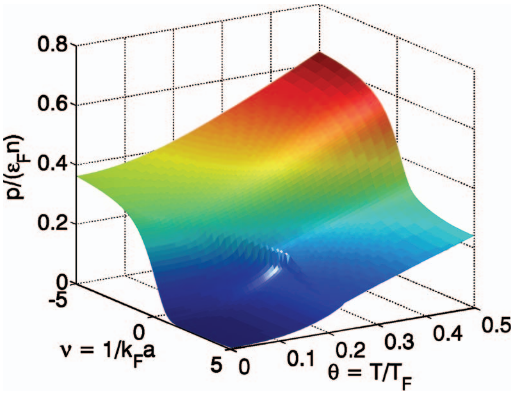


FIG. 7. (Color) Pressure as a function of θ and v obtained using Eqs. (2.48) and (2.58).

proximations involved. In particular the spectrum of excitations right at T_c is free particle like in our approximation rather than $\omega_K \sim K^{3/2}$ [56].

In order to determine the proper critical temperature within our approximation, we have used two essentially equivalent criteria: the fact that the exact entropy is continuous at T_c suggests that our best approximation for the critical temperature is where the jump in the entropy between the two branches characterizing the superfluid and the normal regime has a minimum. Essentially the same value is obtained by defining T_c through the criterion that it be the maximum temperature at which the order parameter $\Delta(T)$ is nonzero. Remarkably, these criteria lead to a critical temperature (shown as $\theta_c^{(upper)}$ in Fig. 4) which exhibits a maximum on the BEC side of the crossover around $v \approx 1$ as expected on general grounds. Moreover, our theory predicts the correct asymptotic functional form (3.4) of the T_c enhancement in the BEC limit $v \gg 1$. Even though the dimer-dimer scattering length $a_{dd}^{(B)} = 2a$ and the prefactor $c \approx 0.58$ of our approximate Popov-type theory differ from the exact values $a_{dd} = 0.60a$ and $c \approx 1.31$, respectively, the agreement of our theory with the exact result is very good (see Fig. 4).

A quite sensitive test of the quantitative reliability of our present result for the critical temperature at arbitrary coupling is provided by a comparison with the recent, rather precise numerical results right at the unitarity point by Burovski *et al.* [28]. In fact, our result for the dimensionless ratio $T_c/\varepsilon_F \approx 0.16$ of the critical temperature in units of the bare Fermi energy, which is one of the universal numbers of the BCS-BEC crossover problem (see Sec. III B below), agrees precisely with the numerical results of Burovski *et al.* within the given error bars. As will be shown below, a similar rather precise agreement is obtained with other thermodynamic quantities, except for the chemical potential. Thus, even in the absence of a small parameter which would allow one to control our theory systematically in the crossover regime, the agreement with the numerical results at unitarity gives us confidence that the approach is quantitatively reliable at arbitrary coupling strengths.

In Fig. 5 the temperature evolution of the entropy is shown for various coupling parameters v. Here the multivalued character is clearly seen which reflects the first-order transition. Furthermore, three-dimensional plots of the entropy and of the pressure are presented in Figs. 6 and 7, respectively. In both figures a rather sharp drop is observed in the crossover region from weak coupling $v \lesssim -1$ (fermionic regime) to strong coupling $v \gtrsim +1$ (bosonic regime). In the weak-coupling limit $v \ll -1$ the results of the nearly ideal Fermi gas are approached which are defined by the BCS formulas (2.48)–(2.50) and (2.57). On the other hand, in the strong-coupling limit $v \gg +1$ the results of Shohno's mean-field theory are approached. While the strong-coupling entropy is defined by Eq. (2.83), the other thermodynamic quantities are defined by more complicated formulas [47]. For $v > 1.0$ and very low temperatures the pressure is nearly zero which reflects a special property of Shohno's mean-field theory of weakly interacting bosons. At high temperatures $T \gg \varepsilon_F$ the entropy, the pressure, and the related thermodynamic quantities approach the Boltzmann limit.

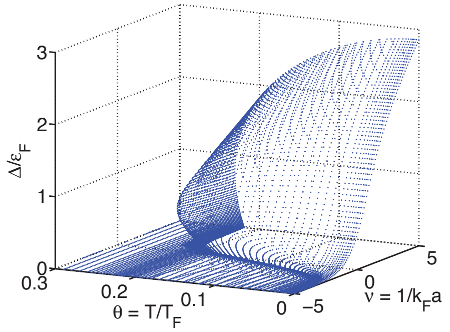


FIG. 8. (Color online) 3D view of the order parameter.

Figure 8 shows the order parameter which vanishes exponentially $\Delta(T=0)/\varepsilon_F \to (8/e^2)\exp(\pi v/2)$ according to the well-known BCS result for $v \ll -1.0$. In the opposite limit of strong coupling the behavior can be derived from $\mu n \to -\Delta^2/2g$ which reflects the fact that the fermion chemical potential in the strong-coupling limit is governed by the potential (i.e., binding) energy. This yields $\Delta(T=0)/\varepsilon_F \to \sqrt{(16/3\pi)v}$ with the square root behavior clearly visible in Fig. 8. Near T_c the gap function displays the multivalued behavior characteristic of a first-order transition.

At low temperatures the entropy has to vanish in accordance with the third law of thermodynamics. The way it does is in fact universal along the full BCS-BEC crossover. Indeed, at low temperatures, the two-component Fermi gas is in a superfluid state, independent of the strength of the attractive interaction. On quite general grounds, therefore, the low-lying excitations above the ground state are sound modes of the Bogoliubov-Anderson type. These modes give rise to an entropy

$$S(T) = V\frac{2\pi^2}{45}\left(\frac{T}{\hbar c}\right)^3 + \cdots, \tag{3.5}$$

which vanishes like T^3 for arbitrary coupling strength. The associated sound velocity c is constant at low T and may be determined from the pressure via $mc^2 = \partial p/\partial n$. Figure 9 displays $(c/v_F)^2$ at $T=0$ as a function of coupling strength with v_F the Fermi velocity. The dilute interacting Fermi gas limit $(c/v_F)^2 = [1+2/(\pi v)]/3$ and the BEC limit $(c/v_F)^2 = k_F a_{dd}/(6\pi)$ for $a_{dd} = 0.60a$ are represented by the blue squares and the green triangles, respectively. The red tri-

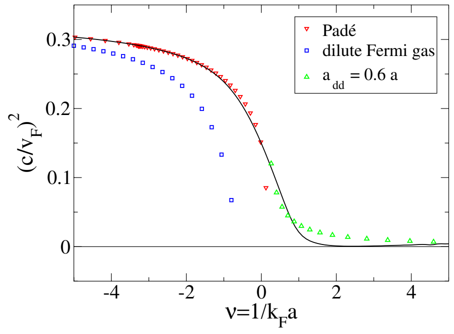


FIG. 9. (Color online) Isothermal sound speed $mc^2 = \partial p/\partial n$ as a function of $v = 1/k_Fa$ for $T=0$. The different curves are explained in the main text.

angles are obtained by extending the expression of the ground-state energy of a dilute weakly interacting Fermi gas [57,58] with the help of a Padé approximation to the strong-coupling regime [8,9],

$$\frac{E}{\varepsilon_F N} \simeq \frac{3}{5} + \frac{\frac{2}{3\pi}k_F a}{1 - \frac{6}{35\pi}(11 - 2\ln 2)k_F a}, \tag{3.6}$$

and the thermodynamic identity

$$c^2 = \frac{1}{m}\frac{\partial}{\partial n}\left(n^2 \frac{\partial E/N}{\partial n}\right). \tag{3.7}$$

Obviously the present crossover theory provides a very good description of the equation of state and sound velocity except in the regime $v > 1$, where our results underestimate both the pressure and its density dependence.

In principle we should be able to independently obtain c from the low-entropy asymptotics (3.5). Our numerical results are consistent with $S(T) \sim T^3$; however, they are not precise enough at such low temperatures to extract the sound velocity in this manner.

B. Thermodynamics in the unitarity limit

After presenting the results for the critical temperature and the thermodynamics at arbitrary coupling, we now turn to a more detailed discussion of the unitarity limit, where the scattering length is infinite. This particular line in the phase diagram has received a lot of attention recently. In particular, precise numerical results are available at this point [28], which provide a sensitive test of analytical approaches to the crossover problem.

As has been mentioned before, the Fermi gas at infinite scattering length $v=0$ is rather special since the only relevant length and energy scales remaining in the problem are the Fermi wavelength set by the density and the Fermi energy ε_F, provided we remain within the zero-range pseudopotential approximation. The free energy has a simple scaling form

$$F(T,V,N) = f(\theta)N\varepsilon_F. \tag{3.8}$$

In particular, there are a number of universal ratios which characterize the crossover problem right at the unitarity point, both at zero temperature and at T_c. Examples, which will be determined below, are the chemical potential and the internal energy in units of the Fermi energy or the entropy per particle at T_c. In addition, also the gap for single-particle excitations and the condensate fraction at zero temperature are universal at the unitarity point.

Figure 10 shows the temperature dependence of the internal energy calculated in two different ways. The solid line is our numerical result which is compared with the internal energy (depicted as the dashed line) as obtained from the numerically calculated pressure $p = -\Omega/V$ via the scaling relation $U = 3pV/2$ valid at the unitarity point. Our numerical results display perfect scaling above T_c. The scaling violation below T_c is a consequence of the modification of the theory. In order to preserve the conserving nature of our theory while obeying the Thouless criterion an extra length scale a_{mod} had to be introduced, leading to a modified dimensionless interaction strength $v_{\mathrm{mod}} = 1/k_F a_{\mathrm{mod}}$ with $\delta v_{\mathrm{mod}} = v_{\mathrm{mod}} - v$ in the range between 0.0 and -0.1 with $v_{\mathrm{mod}} \neq 0$ for $v = 0$ (see Secs. II I and II J for details).

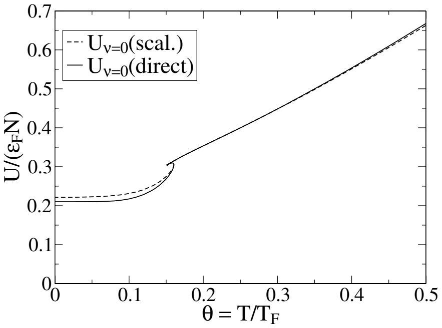


FIG. 10. Internal energy at unitarity as a function of temperature calculated using Eqs. (2.49) and (2.62). The dashed curve is obtained from the calculated pressure using the scaling formula $U = \frac{3}{2}pV$ valid at unitarity.

Figure 11 displays the behavior of the chemical potential $\mu(T)$ as a function of temperature. Using $\mu(T)$ in a local density approximation

$$\mu = \mu_h[n(\mathbf{r}), T(\mathbf{r})/T_F] + V(\mathbf{r}), \tag{3.9}$$

with μ_h the chemical potential of the homogenous case, we can calculate the density profiles of harmonically trapped ultracold gases at unitarity [59]. We have also checked the convergence of our $\mu(T)$ to the high-temperature expansion obtained by Ho and Mueller [60] which, however, only occurs for $T \gg \varepsilon_F$.

Note that below T_c the chemical potential $\mu(T)$ is an increasing function of T. This perhaps counterintuitive result can be understood quite easily from the fact that the low-temperature thermodynamics is determined by the Bogoliubov-Anderson mode. As argued in the previous section, this leads to an entropy which vanishes with a power law $\sim T^3$. Figure 12 displays the entropy at unitarity as a function of temperature. Now, at a given volume, there is a Maxwell relation of the form

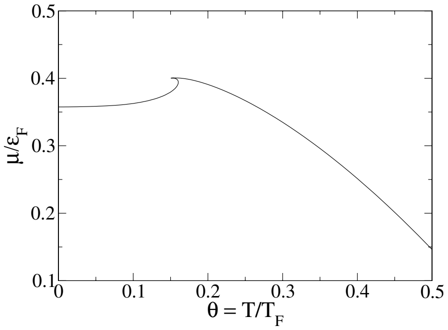


FIG. 11. The single-particle chemical potential at unitarity as a function of temperature obtained from the number conservation constraint (2.26).

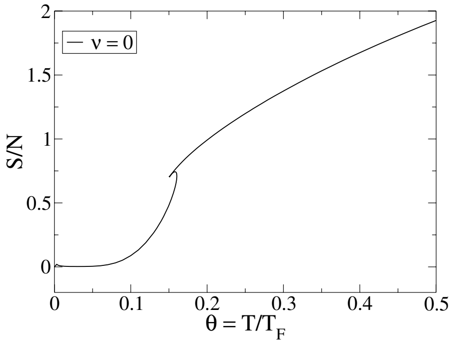


FIG. 12. Entropy at unitarity as a function of temperature.

$$\left.\frac{\partial\mu}{\partial T}\right|_{N,V} = -\left.\frac{\partial S}{\partial N}\right|_{T,V}, \tag{3.10}$$

which connects the temperature dependence of the chemical potential to the density dependence of the entropy. Using the universal result (3.5) for the low-temperature entropy, this relation shows that at low temperatures the chemical potential exhibits a T^4 dependence with a prefactor determined by

$$\frac{\partial\mu}{\partial T} = \frac{3S}{2Vmc_s^2}\frac{\partial^2 p}{\partial n^2} > 0. \tag{3.11}$$

Obviously, this argument is not confined to the unitarity point, showing that the chemical potential at low T has a behavior $\mu(T)=\mu(0)+\mathcal{O}(T^4)$ for arbitrary coupling strengths along the BCS-BEC crossover. A well-documented quantity which determines the density profile of dilute fermions in a trap at unitarity and $T=0$ is the so-called β parameter defined via

$$\mu(T=0) = \varepsilon_F(1+\beta). \tag{3.12}$$

Our value of $\beta \sim -0.640$ is very close to $\beta=-0.67$ obtained via simply Padé-approximating the weak-coupling result for the ground-state energy [8,9] and the experimental results of Bartenstein *et al.* [61], $\beta=-0.68^{+0.13}_{-0.10}$, and Bourdel *et al.* [62], $\beta=-0.64\pm0.15$, but smaller than the results obtained at Duke [63], at Rice [64] and recent QMC results [16,17] (see Table I). Evidently, there is still considerable uncertainty in both the experimental and theoretical results.

A promising route in the direction of thermometry for trapped gases is provided via the reversible adiabatic (isentropic) sweeps [5,61] from the BEC limit. In Fig. 13 we depict the resulting changes in temperature when moving across the unitarity limit for the homogenous case. For the trapped case this cooling mechanism was first advocated by Carr *et al.* [32] and recently quantitatively refined by Hu *et al.* [66]. Finally to facilitate quantitative comparison with various quantum Monte Carlo results we have collected available data from the literature presented in Tables I and II. Apart from the value for T_c which is explicitly quoted in the paper by Bulgac *et al.* [27] (with errors) we have estimated the remaining quantities from their presented results and utilized scaling to fill in the missing data below.

TABLE I. Recent experimental results for β compared with calculated values.

		β
Experimental results	Bartenstein *et al.* [61]	$-0.68^{+0.13}_{-0.10}$
	Bourdel *et al.* [62]	−0.64(15)
	Duke [63]	−0.49(4)
	Partridge *et al.* [64]	−0.54(5)
Calculated values	Astrakharchik *et al.* [17]	−0.58(1)
	Carlson *et al.* [16]	−0.56(1)
	Hu, Liu, and Drummond [67]	−0.599
	Perali *et al.* [65]	−0.545
	Padé approximation[8,9]	−0.67
	Present work	−0.64

The $T=0$ results are fixed-node QM results by Astrakharchik *et al.* [17] and Carlson *et al.* [16] (see Table III). Note that our result for Δ/ε_F is close to the value $\Delta_{\mathrm{GMB}}/\varepsilon_F=(2/e)^{7/3}=0.49$ obtained by a naive extrapolation of the Gorkov-Melik-Barkudarov result to $k_Fa=\infty$.

At T_c our results are in very good agreement with those of Burovski *et al.* except for the value of the dimensionless chemical potential μ/ε_F and that of the entropy per particle at T_c. Now Burovski *et al.* have obtained their values for the pressure $p/n\varepsilon_F$ and the entropy S/N indirectly from the internal energy and the chemical potential by using $3pV=2U$ right at unitarity and the Gibbs-Duhem relation. The different results for the chemical potential then entail a considerable discrepancy in the value of S/N at T_c. Within our numerical scheme, the chemical potential is the most directly—via Eq. (2.26)—obtainable quantity among the thermodynamic data. In light of the excellent agreement of all other quantities with the numerical results of Burovski *et al.*, the discrepancy for the chemical potential is thus quite surprising. Indeed, we believe that our values for both the chemical potential and the entropy, for which the validity of the Gibbs-Duhem relation and of $3pV=2U$ at unitarity has been checked *independently*, are rather close to the exact results. This point of view is supported by considering the evolution of the entropy per particle right at the critical temperature as a function of the dimensionless coupling. In the BCS limit, the entropy associated with single-particle excitations can be calculated

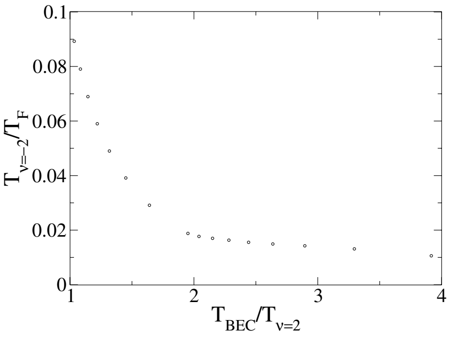


FIG. 13. Temperature reduction on performing an isentropic sweep across $v=0$ from $v=2$ to $v=-2$.

TABLE II. Comparison with diagrammatic determinant Monte Carlo (Burovski *et al.* [28]), quantum Monte Carlo (Bulgac *et al.* [27]), $\varepsilon=4-d$ expansion (Nishida and Son [24,26]), Borel-Padé approximation connecting an expansion in $\varepsilon=4-d$ and one in $\varepsilon=d-2$ [26], and a $1/N$ expansion (Nikolić and Sachdev) [15] at $T=T_c$.

	T_c/ε_F	μ/ε_F	$U/N\varepsilon_F$	$P/n\varepsilon_F$	S/N
Bulgac *et al.*	0.23 (2)	0.45	0.41	0.27	0.99
Burovski *et al.*	0.152 (7)	0.493 (14)	0.31 (1)	0.207 (7)	0.16 (2)
Nikolić and Sachdev ($N=1$)	0.136	0.585	0.164	0.109	
Nishida ($\varepsilon=1$)	0.249	0.18	0.212	0.135	0.698
Borel-Padé	0.183	0.294	0.270	0.172	0.642
Present work	0.160	0.394	0.304	0.204	0.71

from the exactly soluble reduced BCS Hamiltonian and is given by the standard mean-field expression (2.50). At the critical temperature this entropy coincides with that of an ideal Fermi gas:

$$S(T_c)/N=(\pi^2/2)(T_c/T_F). \tag{3.13}$$

Since the ratio T_c/T_F is exponentially small in the weak-coupling limit, the entropy (3.13) associated with fermionic excitations is dominant compared to the contribution arising from the collective Bogoliubov-Anderson mode. Indeed, extrapolating the corresponding low-temperature entropy (3.5) associated with collective excitations up to the critical temperature gives rise to a contribution of order $(T_c/T_F)^3$, which is negligible compared to Eq. (3.13).

At very large coupling strengths, the strongly bound fermion pairs form an eventually ideal Bose gas, for which the entropy per particle right at T_c can again be determined analytically. Recalling that the number of bosons, $N_B=N/2$, in this limit is just half the number of fermions, we obtain a universal number

$$S(T_c)/N=\frac{5\zeta(5/2)}{4\zeta(3/2)}=0.6417\ldots. \tag{3.14}$$

As is evident from Fig. 14, where the complete evolution of the ratio $S(T_c)/N$ is shown as a function of the dimensionless coupling parameter v, the limiting value of the ideal Bose gas is in fact not far from the entropy which is obtained from the Shohno-Popov theory of noninteracting bosonic quasiparticles in the range $v>1$, according to Eq. (2.83).

It is interesting to note that the entropy per particle right at T_c exhibits a maximum as a function of the coupling constant of order $S(T_c)/N\approx0.78$ around the same coupling, where the critical temperature exhibits a maximum. Considering the smooth evolution of $S(T_c)/N$ as a function of v, the value $S(T_c)/N\approx0.16$ at unitarity, which is deduced from the results of Burovski *et al.*, appears to be far too small. On the other hand, the result $S(T_c)/N\approx0.99$ obtained by Bulgac *et al.* seems to be too high.

TABLE III. Comparison with fixed-node Green function Monte Carlo (Astrakharchik *et al.* [17] and Carlson *et al.* [16]) at $T=0$.

	μ/ε_F	$U/N\varepsilon_F$	$P/n\varepsilon_F$	Δ/ε_F
Astrakharchik *et al.*	0.41 (2)	0.25 (1)	0.17 (1)	
Carlson *et al.*	0.43 (1)	0.26 (1)	0.17 (1)	0.54
Present work	0.36	0.21	0.15	0.46

IV. DISCUSSION AND CONCLUSION

In conclusion let us summarize what has been achieved, mention shortcomings of the present approach and indicate possible future extensions.

The formal basis of our results is a self-consistent, conserving theory, which is based on an approach due to Luttinger and Ward and De Dominicis and Martin, in which the exact one- or two-particle Green functions serve as an infinite set of variational parameters. In order for this approach to provide consistent thermodynamic results it is essential that the Green functions satisfy self-consistency conditions which reflect the stationarity of the appropriate thermodynamic potentials. Approximate formulations, in which free Green functions are replaced by full ones according to a choice of G_0G_0, GG_0, or GG, will in general not obey conservation laws or exact thermodynamic identities, in contrast to the Φ derivable formulation presented here. The stationarity conditions were also crucial for the proof of thermody-

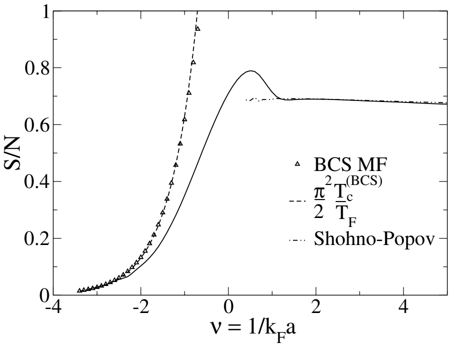


FIG. 14. Entropy at T_c as a function of $v=1/k_Fa$. Numerical result (solid) line obtained with Eqs. (2.50) and (2.63) compared with the limiting results: the BCS mean-field result (triangles) from Eq. (2.50) and (dashed line) from Eq. (3.13) and the Shohno-Popov result (dot-dashed line) from Eq. (2.84).

namic equivalence of the Luttinger-Ward with the De Dominicis–Martin formalism on the level of our approximate functional for the grand canonical potential or the entropy. In fact, to our knowledge, the theory presented here is the first concrete application of the De Dominicis–Martin formulation to the fermionic many-body problem.

An important point we want to emphasize is the necessarily self-consistent nature of the formalism. Indeed, within the Luttinger-Ward or De Dominicis–Martin formulation an approximate functional for the grand canonical potential $\Omega[G]$ or the entropy $S[G,\Gamma]$ is made stationary by determining the space- and time-dependent Green and vertex functions from the variational conditions (2.9) and (2.13), respectively. The solution of these equations *necessarily* leads to a self-consistent mutual dependence of the various Green functions. Self-consistency is thus reached precisely at the stationary point of these functionals. At this point, Eqs. (2.9) and (2.13) are valid, conditions which are necessary for the theory to give consistent thermodynamics, as pointed out, e.g., in the context of Eq. (2.27).

A well-known shortcoming of conserving approximations is the dichotomy with the gapless nature of the collective modes, which reflects the broken continuous symmetry of the superfluid state. For the present theory the formal reason for this dichotomy is a violation of the Ward identity resulting from the global gauge symmetry of the exact theory. In order to overcome this problem an extension of the theory was introduced which forces the gapless nature in the symmetry-broken phase while remaining Φ derivable at the same time to maintain the conserving property.

We have provided quantitative results for essentially all thermodynamic properties at temperatures below half the Fermi temperature, thus covering the relevant regime of the degenerate gas. Overall our results agree remarkably well with recent numerical calculations at the unitarity point, giving confidence that our approach is quantitatively reliable over the full range of couplings between the BCS and BEC limits. In particular, we provide concrete predictions for a number of universal ratios characterizing the unitary Fermi gas both at $T=0$ and at $T=T_c$.

The extensive numerical work entering the solution of the stationarity constraints and thermodynamic potentials is reflected most clearly in the three-dimensional plots of the entropy (Fig. 6), pressure (Fig. 7), and order parameter (Fig. 8). Most noteworthy are the quite abrupt change from fermionic to bosonic character for v in the interval $-1<v<+1$ which are most obvious in the entropy and pressure and the quick convergence to a Shohno-Popov theory of noninteracting bosonic quasiparticles for $v>1$.

An initially unexpected result, which is clearly visible in the numerical data, is the fact that our superfluid phase transition is weakly first order, instead of being continuous as it should be. The origin of this failure to capture the critical behavior correctly is found in the Shohno-Popov theory, which is obtained from our approach in the limit $v \gg 1$. The Shohno-Popov theory of a dilute, repulsive Bose gas generalizes the Bogoliubov theory to finite temperatures. It takes into account the thermal depletion of the condensate by including the effect of bosons with finite-momentum $\mathbf{K}$ in the particle number equation. Long ago Reatto and Straley [44] analyzed Shohno's theory in a self-consistent formulation and obtained a first-order superfluid transition. Physically, the origin of the associated entropy jump is the collapse of the single-particle spectrum right at the transition. Indeed, within the Shohno-Popov theory, the single-particle spectrum changes from initially linear to initially quadratic on raising the temperature through T_c. As a result, the density of states is changed from a ε^2 dependence below T_c to the free particle $\sqrt{\varepsilon}$ result right at and above T_c. The associated drastic increase in the available phase space leads to a jump in the entropy.

For a purely bosonic system, a proper treatment of the behavior near the critical point was recently given by Baym and co-workers [51]. Holzmann and Baym [68] showed that a change of the spectrum for long-wavelength excitations occurs right at T_c. This hardening of the spectrum (the low-$\mathbf{K}$ spectrum is of the form $\mathbf{K}^\alpha$ with $\alpha<2$) leads to the required reduction in the density of states to render the superfluid transition continuous. The subtle low-$\mathbf{K}$ correlations necessary for this change in spectrum are clearly missing in our self-consistent approach.

The BCS-BEC crossover being continuous, however, implies that the first-order result also pertains to the $v \ll -1$ limit of our theory. We have checked that at the transition the discontinuities of all thermodynamic quantities are $\sim\exp(-C|v|)$ for $v \ll -1$ [47]. The associated difficulties of a proper treatment of bosonic excitations do not occur in the reduced BCS Hamiltonian which neglects collective modes altogether, resulting in a continuous superfluid transition. To correctly account for the critical regime $\Delta T/T_c \to 0$ our theory would need to be extended to treat the feedback between different bosonic modes accurately. Bickers and Scalapino [69] have shown that this requires the incorporation of single-particle self-consistency and two-particle self-consistency on the same level of approximation. This may be achieved via so-called parquet resummations. Currently, however, the inclusion of these contributions appears extremely challenging. A systematic and analytically accessible description of the crossover which is uniformly valid in both the normal and superfluid regimes and which gives a proper account of the critical behavior is provided by a $1/N$ expansion as recently shown by Nikolić and Sachdev [15]. This method can in fact be extended in a straigthforward manner to the case of unbalanced spin populations, a subject which has attracted a lot of attention very recently [64,70].

ACKNOWLEDGMENTS

We acknowledge useful discussions with J.N. Fuchs, R. Grimm, and M. Zwierlein and, moreover, would like to acknowledge an illuminating exchange with Y. Nishida and S. Sachdev on their recent work. Part of this work was supported by the Deutsche Forschungsgemeinschaft DFG within the Schwerpunkt “Ultrakalte Gase” (S. C.).

APPENDIX A: REGULARIZATION OF DIVERGENT MATSUBARA-FREQUENCY SUMS

In our formulas of the thermodynamic potentials most sums over Matsubara frequencies are not well defined. The functions which are summed do not decay to zero fast enough so that the Matsubara-frequency sums diverge. However, this problem can be fixed. To do this we first perform a Fourier back transformation to obtain a function in terms of the imaginary time τ. Then we take the limit $\tau \to -0$ or $\tau \to +0$ which is finite and well defined.

We must distinguish between fermion and boson functions which have different Matsubara frequencies. Fermion functions are of the type

$$A(\mathbf{k},\omega_n)=\begin{pmatrix}\mathcal{A}(\mathbf{k},\omega_n) & \mathcal{B}(\mathbf{k},\omega_n)\\ -\mathcal{B}(\mathbf{k},\omega_n)^* & \mathcal{A}(\mathbf{k},\omega_n)^*\end{pmatrix}, \tag{A1}$$

where $A(\mathbf{k},\omega_n)$ may be either $A(\mathbf{k},\omega_n)=-\ln[G(\mathbf{k},\omega_n)]$ or $A(\mathbf{k},\omega_n)=[G_0(\mathbf{k},\omega_n)^{-1}G(\mathbf{k},\omega_n)-1]$. [Note that the lower row of the matrix (A1) has the opposite sign than the lower row of the matrix (2.17). The reason is that in the terms of the thermodynamic potentials always an even number of fermion Green functions are multiplied together.] In this case we define

$$\frac{1}{\beta}\sum_{\omega_n}\mathrm{Tr}\{A(\mathbf{k},\omega_n)\}=2\mathcal{A}(\mathbf{k},\tau=-0), \tag{A2}$$

where we assume that $\mathcal{A}(\mathbf{k},\tau)$ is real. Similarly consider a bosonic function of the form

$$A(\mathbf{K},\Omega_n)=\begin{pmatrix}\mathcal{A}(\mathbf{K},\Omega_n) & \mathcal{B}(\mathbf{K},\Omega_n)\\ \mathcal{B}(\mathbf{K},\Omega_n)^* & \mathcal{A}(\mathbf{K},\Omega_n)^*\end{pmatrix}, \tag{A3}$$

with $A(\mathbf{K},\Omega_n)=\Gamma(\mathbf{K},\Omega_n)$ or $A(\mathbf{K},\Omega_n)=-\ln[\Gamma(\mathbf{K},\Omega_n)]$. In this case we define

$$\frac{1}{\beta}\sum_{\Omega_n}\mathrm{Tr}\{A(\mathbf{K},\omega_n)\}=2\mathcal{A}(\mathbf{K},\tau=-0), \tag{A4}$$

where we assume that $\mathcal{A}(\mathbf{K},\tau)$ is real.

In some terms of our formulas the fermion function $A(\mathbf{k},\omega_n)$ or the boson function $A(\mathbf{K},\Omega_n)$ is proportional to the unit matrix 1. In this case the Fourier back transform $\mathcal{A}(\mathbf{K},\tau)$ is $\delta_F(\tau/\hbar)$ or $\delta_B(\tau/\hbar)$, respectively. Hence, the related Matsubara-frequency sums (A2) and (A4) are zero.

APPENDIX B: NUMERICAL FOURIER TRANSFORMATION

The special numerical Fourier transformation was invented a long time ago by one of the authors in a different context in order to solve the mode-coupling equation for the liquid-glass transition [71]. In this case relaxation phenomena are considered on a logarithmic time scale over many decades, starting at microscopically short times and extending up to very long macroscopic times. Thus, a Fourier transformation is needed which can handle functions with features on logarithmic time and frequency scales extending over ten and more decades. Clearly, a standard fast Fourier transformation cannot be applied because a constant step width would be needed. Rather the function to be transformed has been discretized on a logarithmic scale and interpolated by cubic spline polynomials. Since for polynomial functions the Fourier integrals can be evaluated exactly, we end up with a transformation formula which depends on the spline coefficients of the function.

Later this special numerical Fourier transformation was extended to transform Matsubara Green functions in order to solve the self-consistent equations for the BCS-BEC crossover [30]. Here, three-dimensional spatial Fourier transformations of isotropic functions and discrete Fourier sums with Matsubara frequencies were considered. These Fourier transformations are used also in the present paper for the numerical calculations. Only a few modifications and optimizations have been made over the years. The basic principles of the special numerical Fourier transformation are described in the Appendix of Ref. [30]. Here we present the fundamental formulas in order to make the numerical method available for applications.

In order to perform a discrete Fourier transformation the following sum must be evaluated:

$$f(k)=\sum_{x=x_{\min}}^{x_{\max}}\Delta x e^{ikx}f(x), \tag{B1}$$

where x is a discrete variable with constant step width Δx. In this formula and in the following formulas the sum over x is defined as a trapezoid sum. This means that the first term and the last term in the sum are multiplied by a factor $\frac{1}{2}$, respectively. The continuous Fourier transformation is defined by a related integral which is obtained from Eq. (B1) in the limit $\Delta x \to 0$.

We assume that the function values are known in a finite subset of points x_j according to $f(x_j)=a_j$ where $j=0,1,\ldots,N$. The points x_j cover the whole interval between $x_{\min}$ and $x_{\max}$ on a logarithmic scale so that $x_{\min}=x_0<x_1<\cdots<x_{N-1}<x_N=x_{\max}$. Consequently, the Fourier sum (B1) can be divided into a sum of N trapezoid sums according to

$$f(k)=\sum_{j=0}^{N-1}\left\{\sum_{x=x_j}^{x_{j+1}}\Delta x e^{ikx}f(x)\right\}. \tag{B2}$$

Now, we assume that the function is given by the cubic spline polynomial

$$f(x)=a_j+b_j(x-x_j)+c_j(x-x_j)^2+d_j(x-x_j)^3 \tag{B3}$$

if x is located in the interval $x_j \le x \le x_{j+1}$. The spline coefficients a_j, b_j, c_j, and d_j are calculated numerically. Inserting the cubic spline polynomial (B3) into the formula (B2) we find that the trapezoid sums within the curved brackets can be evaluated exactly. Thus, as a result we obtain the Fourier transform

$$f(k)=\sum_{j=0}^{N-1}\{a_jI_j^{(0)}(k)+b_jI_j^{(1)}(k)+c_jI_j^{(2)}(k)+d_jI_j^{(3)}(k)\}, \tag{B4}$$

where

$$I_j^{(n)}(k)=e^{ikx_j}\left(-i\frac{\partial}{\partial k}\right)^n\left[\frac{\Delta x}{2i}\cot\left(\frac{k\Delta x}{2}\right)[e^{ik(x_{j+1}-x_j)}-1]\right]. \tag{B5}$$

By construction a cubic spline function and its first two derivatives are continuous. These facts imply the following continuity conditions:

$$f(x_{j+1}) = a_j + b_j(x_{j+1}-x_j) + c_j(x_{j+1}-x_j)^2 + d_j(x_{j+1}-x_j)^3 = a_{j+1}, \tag{B6}$$

$$f'(x_{j+1}) = b_j + 2c_j(x_{j+1}-x_j) + 3d_j(x_{j+1}-x_j)^2 = b_{j+1}, \tag{B7}$$

$$f''(x_{j+1}) = 2c_j + 6d_j(x_{j+1}-x_j) = 2c_{j+1}, \tag{B8}$$

which may be used to regroup the terms in Eq. (B4). Consequently, as a result we obtain the alternative formula

$$f(k) = J^{(0)}(k)[e^{ikx_N}a_N - e^{ikx_0}a_0] + J^{(1)}(k)[e^{ikx_N}b_N - e^{ikx_0}b_0] + J^{(2)}(k)[e^{ikx_N}c_N - e^{ikx_0}c_0] + J^{(3)}(k) \times \sum_{j=0}^{N-1} [(e^{ikx_{j+1}} - e^{ikx_j})d_j], \tag{B9}$$

where

$$J^{(n)}(k) = \left(-i\frac{\partial}{\partial k}\right)^n \left[\frac{\Delta x}{2i}\cot\left(\frac{k\Delta x}{2}\right)\right]. \tag{B10}$$

The terms with spline coefficients a_j, b_j, and c_j have canceled for $j=1,2,\ldots,N-1$. In the limit $k\to 0$ the functions (B10) diverge according to $J^{(n)}(k)\sim|k|^{-(n+1)}$. For this reason, the alternative formula (B9) can be applied numerically only for large k so that $|kx_j|\gtrsim 1$ for all $j=0,1,\ldots,N$. On the other hand, the function (B5) is finite in the limit $k\to 0$ so that formula (B4) can be applied numerically for small k where $|kx_j|\lesssim 1$ for all $j=0,1,\ldots,N$. In practice we use a combination of both formulas (B4) and (B9). Which formula is used for a particular j we decide by considering the value of $|kx_j|$ and comparing this value with 1. In this way we obtain a special numerical Fourier transformation which is stable and reliable for points x_j and k_l distributed on a logarithmic scale over many decades.

We have derived our special numerical Fourier transformation for discrete variables x with a finite constant step width Δx. The continuous Fourier transformation is obtained easily and naturally by taking the limit $\Delta x\to 0$ in the functions (B5) and (B10) which is well defined.

In order to transform the Green and vertex functions forward and backward, we need two kinds of Fourier transformations. First, we transform between the Matsubara frequencies and the imaginary time variable. In this case we can apply a continuous (forward) and a discrete (backward) Fourier transformation (B1) directly. Second, we transform between the wave vector and the spatial coordinate in $d=3$ dimensions. Since the functions are spherically symmetric, an integration over the angles can be performed, so that the resulting transformation integrals are one dimensional depending only on radial variables: a radial wave number and a radial space coordinate, respectively. For $d=3$ the transformation integrals can be recast into a one-dimensional continuous Fourier transformation so that our special numerical Fourier transformation (B1) can be used once again.

In practice we use $N=300$ points for all variables. The values of the wave numbers and the values of the space coordinates are distributed on logarithmic scales over six decades, respectively. The Matsubara frequencies are distributed on a logarithmic scale over about 12 decades. The imaginary time variables are distributed appropriately over a finite interval with two logarithmic scales, one for each boundary.

The Green and vertex functions are singular and have slowly decaying long tails. For this reason, reference functions must be subtracted which remove the singularities and the long tails. The reference functions are derived from free Green functions and the two-particle scattering amplitude (T matrix). For these reference functions analytical expressions must be available in all Fourier representations. The difference functions $f(x)$ which are eventually transformed by our numerical method (B1) must be smooth in x and decay according to $f(x)\sim x^{-2}$ or faster for $|x|\to\infty$.

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