Quantum fluctuations in the superfluid state of the BCS-BEC crossover

Roberto B. Diener, Rajdeep Sensarma, and Mohit Randeria
Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA
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We determine the effects of quantum fluctuations about the $T=0$ mean-field solution of the BCS-BEC crossover in a dilute Fermi gas using the functional integral method. These fluctuations are described in terms of the zero-point motion of collective modes and the virtual scattering of gapped quasiparticles. We calculate their effects on various measurable properties, including chemical potential, ground-state energy, the gap, the speed of sound and the Landau critical velocity. At unitarity, we find excellent agreement with quantum Monte Carlo and experimental results. In the BCS limit, we show analytically that we obtain Fermi liquid interaction corrections to thermodynamics including the Hartree shift. In the Bose-Einstein condensation (BEC) limit, we show that the theory leads to an approximate description of the reduction of the scattering length for bosonic molecules and also obtain quantum depletion of the Lee-Yang form. At the end of the paper, we describe a method to include feedback of quantum fluctuations into the gap equation, and discuss the problems of self-consistent calculations in satisfying Goldstone's theorem and obtaining ultraviolet finite results at unitarity.

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I. INTRODUCTION

The BCS-BEC crossover [1–4] is a problem of long-standing interest in many-body physics with implications for a variety of fields including condensed matter, high-energy, nuclear, and atomic and molecular physics. Recent experimental progress in cooling atomic Fermi gases to ultralow temperatures and tuning the interactions between atoms using the Feshbach resonance technique has led to an explosion of interest in the BCS-BEC crossover [5–11].

The theoretical problem is to determine the properties of a system with two species of fermions, spin up and down, with equal masses and densities, interacting via a short-range attractive potential described by a scattering length a_s. The two extremes of the crossover are well understood theoretically. Weak attractive interactions characterized by a small negative scattering length a_s lead to collective Cooper pairing of atoms and BCS superfluidity. In the opposite limit of large attraction, characterized by a small, positive scattering length a_s, one obtains bosonic molecules which exhibit Bose-Einstein Condensation (BEC). The intermediate regime, around the unitary point at which $|a_s| \to \infty$, where one has a strongly interacting Fermi gas, is the most interesting and least well understood theoretically.

The original mean-field (MF) theory of Leggett [1] and Eagles [2] does a decent job of describing the entire $T=0$ crossover at a *qualitative* level [12]. It has only one additional ingredient to the standard BCS theory: the chemical potential must be determined self-consistently along with the pairing gap. This is sufficient to give qualitatively reasonable results [14] which evolve smoothly through unitarity all the way up to the molecular BEC.

Recent theoretical and experimental developments have led to a realization of the quantitative shortcomings of mean-field theory (MFT) at $T=0$, especially at unitarity. The ground-state energy density at unitarity is of the form $\mathcal{E}_0/N = (1+\beta)(3\epsilon_F/5)$, which is a "universal" number [7,16] times the free Fermi gas energy since there is no scale other than ϵ_F as $|a_s| \to \infty$. Quantum Monte Carlo (QMC) calculations [17,18] obtain $(1+\beta)=0.44$, while experiments [8–10] find $(1+\beta)$ in the range 0.32 to 0.44. In contrast the ground-state energy density within MF theory [14] yields $(1+\beta)=0.59$, which is about 34% larger than the QMC result. Furthermore, in the BEC limit ($k_F a_s \to 0^+$), although the MFT correctly predicts a repulsive interaction between the constituent bosons, it misses $O(k_F a_s)^{3/2}$ corrections to thermodynamic quantities, which are present in a weakly repulsive Bose gas.

Our main motivations were to understand this quantitative discrepancy, on which there has been recent progress by several approaches [19–23] (discussed below), and also to obtain a physical picture of the quantum fluctuations missing in MF theory that are responsible for such a large energy difference. We show here that the many-body ground state in the crossover must include, in addition to BCS pairing, the effects of the zero point motion of the collective excitations—the oscillation of the phase (and amplitude) of the order parameter—and the effects of virtual scattering of quasiparticle excitations.

Our central result, from which essentially all our other results follow, is that the thermodynamic potential Ω at $T=0$ is given by

$$\Omega = -\frac{m}{4\pi a_s}\Delta_0^2 - \sum_{\mathbf{k}}\left(E_{\mathbf{k}} - \epsilon_{\mathbf{k}} + \mu - \frac{1}{2}\frac{\Delta_0^2}{\epsilon_{\mathbf{k}}}\right) + \frac{1}{2}\sum_{\mathbf{q}}\left[\omega_0(\mathbf{q}) - E_c(\mathbf{q}) - \int_{-\infty}^{-E_c(\mathbf{q})}\frac{d\omega}{\pi}\delta(\mathbf{q},\omega)\right] + \mathcal{R}. \tag{1}$$

Here the first line represents the "fermionic contribution" to the ground-state energy of the superfluid. It has the same structure as the mean-field result and may be thought of as coming from filling up the negative energy states in a Bogoliubov–de Gennes framework. The second line represents the "bosonic contribution" which arises from Gaussian fluctuations about the saddle point. It consists of the zero-point energy of the collective mode with dispersion $\omega_0(\mathbf{q})$

and of an integral which describes the contribution from the virtual scattering of quasiparticles [with a phase shift $\delta(\mathbf{q},\omega)$], whose two-particle continuum begins at $E_c(\mathbf{q})$. The last term $\mathcal{R}$ regularizes the ultraviolet divergence in the bosonic contribution and will be described in detail later; see Eq. (27).

The problem of determining the ground-state energy density of a strongly interacting system is analogous to that of determining the cosmological constant in quantum-field theories. The latter problem is notorious for being dominated by physics at the scale of the ultraviolet cutoff. Here we will show that our results are independent of the momentum cutoff, which is the inverse of the range r_{eff} of the attractive potential between fermions.

Although there has been considerable attention devoted to "universality" at unitarity ($|a_s|=\infty$), we emphasize the simple but often overlooked point that any observable quantity at $T=0$ is a universal function of the single parameter $1/k_F a_s$. By universal we mean that the results are independent of microscopic details below the ultraviolet cutoff length scale of r_{eff}, provided $k_F r_{\text{eff}} \ll 1$. Thus it does not matter whether one looks at an experiment with ^{6}Li or ^{40}K, the result can only depend on system parameters through the combination $1/k_F a_s$. In the absence of a small parameter in the crossover problem, we judge the validity of our approximations not only by their success at unitarity in comparison with quantum Monte Carlo and experiments, but also by their ability to reproduce known results in the BCS and BEC limits.

We conclude this section with a summary of our main results and an outline of the rest of the paper. In Secs. II–IV, we describe the functional integral formalism used in the paper and results for the chemical potential, gap, ground-state energy, speed of sound, and Landau critical velocity as a function of $1/(k_F a_s)$ are presented in Sec. V. Our main results include the following:

(a) In the extreme BCS limit, the fluctuation corrections are dominated by the virtual scattering of fermionic quasiparticles. We show in Sec. VI that we recover the exact Fermi-liquid corrections to the thermodynamics of a dilute Fermi gas, which are the Hartree shift of order $k_F a_s$ and the Galitskii and Huang-Lee-Yang corrections [24–26] of order $(k_F a_s)^2$, albeit with a negative scattering length a_s. We note that these are obtained from Gaussian fluctuations about the *broken symmetry* state and not by including them in an *ad hoc* way.

(b) In the extreme BEC limit, the zero-point motion of the Bogoliubov sound mode dominates the thermodynamics. From the leading-order corrections we estimate in Sec. VII the effective scattering length between the molecular bosons to be $a_B \simeq 0.55 a_s$, an approximate result which turns out to be close to the exact result [27] for the four-body problem of $0.6 a_s$. At the next order we recover the Lee-Yang form for the quantum depletion [25,26] of the molecular Bose gas with a coefficient that is only 6% less than the correct asymptotic expression.

(c) At unitarity, both the zero-point motion of the collective modes and virtual scattering of quasiparticles are important. Our numerical results (see Table I) for the ground-state energy, the gap, and the speed of sound are in good agreement with experimental data and quantum Monte Carlo results; see Sec. VIII for details.

TABLE I. Comparison of ground-state energy, speed of sound, and gap at unitarity obtained by different methods. The last row gives the results obtained in Secs. V and VIII. The results of a self-consistent calculation are described in Sec. IX.

$\lvert a_s\rvert=\infty$	$\mathcal{E}/(3\epsilon_F/5)$	c/v_F	Δ_0
Mean-field theory [14]	0.59	0.44	0.69
Quantum Monte Carlo method [17,18]	0.44	0.38	0.6 ± 0.1
Experiments [8–10]	0.32–0.51	0.38	—
Mean field + fluctuations	0.40	0.37	0.47

(d) The critical velocity v_c across the crossover is maximum near unitarity, as previously predicted [28,29], and as has been observed in experiments [30]. We estimate an upper bound on v_c using the Landau criterion, and find that quantum fluctuations considerably lower it with respect to mean-field values; see Fig. 4.

(e) The results described above are obtained within a scheme in which the Gaussian fluctuations do not feed back into the saddle-point equation for the functional integral, and they only contribute to the thermodynamic potential (1). This is a natural approximation within the functional integral framework, and we show in Appendix G that it leads to exact answers in the simpler problem of the dilute repulsive Bose gas.

(f) To go beyond this approximation, we next include in Sec. IX the self-consistent feedback of the Gaussian fluctuations into the gap equation. We find that this approach leads to several problems, some of which we can resolve. For instance, we show how the apparent violation of Goldstone's theorem in the self-consistent scheme can be resolved by going to an amplitude-phase representation of the fluctuations. However, we point out that there are other problems which are not under control, such as the instability of the system in the extreme BEC limit. Our detailed analysis of the theory with a gap equation modified by Gaussian corrections shows that imposing self-consistency does not necessarily lead to an improved approximation scheme.

In Sec. X we compare our approach and results with several other methods which have been used to attack the same problem. Our approach has similarities with the $1/N$ expansion [21,22] but there are also differences which are discussed in Sec. X. The equations solved in Sec. V are the same as that obtained from the diagrammatic approach of Hu, Liu and Drummond [19], however, our derivation is different and shows why it is natural not to renormalize the saddle-point condition with fluctuation corrections. Further, our approach also allows us to see what the impact of going beyond this approximation is, as indicated in (f) above. This gives insights into problems faced in other self-consistent calculations [23]. Our main conclusions are summarized at the end in Sec. XI. Technical details of the calculations presented in the text are given in a series of six appendixes. In a seventh appendix we illustrate the methods used in the text

for paired Fermi superfluids for the simpler case of a Bose superfluid.

II. FUNCTIONAL INTEGRAL FORMALISM

We consider a system of fermions of two species, which we call "spin" $\sigma=\uparrow,\downarrow$, each of mass m, described by the Hamiltonian density

$$H=\bar{\psi}_\sigma(x)\left[-\frac{\nabla^2}{2m}-\mu\right]\psi_\sigma(x)-g\bar{\psi}_\uparrow(x)\bar{\psi}_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x). \tag{2}$$

The first term has an implicit sum on the repeated index σ, and the chemical potential μ is tuned to fix the average particle density $n=k_F^3/(3\pi^2)$ in a unit volume. Throughout the paper, we set $\hbar=k_B=1$.

We consider the experimentally relevant case of a "broad" Feshbach resonance which can be adequately described within a single-channel formulation of a dilute gas with $k_F r_{\text{eff}}\ll 1$, where r_{eff} is the range of the potential [31]. The two-body interaction in Eq. (2) is described by a "bare" coupling constant g and a momentum cutoff Λ, not explicitly shown above, which is of the order of $1/r_{\text{eff}}$. The effective interaction at low energies is completely described by the s-wave scattering length a_s for the two-body problem in vacuum. To obtain a given renormalized a_s, the bare coupling $g(\Lambda)$ must be tuned using the relation

$$\frac{m}{4\pi a_s}=\frac{-1}{g(\Lambda)}+\sum_{|\mathbf{k}|<\Lambda}\frac{1}{2\epsilon_{\mathbf{k}}}, \tag{3}$$

where $\epsilon_{\mathbf{k}}=|\mathbf{k}|^2/2m$. We will write most of our equations in terms of the bare g, and only at the end we will use Eq. (3) to take the $\Lambda\to\infty$ limit and express the final results in terms of a_s. (For a detailed discussion of justifying this regularization procedure, we refer the reader to Sec. IV of Ref. [32].)

The partition function Z in the grand canonical ensemble at temperature T, chemical potential μ, and in a unit volume, can be written as the imaginary time functional integral [13–15] over the Grassman fields $\bar{\psi}$ and ψ,

$$Z=\int D\bar{\psi}_\sigma D\psi_\sigma \exp(-S_\psi), \tag{4}$$

with the action

$$S_\psi=\int dx\{\bar{\psi}_\sigma(x)\partial_\tau\psi_\sigma(x)+H[\bar{\psi},\psi]\}. \tag{5}$$

We use x to denote $x=(\mathbf{x},\tau)$, where $\mathbf{x}$ is the spatial coordinate and τ is imaginary time in the interval $0\leqslant\tau\leqslant\beta$, where $\beta=1/T$. $\int dx=\int_0^\beta d\tau\int d^3\mathbf{x}$ denotes an integral over all space and over imaginary time. Even though we are eventually interested in $T=0$, we find it convenient to use the finite T Matsubara formalism and take $\beta\to\infty$ at the end.

We next use a Hubbard-Stratanovich transformation with an auxiliary field $\Delta(x)$ which couples to $\bar{\psi}_\uparrow(x)\bar{\psi}_\downarrow(x)$ to obtain

$$Z=\int D\bar{\psi}_\sigma D\psi_\sigma D\Delta D\Delta^* \exp(-S_{\psi,\Delta}). \tag{6}$$

Using the spinor $\psi^\dagger(x)=(\bar{\psi}_\uparrow(x),\psi_\downarrow(x))$ and its Hermitian conjugate $\psi(x)$ the action can be written as

$$S_{\psi,\Delta}=\int dx\frac{|\Delta(x)|^2}{g}-\int dxdx'\,\psi^\dagger(x)\mathbf{G}^{-1}(x,x')\psi(x') \tag{7}$$

where the inverse Nambu-Gorkov Green's function $\mathbf{G}^{-1}$ is given by

$$\begin{pmatrix}-\partial_\tau+\nabla^2/2m+\mu & \Delta(x)\\ \Delta^*(x) & -\partial_\tau-\nabla^2/2m-\mu\end{pmatrix}\delta(x-x'). \tag{8}$$

The functional integral is now quadratic in the fermion fields and these can be integrated out to obtain

$$Z=\int D\Delta D\Delta^* \exp(-S_\Delta) \tag{9}$$

with the action

$$S_\Delta=\int dx\frac{|\Delta(x)|^2}{g}-\int dx\,\mathrm{Tr}\ln\mathbf{G}^{-1}[\Delta(x)], \tag{10}$$

where the trace is over two-dimensional Nambu space. Equation (9) is a formally exact expression for $Z=\exp(-\beta\Omega)$, where Ω is the thermodynamic potential.

III. MEAN-FIELD THEORY

We briefly discuss the mean-field theory [1,14] of the BCS-BEC crossover to introduce notation used throughout the paper. Technical details highlighting aspects (such as convergence factors) which will be useful later are given in Appendix A.

We begin by finding a spatially uniform, static saddle-point Δ_0 to the functional integral defined by Eqs. (9) and (10). This is determined by the gap equation

$$\delta S_\Delta/\delta\Delta_0=0, \tag{11}$$

where

$$S_\Delta[\Delta_0]=\frac{\beta\Delta_0^2}{g}-\sum_{\mathbf{k},ik_n}\mathrm{Tr}\ln\mathbf{G}_0^{-1}(k)\equiv S_0 \tag{12}$$

with

$$\mathbf{G}^{-1}[\Delta_0]=\begin{pmatrix}ik_n-\xi_{\mathbf{k}} & \Delta_0\\ \Delta_0 & ik_n+\xi_k\end{pmatrix}\equiv\mathbf{G}_0^{-1}(k). \tag{13}$$

Here $ik_n=(2n+1)\pi/\beta$ are fermionic Matsubara frequencies, and $\xi_{\mathbf{k}}=\epsilon_{\mathbf{k}}-\mu$ with $\epsilon_{\mathbf{k}}=|\mathbf{k}|^2/2m$.

After some straightforward algebra (see Appendix A) the $T=0$ gap equation (11) can be finally written as

$$\frac{m}{4\pi a_s}=\sum_{\mathbf{k}}\left(\frac{1}{2\epsilon_{\mathbf{k}}}-\frac{1}{2E_{\mathbf{k}}}\right), \tag{14}$$

where $E_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+\Delta_0^2}$ and we have used Eq. (3) to eliminate g in favor of a_s.

To determine both Δ_0 and the chemical potential μ we need to use $n=-\partial\Omega/\partial\mu$, in addition to Eq. (14). At the level of the mean-field (MF) approximation, the thermodynamic potential is given by its saddle-point estimate $\Omega_0=S_0/\beta$ which leads to the $T=0$ MF number equation

$$n = \sum_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right). \tag{15}$$

Equations (14) and (15) are the Leggett mean-field equations [1] for the $T=0$ BCS-BEC crossover which can be solved to obtain the mean-field values Δ_0 and μ as a function of $(k_F a_s)^{-1}$ [14].

Finally, we can obtain an explicit result for the MF thermodynamic potential at $T=0$ in terms of Δ_0 and μ. We evaluate the Matsubara sum in Eq. (12), take the $T=0$ limit, and use Eq. (3) to obtain

$$\Omega_0 = -\frac{m}{4\pi a_s}\Delta_0^2 - \sum_{\mathbf{k}} \left(E_{\mathbf{k}} - \xi_{\mathbf{k}} - \frac{1}{2}\frac{\Delta_0^2}{\epsilon_{\mathbf{k}}}\right). \tag{16}$$

IV. GAUSSIAN FLUCTUATIONS

To go beyond the MF approximation and include the effects of fluctuations, we write

$$\Delta(x) = \Delta_0 + \eta(x), \tag{17}$$

where the complex bosonic field $\eta(x)$ describes space-time-dependent fluctuations about the real, $(\mathbf{x},\tau)$-independent saddle-point Δ_0. We Fourier transform from $x=(\mathbf{x},\tau)\to q=(\mathbf{q},iq_l)$, where $iq_l=i2\pi l/\beta$ is the Matsubara frequency for the bosonic η fields. We then write Eq. (8) as $\mathbf{G}^{-1}=\mathbf{G}_0^{-1}+\mathbf{K}$, where $\mathbf{G}_0^{-1}$ is defined in Eq. (13) and

$$\mathbf{K}(k,k+q) = \begin{pmatrix} 0 & \eta(q) \\ \eta^*(-q) & 0 \end{pmatrix}. \tag{18}$$

We next expand the action S_Δ to order η^2. The first-order term vanishes by the saddle-point condition (11) and we obtain

$$S_\Delta = S_0 + S_g + \cdots, \tag{19}$$

where the mean-field S_0 was defined in Eq. (12). The Gaussian piece has the form

$$S_g = \frac{1}{2}\sum_{\mathbf{q},iq_l} (\eta^*(q), \eta(-q))\mathbf{M}(q)\begin{pmatrix} \eta(q) \\ \eta^*(-q) \end{pmatrix}. \tag{20}$$

The inverse fluctuation propagator $\mathbf{M}$ is given by [14,33]

$$\begin{aligned}\mathbf{M}_{11}(q) &= \mathbf{M}_{22}(-q) \\ &= \frac{1}{g} + \sum_{\mathbf{k},ik_n} \mathbf{G}_{22}^0(k)\mathbf{G}_{11}^0(k+q) \\ &= \frac{1}{g} + \sum_{\mathbf{k}} \left(\frac{u^2 u'^2}{iq_l - E - E'} - \frac{v^2 v'^2}{iq_l + E + E'}\right)\end{aligned} \tag{21}$$

and

$$\begin{aligned}\mathbf{M}_{12}(q) &= \mathbf{M}_{21}(q) \\ &= \sum_{\mathbf{k},ik_n} \mathbf{G}_{12}^0(k)\mathbf{G}_{12}^0(k+q) \\ &= \sum_{\mathbf{k}} uvu'v'\left(\frac{1}{iq_l + E + E'} - \frac{1}{iq_l - E - E'}\right).\end{aligned} \tag{22}$$

Here we use standard BCS notation

$$v_{\mathbf{k}}^2 = 1 - u_{\mathbf{k}}^2 = \frac{1}{2}(1 - \xi_{\mathbf{k}}/E_{\mathbf{k}}) \tag{23}$$

together with the abbreviations $u=u_{\mathbf{k}}, v=v_{\mathbf{k}}, E=E_{\mathbf{k}}$, and $u'=u_{\mathbf{k}+\mathbf{q}}, v'=v_{\mathbf{k}+\mathbf{q}}, E'=E_{\mathbf{k}+\mathbf{q}}$. The first line in Eqs. (21) and (22) is valid at all temperatures, and the Matsubara sums lead to expressions involving Fermi functions $(1-f-f')$ and $(f-f')$; see Ref. [14]. In the second line of Eqs. (21) and (22) we only give results valid in the $T=0$ limit where both $f(E)=f(E')=0$. The factor of $1/g$ in Eq. (21) has to be regularized as usual using Eq. (3).

Integrating out the Gaussian fluctuations in

$$Z \simeq \exp(-S_0)\int D\eta D\eta^\dagger \exp(-S_g) \tag{24}$$

we obtain an improved estimate of the thermodynamic potential

$$\Omega \simeq \Omega_0 + \frac{1}{2\beta}\sum_{\mathbf{q},iq_l} \ln \mathrm{Det}\,\mathbf{M}(q), \tag{25}$$

where Ω_0 was defined in Eq. (16). We note that this result is true even for a *non*-Hermitian matrix $\mathbf{M}$, provided its Hermitian part is positive definite [34]. In our case, this condition corresponds to $M_{11}+M_{22}-2M_{12}>0$, which is true whenever Eq. (14) is satisfied. Physically this is related to an increase in energy under a distortion of the phase, as can be seen from the analysis of Sec. IX.

There is however a problem with this expression (25), since it is actually ill defined: the Matsubara sum is divergent and we need appropriate convergence factors to make it meaningful as discussed in detail in Appendix B. We only write the final result here:

$$\Omega \simeq \Omega_0 + \frac{1}{2\beta}\sum_{\mathbf{q},iq_l} \ln\left[\frac{\mathbf{M}_{11}(q)}{\mathbf{M}_{22}(q)}\,\mathrm{Det}\,\mathbf{M}(q)\right]e^{iq_l 0^+}. \tag{26}$$

In order to gain physical insight into what Eq. (26) means, we will analytically continue from Matsubara frequencies to real frequencies, $iq_l\to\omega+i0^+$. Using standard manipulations (see Appendix B) the Gaussian part of the thermodynamic potential at $T=0$ can be written as $\Omega_g=-\frac{1}{2}\Sigma_{\mathbf{q}}\int_{-\infty}^0 d\omega/\pi[\delta(\mathbf{q},\omega)-\delta_{22}(\mathbf{q},\omega)+\delta_{11}(\mathbf{q},\omega)]$. Here δ is the phase of $\mathrm{Det}\,\mathbf{M}$ defined by $\delta(\mathbf{q},\omega)=\mathrm{Im}\ln\mathrm{Det}\,\mathbf{M}(\mathbf{q},\omega+i0^+)$ and δ_{22} and δ_{11} are the phases of $\mathbf{M}_{22}$ and $\mathbf{M}_{11}$, respectively. The integral runs only over $\omega<0$ because at $T=0$ the Bose factor $n_B(\omega)=-\Theta(-\omega)$.

The analytical structure of $\mathrm{Det}\,\mathbf{M}(\mathbf{q},z)$ is as follows: It has *zeros* on the real axis at $z=\pm\omega_0(\mathbf{q})$, which correspond to

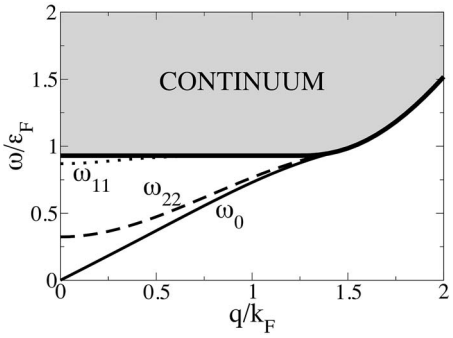

FIG. 1. Spectrum of excitations which contribute to the Gaussian correction to the thermodynamic potential (27). The results shown correspond to unitarity $a_s=\infty$ with $\mu=0.4\epsilon_F$ and $\Delta_0=0.465\epsilon_F$. The full line shows the collective mode dispersion $\omega_0(q)$ (pole of $1/\mathrm{Det}\,\mathbf{M}$) and the shaded region is the two-particle continuum (branch cut). The dashed lines $\omega_{22}(q)$ and $\omega_{11}(q)$ are the zeros of M_{22} and M_{11}, respectively.

poles of the fluctuation propagator, and describe the spectrum of collective excitations. These excitations are oscillations of the phase of the order parameter as $q\to 0$, and is the Goldstone mode arising from the broken symmetry in the superfluid state. We will show that $\omega_0(q)=c_s q$ as $q\to 0$ characteristic of a sound mode. In addition, at higher energies there are *branch cuts* along the real axis at each q, with branch points at $\pm E_c(\mathbf{q})$ with $E_c(\mathbf{q})=\min(E_{\mathbf{k}}+E_{\mathbf{k+q}})$. These branch cuts represent the two-particle *continuum* of states for scattering of gapped quasiparticles; see the lower panel of Fig. 11 in Appendix D.

On the negative ω axis, $\mathbf{M}_{22}(\mathbf{q},\omega)$ and $\mathbf{M}_{11}(\mathbf{q},\omega)$ have zeros at $-\omega_{22}(\mathbf{q})$ and $-\omega_{11}(\mathbf{q})$, respectively, and each has its own scattering continuum. Although the physical meaning of these quantities is less clear, the role that they play in cutting off the ultraviolet divergences in Eq. (26) will be clarified in detail below.

To illustrate these ideas, we show in Fig. 1 the collective mode spectra and the two-particle continuum at the unitary point at which $|a_s|$ diverges. Note that the collective mode frequency $\omega_0(\mathbf{q})$ is initially linear in q, as expected, while the frequencies ω_{22} and ω_{11} have nonzero values in the limit $q\to 0$. All of these frequencies eventually hit the two-particle continuum. Although we keep the integral in the Gaussian part Ω_g over $\omega<0$, as it appears in the algebra, we find it simpler to plot all spectra as for *positive* excitation energies in Fig. 1 and subsequent figures.

We note in passing that even though the unitary Fermi gas is a very strongly interacting system, nevertheless its collective mode spectrum does *not* show a rotonlike minimum observed in superfluid Helium 4. We can understand this within a Feynman approach where the roton minimum arises from a peak in the static structure factor characteristic of a *liquid*, while here we are dealing with a *gas*, even if it is a very strongly interacting gas.

Next we explicitly separate out the collective mode and continuum contributions and write the thermodynamic potential $\Omega(T=0)=\mathcal{E}-\mu N$ as

$$\Omega=\Omega_0+\frac{1}{2}\sum_{\mathbf{q}}[\omega_0(\mathbf{q})-\omega_{22}(\mathbf{q})+\omega_{11}(\mathbf{q})-E_c(\mathbf{q})]$$
$$-\frac{1}{2\pi}\sum_{\mathbf{q}}\int_{-\infty}^{-E_c(\mathbf{q})}d\omega[\delta(\mathbf{q},\omega)-\delta_{22}(\mathbf{q},\omega)+\delta_{11}(\mathbf{q},\omega)]. \tag{27}$$

This is the full expression for the result (1) in the Introduction.

The various contributions to the thermodynamic potential (27) are now much more transparent compared with the Matsubara axis expression (26). Ω_0 is the mean-field contribution (16) to the ground-state energy $\mathcal{E}$. It may be interpreted as arising from filling up the negative energy $(-E_{\mathbf{k}})$ fermionic states of the BCS Hamiltonian, as is made clear in Bogoliubov–de Gennes theory. The Gaussian contribution to $\mathcal{E}$ has three parts to it. The first part $\omega_0(\mathbf{q})/2$ comes from the zero-point motion of the collective mode. The second part, related to the $\delta(\mathbf{q},\omega)$ terms, arises from virtual scattering of the fermionic quasiparticles whose two-particle continuum begins at the energy $E_c(\mathbf{q})$. The third set of contributions, related to the ω_{22}, ω_{11}, δ_{22}, and δ_{11} terms, comes from the convergence factors of Eq. (26) and is essential to obtain a finite answer for Ω.

To obtain a better feel for these various contributions it is useful to look at limiting cases. In the BCS limit (Sec. VI) we will find that the quasiparticle scattering contribution gives the dominant contribution, while in the BEC limit (Sec. VII) it is the zero-point motion of the collective modes. The role of the convergence factors is explained in more detail in Appendix B, and further insight will also be found in the BEC limit.

V. RESULTS FROM MEAN-FIELD THEORY PLUS GAUSSIAN FLUCTUATIONS

Once the thermodynamic potential is obtained, we can find the chemical potential as well as all thermodynamical variables of the system. We must, however, first determine the uniform, static gap parameter Δ_0. From Eq. (24), we see that the Δ_0 used in the expansion is the one that, for a given chemical potential, satisfies the *mean-field* saddle-point equation (11), around which the action S is expanded to quadratic order. Thus, the gap and number equations

$$\delta S_0/\delta\Delta_0=0 \quad \text{and} \quad n=-\partial\Omega/\partial\mu \tag{28}$$

constitute the simplest theory which goes beyond the mean-field approach and is consistent with Goldstone's theorem (see below). As we shall see in this and the next three sections, this approach leads to very useful results and insights. We note that even though the saddle-point gap equation (11) used here retains its mean-field *form*, the *values* of Δ_0 and μ obtained from the simultaneous solution of Eq. (28) will deviate significantly from the mean-field results [which are obtained using Ω_0 of Eq. (16) in the number equation]. Moreover, as we show in Appendix G, an identical approach leads to the known results in a different problem, that of a dilute repulsive Bose gas. In Sec. IX, we will analyze a different

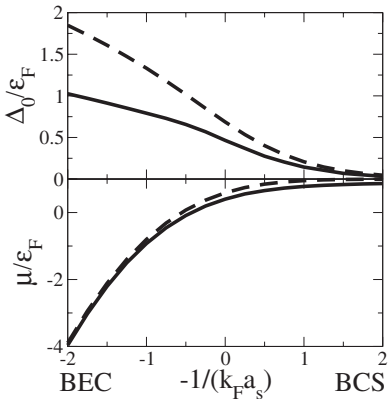

FIG. 2. Gap Δ_0 and chemical potential μ as a function of $-(k_F a_s)^{-1}$ across the BCS-BEC crossover. The dashed line is the mean-field solution while the results of the calculation which includes Gaussian fluctuations are shown as solid lines.

scheme with a modified gap equation which incorporates the self-consistent feedback of Gaussian fluctuations in the calculation of the saddle point, and show that it fails in some important aspects as an appropriate theory throughout the crossover.

In this section we present the results on the following quantities across the BCS-BEC crossover obtained by adding Gaussian corrections to mean-field theory: (i) the gap parameter Δ_0, (ii) the chemical potential μ, (iii) the ground-state energy $\mathcal{E}$, (iv) the speed of sound c_s, and (v) the Landau critical velocity. In the next three sections we will discuss the asymptotic results in the BCS and BEC limits and detailed numerical results at unitarity.

In order to obtain Δ_0 and μ from Eq. (28), we solve the gap equation (14) for $\Delta_0(\mu)$ together with the number equation written as

$$n = -\frac{\partial \Omega_0}{\partial \mu} - \frac{\partial \Omega_g[\mu, \Delta_0(\mu)]}{\partial \mu}. \tag{29}$$

Note that the thermodynamic μ derivative (keeping volume and $T=0$ fixed) in Eq. (29) must take into account the μ dependence of the saddle-point $\Delta_0(\mu)$. (An analogous point for the possibly more familiar case of the dilute Bose gas is emphasized in Appendix G.)

To solve the above number equations we must numerically evaluate $\Omega_g[\mu, \Delta_0(\mu)]$. Even though the real-frequency representation (27) gives physical insight, we find it simpler to numerically evaluate Ω_g on the Matsubara axis, as described in Appendix C. Finally, we calculate $F(\mu)=\Omega_0 + \Omega_g[\mu, \Delta_0(\mu)] + \mu n$ and look for an extremum (maximum) as a function of the chemical potential μ.

The gap Δ_0 and the chemical potential μ are plotted as a function of $-(k_F a_s)^{-1}$ in Fig. 2, where the dashed line is the MF value for comparison. As expected, the inclusion of fluctuations reduces the value of Δ_0. We note that the auxiliary field Δ_0 continues to determine the energy gap $E_g=\Delta_0$ for $\mu>0$ and $E_g=\sqrt{|\mu|^2+\Delta_0^2}$ for $\mu<0$ (just as in MF theory), so long as we ignore the feedback of the fluctuations on the single-particle propagator.

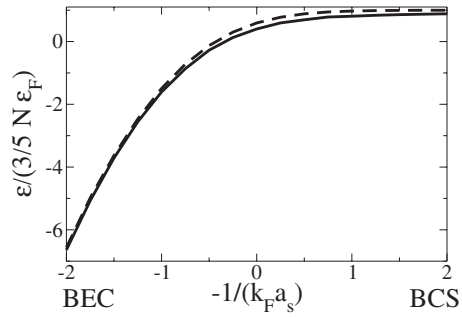

FIG. 3. Ground-state energy per particle $\mathcal{E}$ in units of the noninteracting result $3\epsilon_F/5$ as a function of $-1/(k_F a_s)$. The difference between the mean-field result (dashed line) and the Gaussian fluctuation calculation (solid line) is small and more clearly shown in Fig. 6 (BCS limit), Fig. 8 (BEC limit), and Table I (unitarity).

The ground-state energy of the system is obtained from the thermodynamical potential using $\mathcal{E}=\Omega(T=0)+\mu n$ is plotted in Fig. 3. We see that although the difference between the MF and Gaussian results is quite small, fluctuations reduce the ground-state energy through the entire crossover. The quantitative superiority and the physical insights of the Gaussian results are discussed in detail later: see Fig. 6 for the BCS limit, Fig. 8 for the BEC limit, and Table I for the results at unitarity.

We next compute the speed of sound through the BCS-BEC crossover. First, we emphasize that Goldstone's theorem is necessarily obeyed by the theory defined by Eq. (28); this is in contrast to the self-consistent calculation to be described in Sec. IX. The existence of a zero-energy Goldstone mode is guaranteed by the form of the gap equation (11), which implies that $\mathrm{Det}\, M(\mathbf{q}=0, \omega=0)=0$. To see this fact, note that we can write

$$\mathrm{Det}\, \mathbf{M}(0,0) = \left(\frac{1}{g} + \sum_k \mathrm{Det}\, \mathbf{G}\right)\left(\frac{1}{g} + \sum_k \mathbf{G}_{22}\mathbf{G}_{11} + \mathbf{G}_{12}^2\right) \tag{30}$$

and the saddle-point condition is $1/g=-\Sigma_k \mathrm{Det}\, \mathbf{G}$.

The collective mode spectrum has the form $\omega_0(\mathbf{q})=c_s|\mathbf{q}|$ for $q\to 0$ where c_s is the speed of sound. We calculate c_s following the approach of [14]; we include the expressions here to correct a typographical error [33] in that reference. Rotating the frequency from the Matsubara axis to the real line ($iq_l \to -\omega$) and expanding to quadratic order in both momentum and frequency, we obtain $M_{11}(-\omega, \mathbf{q})=[A+2B\omega + (C+Q)|\mathbf{q}|^2-(D+R)\omega^2]/2$, $M_{22}(-\omega, \mathbf{q})=M_{11}(\omega, \mathbf{q})$, and $M_{12}(-\omega, \mathbf{q})=[A+(C-Q)|\mathbf{q}|^2-(D-R)\omega^2]/2$. Here $A=\Sigma_{\mathbf{k}}\Delta_0^2/2E^3$, $B=\Sigma_{\mathbf{k}}\xi/2E^3$, $C=\Sigma_{\mathbf{k}}\{(1-3X)\xi/m-[1-10X(1-X)]Y\}/8E^3$, $D=\Sigma_{\mathbf{k}}(1-X)/8E^3$, $Q=\Sigma_{\mathbf{k}}\{\xi/m-(1-3X)Y\}/8E^3$, and finally $R=\Sigma_{\mathbf{k}}1/8E^3$, with the notation $X=\Delta_0^2/E^2$ and $Y=|\mathbf{k}|^2/3m^2$. We thus obtain

$$c_s = \sqrt{Q/(B^2/A + R)}. \tag{31}$$

The results for the speed of sound across the BCS-BEC crossover are shown as the black curve in Fig. 4. The solid line is the result obtained after inclusion of Gaussian fluctua-

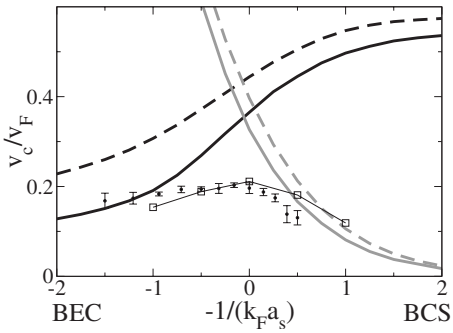

FIG. 4. The Landau critical velocity as a function of $-1/(k_F a_S)$ in the BCS-BEC crossover is given by $\min\{\mathcal{E}(k)/k\}$. The black lines represent the speed of sound c_s and the gray lines the pair breaking estimate obtained using Eq. (32). In each case the dashed line is the result using the MF gap and chemical potential, while the solid line is the result obtained after inclusion of Gaussian fluctuations. The black data points (with error bars) are the experimental results from Ref. [30]. The open squares are the result of a Bogoliubov–de Gennes vortex calculation from Ref. [28].

tions, while the dashed line is the result using the MF values for Δ_0 and μ. The other curves shown in this figure are discussed below.

To conclude this section, we turn to the calculation of the Landau critical velocity v_c as a function of $-1/(k_F a_S)$. As we have seen, most observables—gap, chemical potential, ground-state energy, speed of sound—are monotonic functions of $1/k_F a_s$ through the crossover. The same is true of the transition temperature T_c which shows a slight maximum near unitarity [13] but is essentially the same, of order $0.2\epsilon_F$ for all positive scattering lengths, i.e., to the BEC side of unitarity. In other words there seems to be nothing particularly dramatic about the properties of the most strongly interacting unitary regime. However, as first pointed out in Ref. [28] based on the study of the current flow around a vortex, the critical velocity as a function of $1/k_F a_s$ has a strongly nonmonotic behavior through the crossover with a pronounced peak at (or close to) unitarity. The reason for this behavior is that very different excitations are responsible for the destruction of superfluidity [28,29]: breaking of pairs on the BCS side and generation of phonons on the BEC side of unitarity.

To understand this better and to compare with recent experimental data, we use the Landau criterion which gives an upper bound on the critical velocity of the form $v_c = \min\{\mathcal{E}(k)/k\}$, where $\mathcal{E}(k)$ is the energy of an excitation carrying momentum k. We separately consider single-particle (fermionic) and collective (bosonic) excitations. For single-particle (SP) excitations, the excitation energy is $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}}-\mu)^2+\Delta_0^2}$, which then leads to the v_c estimate

$$\left(\frac{v_c}{v_f}\right)_{\mathrm{SP}} = \left(\frac{(\sqrt{\mu^2+\Delta_0^2}-\mu)^2+\Delta_0^2}{4\epsilon_F\sqrt{\mu^2+\Delta_0^2}}\right)^{1/2}. \tag{32}$$

As we shall see, this is most relevant on the BCS side of unitarity, and in the BCS limit $\mu \gg \Delta_0$, it simply reduces to the well-known result for pair-breaking $v_c \simeq \Delta_0/k_F$. The pair breaking estimate of Eq. (32) is plotted in gray in Fig. 4. The dashed gray line is the result using the MF gap and chemical potential, while the solid gray line is the result obtained after inclusion of Gaussian fluctuations.

For collective excitations, we find that the Landau critical velocity is given by the slope of the tangent to the $\omega_0(k)$ curve. Since there is no roton dip for the superfluid Fermi gas (as already remarked), one simply obtains the speed of sound,

$$(v_c)_{\mathrm{coll.}} = c_s. \tag{33}$$

The actual critical velocity is then bounded above by the minimum of the single-particle $(v_c)_{\mathrm{SP}}$ and collective $(v_c)_{\mathrm{coll.}}$. An estimate of the Landau critical velocity at the mean-field level, which corresponds to the dashed curves in Fig. 4, was given in [29]. We find that quantum fluctuations lead an appreciable reduction in v_c, as seen in the full curves in the figure. We also plot the results of a recent experimental study of the critical velocity [30], for which $v_F = 30$ mm/s. The theoretical predictions of the nonmonotocity of v_c with a peak around unitarity and their experimental confirmation show that the unitary Fermi gas is the most robust superfluid in the entire crossover.

VI. BCS LIMIT: HARTREE SHIFT AND FERMI-LIQUID CORRECTIONS

We now describe in detail the BCS limit solution for $1/k_F a_s \to -\infty$. We will show that the collective mode contribution in Eq. (27) is very small because of phase space restrictions, and the dominant correction to $\Omega(T=0)$ comes from virtual scattering of quasiparticles. We find that the Gaussian theory recovers the well-known "normal state" correction to the ground-state energy of a dilute Fermi gas originally studied by Huang, Yang, and Lee and by Galitskii. The leading term in this correction, which is of order $k_F a_s$, is the Hartree shift of the ground-state energy. We note that the BCS mean-field ground state energy differs from the free Fermi gas by a condensation energy of order Δ_0^2/ϵ_F and represents an exponentially small correction of order $\exp(-1/k_F|a_s|)$ relative to ϵ_F. In contrast, the Gaussian fluctuation contributions will be found to be power-law corrections in $k_F|a_s|$.

The BCS limit is characterized by an exponentially small gap Δ_0 and $\mu \approx \epsilon_F$. The spectrum of collective excitations found in the BCS regime is shown in Fig. 5 for $1/(k_F a_s) = -2$ with $\mu = 0.867\epsilon_F$ and $\Delta_0 = 0.0311\epsilon_F$. In this case, at $q = 0$ the continuum starts at a frequency equal to $2\Delta_0$, and the collective modes are restricted to a small frequency interval, magnified in the inset. Due to particle-hole symmetry in the BCS limit, the zeros ω_{22} and ω_{11} coincide and hence do not contribute to the energy (27). The speed of sound in this limit becomes $c_s \simeq v_F/\sqrt{3}$ [35] as we show at the end of this section.

The MF ground-state energy of the superfluid state is given by the well-known BCS result $\mathcal{E}_0 = 3n\epsilon_F/5 - (3n\Delta_0^2/8\epsilon_F)$. We first show that the contribution of the zero-point motion of the collective modes to Ω is exponentially smaller than the (already small) MF condensation energy,

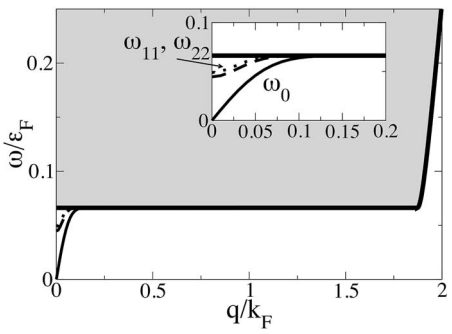

FIG. 5. Spectrum of excitations which contribute to the Gaussian correction to the thermodynamic potential (27). The results shown correspond to the BCS regime $1/(k_F a_s)=-2$, with $\mu=0.867\epsilon_F$ and $\Delta_0=0.0311\epsilon_F$. The full line shows the collective mode dispersion $\omega_0(q)$ (pole of $1/\mathrm{Det}\,\mathbf{M}$) and the shaded region is the two-particle continuum (branch cut). The dashed lines $\omega_{22}(q)$ and $\omega_{11}(q)$ are the zeros of M_{22} and M_{11}, respectively, which coincide in the particle-hole symmetric BCS limit. The inset shows long-wavelength low-energy spectra.

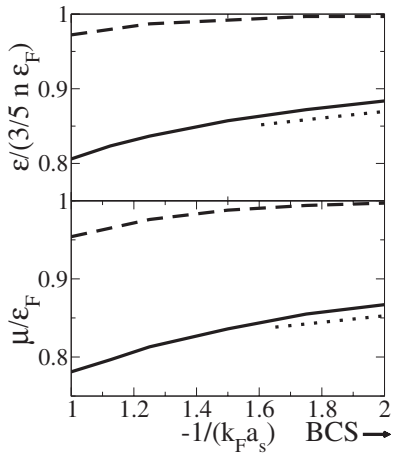

FIG. 6. Energy and chemical potential in the BCS regime for $-(k_F a_s)^{-1}$ between 1 and 2. The solid lines are our calculations including Gaussian fluctuations, the dashed lines the mean-field values, and the dotted lines the results of formulas (34) and (35), in the top and bottom panels, respectively.

and may be neglected. The momentum q_c where the pole hits the continuum at $2\Delta_0$ is given by $q_c \sim \Delta_0/v_F \sim \xi^{-1}$, where ξ is the correlation length. Thus the phase space available for the collective mode contribution is tiny because $q_c \ll k_F$. The contribution per particle to Eq. (27) coming from the poles is seen to be $\sim \epsilon_F (k_F\xi)^{-4} \sim \epsilon_F (\Delta_0/\epsilon_F)^4$, which is negligible.

We next turn to the continuum contribution to Eq. (27). In the BCS limit it is justified to set $\Delta_0=0$ here to obtain the leading-order terms in the ground-state energy. Any corrections due to nonzero Δ_0 are at least down by a factor of $O(\Delta_0^2/\epsilon_F)$ and thus negligible. As already remarked, the ground state is a superfluid which leads to a MF energy reduction of $O(\Delta_0^2/\epsilon_F)$, with respect to the energy that we will calculate. This exponentially small contribution is vital to obtain a stable ground state, but once this is done, we can set the gap to zero in computing leading-order corrections to the ground-state energy, as explained in Appendix D.

In the BCS limit, our result for Ω_g is exactly of the form of the well-known results for the dilute Fermi gas in its *normal* state [26], but with $a_s<0$, as shown in Appendix D. We find that the total energy is given by

$$\frac{\mathcal{E}}{n\epsilon_F} = \frac{3}{5} - \frac{3\Delta_0^2}{8\epsilon_F^2} + \frac{2}{3\pi}k_F a_s + \frac{4(11-2\ln 2)}{35\pi^2}(k_F a_s)^2 + \cdots \tag{34}$$

and the chemical potential

$$\frac{\mu}{\epsilon_F} = 1 - O(\Delta_0/\epsilon_F)^2 + \frac{4}{3\pi}k_F a_s + \frac{4(11-2\ln 2)}{15\pi^2}(k_F a_s)^2 + \cdots . \tag{35}$$

The first-order term is the Hartree term while the second-order contributions have the same form as those obtained by Huang, Yang, and Lee and by Galitskii [24,25] for the dilute Fermi gas, except that in our case $a_s<0$.

It is worth commenting that, although it is customary to think of the Hartree term as a "mean field shift," it arises in our approach as the first term in the *fluctuation* correction to the saddle-point thermodynamic potential in the BCS limit. This is also seen clearly from Fig. 10 in Appendix D where the first diagram is clearly the Hartree term. Once we move away from the BCS limit toward unitarity, the Gaussian fluctuation contribution is still well defined even in absence of a small parameter, however a "Hartree term" becomes hard to identify.

In Fig. 6 we plot the energy per particle as well as the chemical potential as function of interaction in the BCS regime: $-2<(k_F a_s)^{-1}<-1$. We have also included the mean-field result and the asymptotic values given by Eqs. (34) and (35). As we can see, quantum fluctuations reduce the energy and the chemical potential in a way that is consistent with the corrections obtained from our analysis.

In order to calculate the speed of sound, one needs to look at the slope of the pole dispersions, which in a superfluid is given by $c=\sqrt{\rho_s/\kappa}$, where ρ_s is the superfluid density and $\kappa = m\partial n/\partial\mu$ is the compressibility of the system. In a homogeneous system, Galilean invariance implies that $\rho_s=n$ at $T=0$. Keeping only the Hartree term in the formula for the chemical potential, we obtain to linear order in the scattering length $c_s=v_f/\sqrt{3}\left(1+\frac{1}{\pi}k_f a_s\right)$, which was first obtained for BCS superconductors by Anderson [35].

We conclude this section with a comment on the Gorkov–Melik-Barkhudarov correction [36] which enters the preexponential factor in the BCS expression for the gap. It arises from the renormalization of the effective attraction by particle-hole excitations in the medium. Such effects are *not* accounted for in our theory which effectively considers only particle-particle channel diagrams. At the present time we do not know of any theory which recovers this correction in the extreme BCS limit and shows how this correction evolves through unitarity.

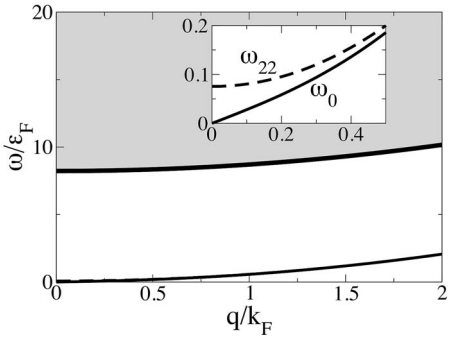

FIG. 7. Spectrum of excitations which contribute to the Gaussian correction to the thermodynamic potential (27). The results shown correspond to the BEC regime with $1/(k_F a_s)=2$ with $\mu=-3.967\epsilon_F$ and $\Delta_0=1.025\epsilon_F$. The full line shows the collective mode dispersion $\omega_0(q)$ (pole of $1/\mathrm{Det}\,\mathbf{M}$) and the shaded region is the two-particle continuum (branch cut). The dashed line $\omega_{22}(q)$ are the zeros of M_{22}. We do not show $\omega_{11}(q)$, the zeros of M_{11}, because they coincide with the continuum in the BEC limit. The inset shows the long-wavelength low-energy spectra.

VII. BEC LIMIT: DIMER SCATTERING AND LEE-YANG CORRECTIONS

We next describe in detail the BEC limit solution for $1/k_F a_s \to +\infty$. We will see that the zero-point motion of collective modes entirely dominates over the continuum contribution in the thermodynamic potential. We will find that this leads to two important effects in the BEC limit: first, a reduction of the effective dimer-dimer scattering length relative to its mean-field value of $2a_s$ and second, a Lee-Yang correction to the equation of state of the dilute gas of dimers. While our theory is able to obtain both these effects semiquantitatively, it does not give the exact asymptotic answers. The scattering length for bosonic molecules, or dimers, is found to be $\simeq 0.55a_s$, while the exact solution of the four-body problem yields $0.6a_s$ [27], and the coefficient of the Lee-Yang correction is only 6% smaller than the exact result.

In the BEC limit the chemical potential is large and negative and, to leading order, goes to one half of the binding energy of the molecules: $\mu=-E_b/2$ where $E_b=1/ma_s^2$. The spectrum for collective excitations is shown in Fig. 7 for $1/k_F a_s=2$. The two-particle continuum then sits at a very high energy; at $|\mathbf{q}|=\mathbf{0}$ it begins at an energy of $2\sqrt{|\mu|^2+\Delta_0^2} \approx E_b$. The virtual scattering of the very high energy fermionic excitations makes a negligible contribution to the thermodynamic potential in the molecular BEC limit.

The Gaussian contribution is then entirely dominated by the low-frequency collective mode $\omega_0(q)$, which is the Bogoliubov excitation of the molecular Bose gas, and the mode $\omega_{22}(q)$ coming from the convergence factor. These modes are shown in more detail in the inset of Fig. 7. Note that for $\mu<0$, ω_{11}, the zeros of M_{11}, are pushed to the continuum and do not enter the calculation. The thermodynamic potential then simplifies to $\Omega_g \simeq \frac{1}{2}\Sigma_{\mathbf{q}}[\omega_0(\mathbf{q})-\omega_{22}(\mathbf{q})]$. In the BEC limit the pole always remains below the continuum for all q and the phase space for the zero-point oscillations extend formally to $q=\infty$.

This raises the question: how can we obtain a finite answer for the sum in Ω_g? The dispersion of the pole is given by the standard Bogoliubov expression $\omega_0(\mathbf{q})=\sqrt{c_s^2\mathbf{q}^2+(\mathbf{q}^2/2m_b)^2}$, where $m_b=2m$ is the mass of the bosonic molecule as shown in Ref. [14]. The large $\mathbf{q}$ limit of this dispersion is just the kinetic energy of the bosonic molecule, which should *not* be part of the zero-point motion of the fluctuations. This is exactly where the convergence factors come in. One finds that $\omega_{22}(\mathbf{q}) \to \mathbf{q}^2/2m_b$ for large $\mathbf{q}$ and cancels the contribution of the free boson dispersion. Thus the convergence factor gives rise to manifestly finite results by eliminating the free particle dispersion of the pole spectrum from contributing to the zero-point motion of the phase fluctuations. (See Appendix G for an analogous discussion for the dilute Bose gas.)

We now calculate the leading-order correction to the mean-field thermodynamic potential in the BEC limit, which will in turn determine the effective interaction between the bosonic molecules. The idea is to use an expansion in the small parameter $\Delta_0/|\mu| \ll 1$ in the BEC limit. The calculation is most easily done on the Matsubara axis as detailed in Appendix E. Here we only quote the leading-order result,

$$\Omega_g \simeq -\frac{\alpha}{256\pi}(2m)^{3/2}\frac{\Delta_0^4}{|\mu|^{3/2}}, \tag{36}$$

where we have included the factor of 256π in order to simplify later expressions. The m, Δ_0, and μ dependence can be determined analytically and the dimensionless prefactor $\alpha=2.61$ has to be evaluated by a numerical integration, as shown in Appendix E.

To find the effective scattering length between the molecules we calculate the shift in the bosonic chemical potential as a result of interactions. Toward this end we proceed as follows. We expand the gap equation (14) in powers of $\Delta_0/|\mu| \ll 1$ to recover the Gross-Pitaevskii equation for bosons. We then obtain

$$\frac{1}{a_s}=\sqrt{2m|\mu|}\left(1+\frac{1}{16}\frac{\Delta_0^2}{|\mu|^2}\right). \tag{37}$$

As noted earlier, the leading-order result is $\mu=-1/(2ma_s^2)$. The above result allows us to relate the next order correction in μ to Δ_0. We find

$$\mu=-1/(2ma_s^2)+\delta\mu, \quad \delta\mu=ma_s^2\Delta_0^2/4. \tag{38}$$

Next we determine Δ_0 from the number equation (29). We find

$$n=n_{\mathrm{MF}}-\left(\frac{\partial\Omega_g}{\partial\mu}\right)_{\Delta_0}-\left(\frac{\partial\Omega_g}{\partial\Delta_0^2}\right)_{\mu}\frac{\partial\Delta_0^2}{\partial\mu}, \tag{39}$$

where $n_{\mathrm{MF}}=\Delta_0^2 m^{3/2}/(4\sqrt{2}\pi|\mu|^{1/2})$ is the MF result in the BEC limit. (See Appendix G for an analogous discussion of keeping track of the μ dependence of the saddle point for a dilute Bose gas.) Using Eq. (36) we obtain $\partial\Omega_g/\partial\mu=(\alpha/256\pi)\times(2m)^{3/2}(3/2)\Delta_0^4/|\mu|^{5/2}$ and the last term in Eq. (39) is given by $(\alpha/32\pi)(2m)^{3/2}\Delta_0^2/(|\mu|^{3/2}ma_s^2)$. It is easily seen that $-\partial\Omega_g/\partial\mu \sim (k_F a_s)^3$ and can be neglected in the BEC limit. Now, using $|\mu|=1/(2ma_s^2)$ to leading order, we obtain

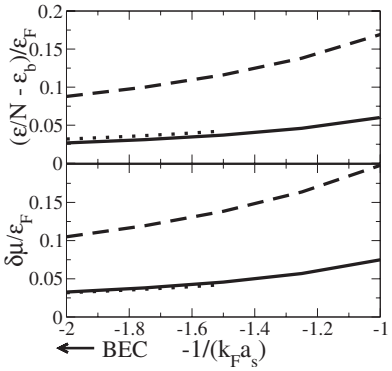

FIG. 8. Energy and chemical potential in the BEC regime, for $(k_F a_s)^{-1}$ between 1 and 2. The solid lines are our calculations including Gaussian fluctuations, the dashed lines the mean-field result, and the dotted lines the leading-order result for a dilute Bose gas with an effective repulsion $a_b=0.6a_s$.

$$\Delta_0^2 = \left(\frac{16}{3\pi}\right)\epsilon_F^2 \frac{1}{k_F a_s}\left(\frac{1}{1+\alpha}\right). \tag{40}$$

This leads to $\delta\mu=(2/3\pi)\epsilon_F k_F a_s[1/(1+\alpha)]$. Comparing the chemical potential for the bosons $\mu_b=2\delta\mu$ with the weakly interacting Bose gas result $\mu_b=4\pi a_b n_b/m_b$ with $n_b=n/2$ and $m_b=2m$, we obtain the effective scattering length for the bosons to be

$$a_b = 2a_s/(1+\alpha) \simeq 0.55a_s, \tag{41}$$

using our numerical result $\alpha=2.61$. This result for a_b is identical with the one obtained by Hu *et al.* [19]; see Sec. X for further discussion.

Going beyond the leading-order term we find that the next-order correction to the chemical potential is of order $(n_b a_b^3)^{1/2}(n_b a_b/m_b)$, which has the same form as the Lee-Yang corrections for a weakly repulsive Bose gas [25]. To see this we analyze our numerical results for Ω in the BEC limit as follows. Scaling out energies with $1/(2ma_s^2)$ and lengths with a_s, we find that we can fit Ω_g to the functional form $\Omega_g=(1/2ma_s^2)a_s^{-3}[A(\tilde{\delta\mu})^2+B(\tilde{\delta\mu})^{5/2}+\cdots]$ where $\tilde{\delta\mu}=2ma_s^2\mu-1$. Solving for the molecular chemical potential $\mu_b=2\delta\mu$ we obtain

$$\mu_b = \frac{4\pi n_b a_b}{m_b}\left(1+\gamma\frac{32}{3\sqrt{\pi}}(n_b a_b^3)^{1/2}+\cdots\right), \tag{42}$$

where we find that the coefficient $\gamma=0.94$ is 6% smaller than the Lee-Yang result $\gamma=1$ (see Appendix G).

In Fig. 8 we show the total energy and the chemical potential for interactions in the BEC regime $1<1/k_F a_s<2$. For comparison we also show the mean-field results (dashed lines) and the leading-order result for a gas of bosons interacting with $a_b=0.6a_s$ (dotted lines).

VIII. UNITARITY

At unitarity $(1/k_F a_s=0)$, there is no small parameter and the problem can only be solved numerically. At this point both the pole and the continuum corrections are of comparable magnitude in the thermodynamic potential. We present the results for the gap, chemical potential, ground-state energy, and the speed of sound and compare with quantum Monte Carlo and experimental results in Table I.

At unitarity $|a_s|$ diverges and this leads to the concept of universality, i.e., all energies scale with the Fermi energy ϵ_F and all lengths scale with k_F^{-1}. A consequence of universality is the relation between the ground-state energy per particle and the chemical potential $\mu=(5/3)(\mathcal{E}/N)$, which acts as a check on our numerical calculation. The ground-state energy is generally written in terms of the noninteracting energy $\mathcal{E}/N=(1+\beta)3\epsilon_F/5$. (Note that in this section β is used to denote the universal interaction correction to the ground-state energy, and *not* the inverse temperature.) We obtain a numerical value of $\beta=-0.598(1)$. The mean-field theory gives $\beta=-0.41$ [14], while quantum Monte Carlo methods give a β of -0.56 [17]. The experimentally obtained values range from -0.68 to -0.49 [8–10]. We thus see that at unitarity the Gaussian quantum fluctuations—zero-point motion of collective modes and virtual quasiparticle scattering—account for most of the difference between the exact ground-state energy (i.e., that obtained from QMC or experiments) and the simple mean-field estimate.

The speed of sound is obtained from the dispersion of the pole $\omega=c_s|\mathbf{q}|$ at small momenta, or alternatively in our theory from Eq. (31). However, we can also calculate the speed of sound once we know the equation of state. Using that $\partial\mu/\partial n=(2\mu)/(3n)$, we arrive at the expression $c_s/v_F=\sqrt{(1+\beta)/3}$. Our theory predicts a speed of sound at unitarity of $c_s=0.37\ v_F$, using either one of the mentioned methods. For comparison, the answer [14] obtained by using the mean-field gap and chemical potential is $0.44v_F$. The quantum Monte Carlo estimate is $c_s=0.38v_F$, while the experimentally measured value of the speed of sound at unitarity is $0.38v_F$ [37].

We also show in the last column of Table I various gap estimates. The inclusion of fluctuations reduces the value of Δ_0 relative to the MF estimate. As already noted above, Δ_0 continues to determine the energy gap $E_g=\Delta_0$ for $\mu>0$, so long as we ignore the feedback of the fluctuations on the single-particle propagator. We do not include an experimental value for the energy gap as we believe that it is not clear how to quantitatively extract this from rf spectroscopy data, taking into account the interactions between atoms in the final and initial states [38].

IX. SELF-CONSISTENT FEEDBACK OF GAUSSIAN FLUCTUATIONS ON THE SADDLE POINT

In this section we describe how one can include the feedback of the Gaussian fluctuations on the saddle-point equation in a self-consistent manner. We show here that it is straightforward to accomplish this using a fluctuation formalism similar to the one used in Sec. IV. However, one finds, quite generally, that Goldstone's theorem is violated if one uses such a Cartesian representation for the fluctuations, as soon as one modifies the saddle point equation. We next show that a polar representation of the fluctuations in terms of the amplitude and phase of the auxiliary field allows one

to recover the Goldstone mode, even when the saddle point condition is modified away from its mean-field form. There is still a problem with obtaining an ultraviolet convergent expression for the thermodynamic potential in terms of the fluctuations. The polar representation respects Goldstone's theorem at low energies but has unacceptable high-energy properties, while the Cartesian representation violates Goldstone in the infrared but is well controlled in the ultraviolet. We thus construct a hybrid representation which interpolates between the polar in the infrared and the Cartesian in the ultraviolet, and compute the thermodynamic potential. In the end, we are not convinced from the solutions of the new gap and number equations that the self-consistent theory is worth the effort. In fact we find results which are not an improvement relative to those presented in Sec. VIII at unitarity and the theory has problems in the BEC limit.

Formally the calculation proceeds in much the same way as in Sec. IV with one important difference. We again write $\Delta(x)=\Delta_0+\eta(x)$, where Δ_0 is a real number, which is the $(\mathbf{x},\tau)$-independent part of $\Delta(x)$, and $\eta(x)$ are the complex fluctuations about it. We call this the Cartesian representation of fluctuations to be contrasted with the polar representation to be introduced below. The main difference with Sec. IV is this: Here Δ_0 does *not* follow the mean-field gap equation and its value will be determined only *after* including the effect of fluctuations, as explained in detail below. In this sense, the η's are *not* the fluctuations about the mean-field saddle point, but rather about a uniform static value Δ_0 which will be determined self-consistently *after* integrating out the fluctuations.

We again find that to order η^2 we obtain the action $S_\Delta=S_0+S_g+\cdots$ where S_0 has the mean-field–like form (12) even though Δ_0 is *not* set to its mean-field value. The Gaussian piece too has the same form as Eq. (20). We emphasize that there is *no linear term* in η in Eq. (19), despite the fact that we are not expanding around a saddle point. The reason for the absence of a linear term is that such a term would be proportional to $\eta(q=0)$. However, $\eta(q=0)\equiv 0$ since the uniform $(\mathbf{q}=\mathbf{0})$ static $(iq_l=0)$ piece of $\Delta(q)$ is described by the (as yet undetermined) Δ_0.

Integrating out the Gaussian fluctuations, we obtain

$$Z \simeq \int d\Delta_0 \int D\eta D\eta^\dagger \exp(-S_0 - S_g) \tag{43}$$

$$= \int d\Delta_0 \exp[-S_{\text{eff}}(\Delta_0)] \tag{44}$$

with the effective action

$$S_{\text{eff}} = S_0 + (1/2)\sum_{\mathbf{q},iq_l} \ln \text{Det}\, \mathbf{M}(q), \tag{45}$$

where S_0 was defined in Eq. (12) [39]. Using the convergence factors described in Sec. IV and Appendix B we obtain the final result

$$\frac{S_{\text{eff}}}{\beta} = \frac{\Delta_0^2}{g} - \frac{1}{\beta}\sum_{\mathbf{k},ik_n} \text{tr} \ln \mathbf{G}_0^{-1}(k) + \frac{1}{2\beta}\sum_{\mathbf{q},iq_l} \ln\left[\frac{\mathbf{M}_{11}(q)}{\mathbf{M}_{22}(q)} \text{Det}\, \mathbf{M}(q)\right] e^{iq_l 0^+}. \tag{46}$$

The parameters Δ_0 and μ are then fixed by solving the gap equation given by

$$\delta S_{\text{eff}}/\delta\Delta_0 = \delta S_0/\delta\Delta_0 + \delta S_g/\delta\Delta_0 = 0 \tag{47}$$

and the number equation given by

$$n = -\partial\Omega/\partial\mu = -\partial[S_0/\beta]/\partial\mu - \partial[S_g/\beta]/\partial\mu. \tag{48}$$

The theory developed above has a serious problem: there is no zero-energy Goldstone mode in the system. To see this recall Eq. (30) for Det $\mathbf{M}(0,0)$ (which continues to be valid here). We immediately see Det $M(\mathbf{q}=\mathbf{0},\omega=0)\neq 0$ unless $1/g=-\Sigma_{\mathbf{k}}\text{Det}\,\mathbf{G}$. The last condition is however the *mean-field* gap equation which is *not* satisfied by solutions Δ_0 and μ of the self-consistent gap equation (47) and the number equation (48). We thus see that in the Cartesian representation, the Goldstone mode is lost as soon as one moves away from the mean-field saddle point.

A. Amplitude and phase fluctuations in the self-consistent theory

How can we restore the gapless Goldstone mode in a self-consistent Gaussian calculation? This can be achieved by using a *polar* representation for the fluctuations in terms of amplitude and phase:

$$\Delta(x) = \Delta_0[1+\lambda(x)]e^{i\theta(x)} \tag{49}$$

in place of the Cartesian representation $\Delta(x)=\Delta_0+\eta(x)$ used above. We will first show that the phase excitations $\theta(x)$ are necessarily gapless in the long-wavelength limit, even when the saddle point shifts away from the mean-field value. However, we will find that there is a price to pay for obtaining the correct low-energy, small-$|\mathbf{q}|$ physics. The high-energy large-$|\mathbf{q}|$ behavior of the amplitude-phase fluctuation propagator has unphysical properties, and finally we will be forced to an interpolation scheme between the polar representation at low energies and the Cartesian representation at high energies.

Working with the amplitude $\lambda(x)$ and phase $\theta(x)$ we obtain

$$Z = \int d\Delta_0 \int D\lambda D\theta J \exp(-S_{\Delta_0,\lambda,\theta}). \tag{50}$$

A detailed derivation of the results stated here is given in Appendix F. As shown there, the action is the sum of two terms

$$S_{\Delta_0,\lambda,\theta} = S_0 + \tilde{S}_g, \tag{51}$$

where S_0 defined in Eq. (12) has the mean-field form, and the Jacobian J of the transformation is approximated by

$$J = \prod_{\mathbf{r},\tau} \Delta_0^2. \tag{52}$$

This is the same approximation used in Sec. IV a of [40]. We will see later that the contribution from J is exactly canceled by another contribution [see below Eq. (55)].

The Gaussian term $\tilde{S}_g$ can be written as

$$\tilde{S}_g = \frac{1}{2}\sum_q (\lambda^*(q), \theta^*(q))\mathbf{D}\begin{pmatrix}\lambda(q)\\ \theta(q)\end{pmatrix}. \tag{53}$$

We use the notation $\tilde{S}_g$ here to distinguish it from the Gaussian action S_g in the Cartesian case (20). The inverse fluctuation propagator $\mathbf{D}$ is given by

$$\mathbf{D}_{11} = \frac{\Delta_0^2}{g} + \frac{\Delta_0^2}{2}\sum_{\mathbf{k},ik_n} \mathrm{tr}\, \mathbf{G}_0(k)\sigma_1\mathbf{G}_0(k+q)\sigma_1,$$

$$\mathbf{D}_{22} = \frac{q^2}{8m}\sum_{\mathbf{k},ik_n} \mathrm{tr}\, \mathbf{G}_0(k)\sigma_3 + \frac{1}{8}\mathrm{tr}\, \mathbf{G}_0(k)(iq_l\sigma_3 - \delta\xi)\mathbf{G}_0(k+q) \times (iq_l\sigma_3 - \delta\xi),$$

$$\mathbf{D}_{12} = \frac{i\Delta_0}{4}\sum_{\mathbf{k},ik_n} \mathrm{tr}\, \mathbf{G}_0(k)(iq_l\sigma_3 - \delta\xi)\mathbf{G}_0(k+q)\sigma_1,$$

$$\mathbf{D}_{21} = -\mathbf{D}_{12} \tag{54}$$

where the Pauli matrices σ_i operate in Nambu space and $\delta\xi = \xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}} = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}$.

Infrared behavior. The long-wavelength low-energy limit of the amplitude and phase fluctuations described by Eq. (54) have the following properties: (i) $\mathbf{D}_{12}$ $(\mathbf{q}=\mathbf{0}, iq_l=0)=0$, so that the amplitude and phase modes decouple in the $q=0$ limit. (ii) The $\mathbf{D}_{22}(q)|\theta(q)|^2$ term, upon transforming to space-time, has form $\rho_s|\nabla\theta|^2/2 - \kappa(\partial\theta/\partial t)^2 + \cdots$, where ρ_s is the superfluid density and κ the compressibility. In particular, we note that $\mathbf{D}_{22}$ $(\mathbf{q}=\mathbf{0}, iq_l=0)=0$ for any choice of Δ_0 and μ, so that the phase mode is gapless in the long wavelength limit. Thus Goldstone's theorem is respected even when one moves away from the mean-field saddle point, in marked contrast to the case of Cartesian fluctuations.

Now, it would seem that fluctuations in the amplitude-phase representation appear to solve all our problems. It is tempting to argue that one can simply integrate out the λ and θ fields in Eq. (50) and obtain an effective action which is the analog of Eq. (45) with $\Sigma_{\mathbf{q},iq_l} \ln \mathrm{Det}\, \mathbf{M}(q)$ replaced by $\Sigma_{\mathbf{q},iq_l} \ln \mathrm{Det}\, \mathbf{D}(q)$. However the situation is *not* so simple. As we show next, the high-energy behavior of $\mathrm{Det}\, \mathbf{D}(q)$ is such that the required Matsubara sum diverges, and there is no analog of the convergence factors in Eq. (46).

Ultraviolet behavior. We find it useful to rewrite the $\mathbf{D}$ matrix in a form which permits us to better understand its high-energy properties and also to see its relationship to the $\mathbf{M}$ matrix used to describe the fluctuations in the Cartesian representation. Omitting the rather lengthy algebra involved (which is sketched in Appendix F), we find that

$$\mathbf{D}_{11} = \frac{\Delta_0^2}{g} + \frac{\Delta_0^2}{2}\sum_{\mathbf{k},ik_n} [\mathbf{G}^0_{22}\mathbf{G}^{0\prime}_{11} + \mathbf{G}^0_{11}\mathbf{G}^{0\prime}_{22} + 2\mathbf{G}^0_{12}\mathbf{G}^{0\prime}_{12}],$$

$$\mathbf{D}_{22} = \frac{\Delta_0^2}{2}\sum_{\mathbf{k},ik_n} [\mathbf{G}^0_{22}\mathbf{G}^{0\prime}_{11} + \mathbf{G}^{0\prime}_{22}\mathbf{G}^0_{11} - 2\mathbf{G}^0_{12}\mathbf{G}^{0\prime}_{12} - 2\,\mathrm{Det}\,\mathbf{G}^0],$$

$$\mathbf{D}_{12} = -\mathbf{D}_{21} = \frac{i\Delta_0^2}{2}\sum_{\mathbf{k},ik_n} [\mathbf{G}^0_{22}\mathbf{G}^{0\prime}_{11} - \mathbf{G}^0_{11}\mathbf{G}^{0\prime}_{22}], \tag{55}$$

where we have used the notation $\mathbf{G}^0 = \mathbf{G}^0(k)$ and $\mathbf{G}^{0\prime} = \mathbf{G}^0(k+q)$. Note that both the properties discussed below Eq. (54)—the decoupling of the amplitude and phase modes at $q=0$ and the Goldstone theorem—are also evident in the new expression for the $\mathbf{D}$ matrix.

From the expansion of the order parameter field in Eq. (49) to linear order, we see that the fluctuations of the order parameter are of the form $\tilde{\lambda} = \Delta_0\lambda$ and $\tilde{\theta} = \Delta_0\theta$. It is useful to rescale the fluctuation fields to $\tilde{\lambda}$ and $\tilde{\theta}$, so that $\tilde{\mathbf{D}} = \mathbf{D}/\Delta_0^2$. This leads to a factor of $2\ln\Delta_0$ in the action which exactly cancels the factor J in Eq. (52). In this form it is also easier to make connection with the Cartesian η fields, as shown below.

At sufficiently high energy and/or short distance scales, the system must "look normal" (i.e., nonsuperfluid) and the natural variables to describe the fluctuations are the Cartesian η's:

$$\begin{pmatrix}\eta_q\\ \eta^*_{-q}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & +i\\ 1 & -i\end{pmatrix}\begin{pmatrix}\tilde{\lambda}_q\\ \tilde{\theta}_q\end{pmatrix} = \mathbf{W}\begin{pmatrix}\tilde{\lambda}_q\\ \tilde{\theta}_q\end{pmatrix}. \tag{56}$$

In this basis the matrix $\tilde{\mathbf{D}} \to \mathbf{L} = \mathbf{W}\tilde{\mathbf{D}}\mathbf{W}^\dagger$ where

$$\mathbf{L}_{11} = \frac{1}{2}(\tilde{\mathbf{D}}_{22} + \tilde{\mathbf{D}}_{11} - 2i\tilde{\mathbf{D}}_{12}) = \mathbf{M}_{11} - \frac{X}{2},$$

$$\mathbf{L}_{22} = \frac{1}{2}(\tilde{\mathbf{D}}_{22} + \tilde{\mathbf{D}}_{11} + 2i\tilde{\mathbf{D}}_{12}) = \mathbf{M}_{22} - \frac{X}{2},$$

$$\mathbf{L}_{12} = \mathbf{L}_{21} = \frac{1}{2}(\tilde{\mathbf{D}}_{11} - \tilde{\mathbf{D}}_{22}) = \mathbf{M}_{12} + \frac{X}{2}, \tag{57}$$

where the $\mathbf{M}$ matrix was defined in Eqs. (21) and (22) and

$$X = 1/g + \sum_k \mathrm{Det}\, \mathbf{G}_0(k) = 1/g - \sum_{\mathbf{k}} 1/(2E_{\mathbf{k}}). \tag{58}$$

We now see that, insofar as fluctuations about the mean-field saddle point are concerned, the $\mathbf{L}$ and $\mathbf{M}$ matrices are identical. This follows from the fact that $X \equiv 0$ when the saddle-point equation has the mean-field form. (This was the case in the calculation described in Secs. V–VIII, even though Δ_0 and μ did not have their mean-field values.)

Conversely, if we look at fluctuations about a saddle point defined by an equation which does not have the mean-field form—which is the case here—then $X \neq 0$ and the inverse fluctuation propagators $\mathbf{M}$ (directly obtained in the Cartesian representation) and $\mathbf{L}$ (obtained by transformation from the polar $\mathbf{D}$ to the Cartesian representation) necessarily differ. It

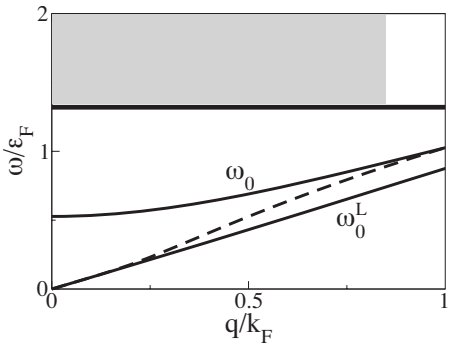

FIG. 9. Spectra used in the self-consistent calculation of Gaussian fluctuations. As explained in the text, the method requires to modify the contribution of the poles of the fluctuation matrix at low energies, from that of the Cartesian representation to that of the amplitude-phase representation. The interpolated values used in the calculation are included in the dashed line.

is only $\mathbf{L}$, derived from a polar representation, that respects Goldstone's theorem. The presence of the X factors which ensure the Goldstone mode in the infrared, however, spoils the ultraviolet behavior of $\mathbf{L}$ and prevents one from obtaining a convergent answer for $\Sigma_{iq_l} \ln \mathrm{Det}\, \mathbf{L}(\mathbf{q}, iq_l)$. The mathematical analysis showing this difficulty is sketched in Appendix E; here we give a simple argument which indicates the problem.

After analytic continuation from $iq_l \to \omega + i0^+$ we find that in the $\omega \to -\infty$ limit, the $\mathbf{L}$ matrix looks schematically like $\mathbf{L}_{22}(\mathbf{q},\omega) \sim -1/a_s + i\sqrt{|\omega|} - X/2 + \cdots$ and $\mathbf{L}_{11}(\mathbf{q},\omega) \sim -1/a_s + \sqrt{|\omega|} - X/2 + \cdots$ and $\mathbf{L}_{12}(\mathbf{q},\omega) \sim |\omega|^{-3/2} + X/2$. (We omit multiplicative constants here in various terms and simply focus on their dependence on a_s, ω, and X.) The presence of the $X/2$ factor in the $\mathbf{L}_{12}$ fundamentally changes its asymptotic behavior from the $\omega^{-3/2}$ in the $\mathbf{M}$ matrix to a constant $X/2$. This leads to convergence problems discussed in Appendix F.

B. Results of the self-consistent calculation

We resolve the problem described above by choosing a scheme that interpolates between the polar representation in the infrared and the Cartesian representation in the ultraviolet. We define an "interpolating" collective mode energy $\omega_0^I(\mathbf{q}) = \omega_0(\mathbf{q}) + f(\mathbf{q})[\omega_0^L(\mathbf{q}) - \omega_0(\mathbf{q})]$ where we choose $f(|\mathbf{q}|) = 1 - \exp(1 - q_c/|\mathbf{q}|)$ for $|\mathbf{q}| < q_c$ and $f(|\mathbf{q}|) = 0$ for $|\mathbf{q}| \geq q_c$, with $q_c = k_F$ (the only scale at unitarity). This formula goes smoothly from $\omega_0^I \simeq \omega_0^L$, the polar result at small q to $\omega_0^I \simeq \omega_0$, the Cartesian result at large q, as shown in Fig. 9. Since the continuum contributions occur at high enough energies (at unitarity) we have left these (Cartesian representation) contributions untouched. Operationally, we implement this by adding the following term into the thermodynamical potential:

$$\delta\Omega_{sc} = \frac{1}{2}\sum_{\mathbf{q}} f(\mathbf{q})[\omega_0^L(q) - \omega_0(\mathbf{q}) - \omega_{22}^L(\mathbf{q}) + \omega_{22}(\mathbf{q}) + \omega_{11}^L(\mathbf{q}) - \omega_{11}(\mathbf{q})]. \tag{59}$$

Using this method and solving the modified gap and number equations (47) and (48) we obtained that at unitarity the chemical potential is $\mu_{sc} = 0.35\epsilon_F$ with a gap of $\Delta_{0,sc} = 0.68\epsilon_F$. These values compare rather unfavorably with the quantum Monte Carlo values as well as the experimentally measured values.

We next show that the self-consistent calculation has serious problems in the BEC limit: the effective interaction between the bosons is attractive and the system is thermodynamically unstable. Clearly this is an artifact of the modified gap equation. In parallel with the analysis in Sec. VII we can show that, just as in Eq. (36), $\Omega_g \simeq -\alpha(2m)^{3/2}\Delta_0^4/|\mu|^{3/2}/(256\pi)$. Although the values of Δ_0 and $|\mu|$ will change because now we are using a modified gap equation, the dimensionless constant α remains the same as before. As shown in Appendix E, it is given by $\alpha = 2.61$. From the new gap equation we can show that Eq. (37) is now modified to

$$\frac{1}{a_s} = \sqrt{2m|\mu|}\left(1 + (1-\alpha)\frac{\Delta_0^2}{16|\mu|^2}\right), \tag{60}$$

from which we find $\mu = -1/(2ma_s^2) + \delta\mu$ with

$$\delta\mu = (1-\alpha)\frac{ma_s^2\Delta_0^2}{4} = -1.61\frac{ma_s^2\Delta_0^2}{4}. \tag{61}$$

Unlike the result (38) for $\delta\mu$ in Sec. VII, we find that the self-consistent calculation yields $\delta\mu < 0$ in the BEC limit. A reduction in μ relative to the noninteracting boson value is equivalent to an effective attraction between the bosons or a negative compressibility.

X. RELATION TO OTHER APPROACHES

We now turn to a discussion of the relation of our work to that of other authors. First, the idea of writing the ground-state energy density of a many-body system in terms of the zero-point motion of collective excitations (plasmons) goes back to early work on the electron gas using the "random phase approximation" (RPA) [41]. The RPA was generalized to the BCS superfluid in the early work of Anderson [35], where the collective mode spectrum and its modification by long-range Coulomb interactions was discussed, but the question of the ground-state energy density was not fully addressed as far as we can see. The inclusion of thermally populated collective excitations was central to the Noziéres–Schmitt-Rink theory of T_c in the BCS-BEC crossover [3,13]. In fact that was the dominant contribution on the BEC side of the crossover. The difference here is that we are looking at quantum corrections about the broken symmetry state where we have to deal with matrix propagators.

Several recent works introduce a small parameter by hand; either by expanding in dimensionality around four or two dimensions [20] or by introducing a large number $2N$ of fermion flavors with a Sp($2N$)-invariant Hamiltonian [21,22]. Our self-consistent calculation in Sec. IX is closely related to the "$1/N$ expansion" approach. At zero order in $1/N$ one obtains the mean-field results and first order in $1/N$ gives the RPA or Gaussian fluctuations. The saddle point is

then recalculated to lowest order in a $1/N$ expansion, with changes in the gap and chemical potential from their MF values obtained perturbatively in $1/N$, which is treated as a small parameter. In practice the calculation is done to first order in $1/N$ (although in principle it could be done to higher order) and N is set equal to unity at the end. On the other hand, we keep $N=1$ throughout the self-consistent calculation. Thus the actual values of the Δ_0 and μ obtained at unitarity, for instance, are quite different in our approach and in the large N approach, even though if one was to set $N=1$ throughout the equations would look the same. One has to be rather careful about how various physical quantities are calculated in the $1/N$ expansion. For example, in the BEC limit we can show that $\mu_b=(4\pi n_b/m_b)2a_s(1-\alpha/N)$, which is negative for $N=1$ and would lead to a negative bulk modulus $\partial\mu_b/\partial n_b$. On the other hand, the more natural quantity to compute in the grand canonical ensemble is the compressibility $\partial n_b/\partial\mu_b$ and this is proportional to $1/a_b=(1+\alpha/N)/(2a_s)$ which is found to be positive even when N is set to unity.

There have been several diagrammatic and field-theoretical approaches to the crossover problem [19,23,42–45]. Our results in Sec. V are essentially the same as the diagrammatic approach of Hu, Liu and Drummond [19], although the derivations are somewhat different. In particular, in the diagrammatic approach the form of the gap equation was unchanged for convenience and only the thermodynamic potential was altered. In our functional integral framework we can justify this as a natural approximation, and, in Sec. IX we go beyond this approximation and discuss the problems of self-consistently including the feedback of Gaussian fluctuations in the gap equation.

The problems that we uncover in the self-consistent approach give insight into the conserving approximation scheme used by Haussmann *et al.* [23]. They too find that, within their approach, as soon as one changes the gap equation from its mean-field–like form, one has problems with Goldstone's theorem. They fix this problem by simply redefining the scattering length in an *ad hoc* manner to impose Goldstone's theorem. Our approach is fundamentally different, as it is based on the observation that the Goldstone mode is associated with the presence of soft phase modes in the superfluid phase, amenable to an amplitude-phase decomposition.

XI. CONCLUSIONS

To conclude, we have studied in this paper the BCS-BEC crossover in an attractive Fermi gas at $T=0$ which is relevant to experiments on ultracold gases with a wide Feshbach resonance. We have gone beyond the mean-field approximation and included the effects of quantum fluctuations at the Gaussian level. There is no small parameter which controls this calculation, as we have *not* introduced a parameter such as dimensionality $(4-\epsilon)$ or number of Fermion species $2N$. Instead we have attempted to see whether there is an approximation scheme which can capture the known physics in both the BCS and BEC limits and in addition interpolate between them through unitarity.

In summary:

(1) We include the effect of quantum fluctuations which go beyond mean-field theory using a functional integral approach at $T=0$. We find that at the Gaussian level these fluctuations are the zero-point motion of the collective modes and the virtual scattering of fermionic quasiparticles.

(2) In the BCS limit, the virtual scattering of quasiparticles dominates the Gaussian correction and leads to Fermi-liquid corrections to the ground-state properties.

(3) In contrast, in the BEC limit the zero-point oscillations dominate the correction term. We can obtain an approximate understanding of the renormalization of the effective repulsion between molecular bosons and recover the Lee-Yang form for the quantum depletion.

(4) At unitarity we find that both collective modes and quasiparticle scattering contribute to the thermodynamic potential. Our results are in good agreement with both quantum Monte Carlo and experimental results.

(5) We discuss in Sec. IX the problems of self-consistently including the feedback of fluctuations into the gap equation. Although the problem of imposing a gapless Goldstone mode is solved by going to the amplitude-phase representation for the fluctuations, there are still some unsatisfactory aspects to the calculation. One is the somewhat *ad hoc* manner in which the ultraviolet divergences have to be regulated by interpolating between the polar and Cartesian representations. The results are not quantitatively superior to the simpler approach at unitarity and there is the further problem of thermodynamic instability in the BEC limit. In conclusion, we feel it is best to not modify the gap equation by feeding back the Gaussian fluctuations and to stick to the simpler set of equations dealt with in Secs. V–VIII.

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APPENDIX A: MEAN-FIELD THEORY

We review the derivation of the mean-field gap and number equations with special attention to convergence factors, which will play a central role in a more complicated setting later on (see Appendix B).

The saddle-point equation $\delta S_0/\delta\Delta_0=0$, with S_0 given by Eq. (12), leads to the MF gap equation

$$\frac{2\Delta_0}{g}=\frac{1}{\beta}\sum_{\mathbf{k},ik_n}\mathrm{Tr}\,\mathbf{G}_0(k)\frac{\partial\mathbf{G}_0^{-1}(k)}{\partial\Delta_0}. \tag{A1}$$

The Nambu Green's function

$$\mathbf{G}_0(k)=\frac{1}{(ik_n)^2-E_{\mathbf{k}}^2}\begin{pmatrix} ik_n+\xi_{\mathbf{k}} & -\Delta_0 \\ -\Delta_0 & ik_n-\xi_k \end{pmatrix} \tag{A2}$$

is the inverse of $\mathbf{G}_0^{-1}(k)$ defined in Eq. (13). Doing the Matsubara sum we obtain

$$\frac{1}{g} = -\frac{1}{\beta}\sum_{\mathbf{k},ik_n}\frac{1}{(ik_n)^2 - E_{\mathbf{k}}^2} = \sum_{\mathbf{k}}\frac{1-2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}}. \tag{A3}$$

To obtain the final result (14), we set the Fermi function $f(E_{\mathbf{k}})=0$ at $T=0$ in the equation above, and use Eq. (3) to take the infinite Λ limit and eliminate the coupling g in favor of the s-wave scattering length a_s.

Evaluating $n=-\partial\Omega_0/\partial\mu$ with $\Omega_0=S_0/\beta$ we obtain

$$n = \frac{1}{\beta}\sum_{\mathbf{k},ik_n}[\mathbf{G}_{11}^0(k) - \mathbf{G}_{22}^0(k)]. \tag{A4}$$

The Matsubara sum is formally divergent and we must introduce *convergence factors*. These factors arise because we need to calculate the equal time limit of $\mathbf{G}_{11}^0(\mathbf{k},\tau) = -\langle Tc_{\mathbf{k}\uparrow}(\tau)c^{\dagger}_{\mathbf{k}\uparrow}(0)\rangle$ and $\mathbf{G}_{22}^0(\mathbf{k},\tau) = -\langle Tc^{\dagger}_{\mathbf{k}\downarrow}(\tau)c_{\mathbf{k}\downarrow}(0)\rangle$ to obtain $n_{\mathbf{k}\uparrow}=\mathbf{G}_{11}^0(\mathbf{k},\tau\to 0^-)$ and $n_{\mathbf{k}\downarrow}=-\mathbf{G}_{22}^0(\mathbf{k},\tau\to 0^+)$. We thus rewrite Eq. (A4) as

$$n = \frac{1}{\beta}\sum_{\mathbf{k},ik_n}[\mathbf{G}_{11}^0(k)e^{ik_n0^+} - \mathbf{G}_{22}^0(k)e^{-ik_n0^+}], \tag{A5}$$

and evaluate Σ_{ik_n} as a contour integral in the complex z plane, with $ik_n\to z$. The Fermi factors $f(z)=1/(e^{\beta z}+1)$ ensure convergence for $z\to+\infty$. For $z\to-\infty$, e^{z0^+} leads to the convergence of the first term, but the second term is divergent. To convert the offending $e^{-ik_n0^+}$ in Eq. (A5) to the desired $e^{ik_n0^+}$, we exploit the fact that the sum is over both positive and negative k and even under $k\to-k$, since $\mathbf{G}_{22}^0(-k)=-\mathbf{G}_{11}^0(k)$ from Eq. (A2). Thus

$$n = 2\sum_{\mathbf{k},ik_n}\mathbf{G}_{11}^0(k)e^{ik_n0^+} = \sum_{\mathbf{k}}\left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\tanh(\beta E_{\mathbf{k}}/2)\right]. \tag{A6}$$

The final result going from (A4) to (A6) could have been simply obtained by physical reasoning. The only point of going through the convergence factors in detail here is that it will streamline the discussion in Appendix B.

APPENDIX B: CONVERGENCE FACTORS FOR BOSE MATSUBARA SUMS

In this appendix, we collect useful results for the asymptotic expansion of $\mathbf{M}_{ij}$ for large frequencies and show that the integral of the phase $\delta(\mathbf{q},\omega)$ of $\mathrm{Det}\,\mathbf{M}(\mathbf{q},\omega+i0^+)$ diverges for large negative ω. This forces us to introduce convergence factors to obtain a finite answer for the thermodynamic potential, leading us from the formal expression (25) to the convergent result (26).

We use Eqs. (21) and (22) to find the large q_l expansion valid for $q_l \gg \max(\Delta_0,|\mu|)$. By neglecting the dependence on Δ_0 and μ we obtain

$$M_{11}(\mathbf{q},iq_l) = M_{22}(\mathbf{q},-iq_l) \simeq -\frac{m}{4\pi a_s} + \sum_{\mathbf{k}}\left(\frac{1}{iq_l - \epsilon_{\mathbf{k}+\mathbf{q}/2} - \epsilon_{\mathbf{k}-\mathbf{q}/2}} + \frac{1}{2\epsilon_{\mathbf{k}}}\right) = -\frac{m}{4\pi a_s} + (m^{3/2}/4\pi)\sqrt{\epsilon_{\mathbf{q}}/2 - iq_l}, \tag{B1}$$

where $\epsilon_{\mathbf{q}}=\mathbf{q}^2/2m$. For the slightly more restrictive case when q_l further satisfies $q_l \gg \epsilon_{\mathbf{q}}/2$, we obtain

$$M_{12} = \Delta_0^2 m^{3/2} q_l^{-3/2}/(2\sqrt{2}\pi). \tag{B2}$$

On the real frequency axis, we are interested in large negative ω [at $T=0$, the positive frequency contributions go to zero due to the Bose occupation factors $n_B(\omega)$]. With $|\omega| \gg \max(\Delta_0,|\mu|)$ we find

$$\mathbf{M}_{11}(\mathbf{q},\omega) = -\frac{m}{4\pi a_s} + \frac{m^{3/2}}{4\pi}\sqrt{|\omega| + \epsilon_{\mathbf{q}}/2} + iO(|\omega^{-7/2}|),$$

$$\mathbf{M}_{22}(\mathbf{q},\omega) = -\frac{m}{4\pi a_s} + i\frac{m^{3/2}}{4\pi}\sqrt{|\omega| - \epsilon_{\mathbf{q}}/2}. \tag{B3}$$

Here the imaginary part of $\mathbf{M}_{11}$ comes from just the first term in the sum in Eq. (21), for which the branch cut appears on the negative real frequency line. Using the slightly more restrictive condition $|\omega| \gg \epsilon_{\mathbf{q}}/2$

$$\mathbf{M}_{12}(\mathbf{q},\omega) = -\frac{\Delta_0^2 m^{3/2}}{4\pi}|\omega|^{-3/2}(1+i). \tag{B4}$$

Thus in the limit of large and negative ω we can neglect $\mathbf{M}_{12}$ and go to the leading order

$$\mathrm{Det}\,\mathbf{M} \simeq -\frac{m^{5/2}}{16\pi^2 a_s}\sqrt{|\omega|} + i\frac{m^3}{16\pi^2}|\omega|. \tag{B5}$$

The phase is given by $\mathrm{Im}\ln\mathrm{Det}\,\mathbf{M}=\delta\approx\tan^{-1}(a_s\sqrt{m|\omega|}) \approx \pi/2$ as $\omega\to-\infty$. Thus the Matsubara sum in Eq. (25) is divergent.

We next turn to the derivation of the convergence factors in Eq. (26) and how they lead to finite results. We begin with looking at the sum on Matsubara frequencies for a fixed $\mathbf{q}$,

$$\sum_{iq_l}\ln\mathrm{Det}\,\mathbf{M}(q) = \sum_{iq_l}\left[\ln\mathbf{M}_{11} + \ln\mathbf{M}_{22} + \ln\left(1 - \frac{\mathbf{M}_{12}^2}{\mathbf{M}_{11}\mathbf{M}_{22}}\right)\right] \tag{B6}$$

and show that the first two terms should be written as $\Sigma_{iq_l}[\ln\mathbf{M}_{11}e^{iq_l0^+} + \ln\mathbf{M}_{22}e^{-iq_l0^+}]$, while the third term does not need a convergence factor. We can rewrite Eq. (21) as

$$\mathbf{M}_{11}(q) = \mathbf{M}_{22}(-q) = \frac{1}{g} + \sum_{\mathbf{k},ik_n}\mathbf{G}_{22}^0\mathbf{G}_{11}^{0\prime}, \tag{B7}$$

with $\mathbf{G}^0=\mathbf{G}^0(k)$ and $\mathbf{G}^{0\prime}=\mathbf{G}^0(k+q)$. We then expand the logarithm in powers of g so that $\Sigma_q\ln\mathbf{M}_{22}=\Sigma_q[\ln(1/g) + g\Sigma_k\mathbf{G}_{22}^0\mathbf{G}_{11}^{0\prime}+\cdots]$. Using the argument given in Appendix A below Eq. (A4), we see that the *equal time limit* requires that $\mathbf{G}_{22}$ carries a factor of e^{-i-0^+} and $\mathbf{G}_{11}'$ a factor of $e^{i(k_n+q_l)0^+}$. We

thus see that order by order in g each term in $\ln \mathbf{M}_{22}$ comes with a factor of $e^{-iq_l 0^+}$ and $\ln \mathbf{M}_{11}$ comes with $e^{+iq_l 0^+}$. We also note that, using this prescription, $\mathbf{M}_{12}(q)=\mathbf{M}_{21}(q)=\Sigma_{\mathbf{k},ik_n}\mathbf{G}^0_{12}\mathbf{G}^{0\prime}_{12}$ does not acquire a convergence factor and, in fact, none is needed.

The Matsubara sum Σ_{iq_l} is converted to a standard contour integral. Convergence for $z\to+\infty$ is guaranteed by the Bose function $n_B(z)=1/(e^{\beta z}-1)$. For $z\to-\infty$, convergence is ensured by converting the problematical factor of $e^{-iq_l 0^+}$ into the convergence factor $e^{iq_l 0^+}$, following the same reasoning as in Appendix A. Using the fact that the sum is over both positive and negative q and $\mathbf{M}_{22}(q)=\mathbf{M}_{11}(-q)$ [see Eq. (21)] we obtain

$$\sum_{iq_l} \ln \mathrm{Det}\, \mathbf{M}(q) = \sum_{iq_l}\left[2\ln \mathbf{M}_{11}e^{iq_l 0^+} + \ln\left(1-\frac{\mathbf{M}_{12}^2}{\mathbf{M}_{22}\mathbf{M}_{11}}\right)\right] = \sum_{iq_l} \ln\left(\frac{\mathbf{M}_{11}\mathrm{Det}\,\mathbf{M}}{\mathbf{M}_{22}}\right)e^{iq_l 0^+}, \tag{B8}$$

which is exactly the expression in Eq. (26).

We finally show explicitly that the Matsubara sum in Eq. (B8) is convergent. The Matsubara sum in Eq. (B8) can be written as the contour integral $\oint_{\mathcal{C}} dz/(2\pi i) n_B(z)\ln[\mathbf{M}_{11}(\mathbf{q},z)\mathrm{Det}\,\mathbf{M}(\mathbf{q},z)/\mathbf{M}_{22}(\mathbf{q},z)]$, where $\mathcal{C}$ runs on either side of the imaginary z axis, enclosing it counterclockwise. We distort the contour to run above and below the real axis and at $T=0$ obtain for the thermodynamic potential

$$\Omega_g = -\frac{1}{2}\sum_{\mathbf{q}}\int_{-\infty}^{0}\frac{d\omega}{\pi}[\delta(\mathbf{q},\omega)+\delta_{11}(\mathbf{q},\omega)-\delta_{22}(\mathbf{q},\omega)], \tag{B9}$$

where $\delta(\mathbf{q},\omega)=\mathrm{Im}\ln\mathrm{Det}\,\mathbf{M}(\mathbf{q},\omega+i0^+)$ and δ_{11} and δ_{22} are the corresponding phases for $\mathbf{M}_{11}$ and $\mathbf{M}_{22}$.

From the leading order expression for $\mathbf{M}_{11}$ in Eq. (B3), we see that for large negative ω, $\delta_{11}\sim|\omega|^{-4}$ and hence that term is convergent. To look at $\delta-\delta_{22}$, we recognize that this is the phase of $\mathrm{Det}\,\mathbf{M}/\mathbf{M}_{22}=\mathbf{M}_{11}-\mathbf{M}_{12}^2/\mathbf{M}_{22}$. Now for large negative ω, $\mathbf{M}_{12}^2/M_{22}\sim|\omega|^{-7/2}+i|\omega|^{-4}$ and can be neglected in comparison to $\mathbf{M}_{11}$. Thus the integrand in Eq. (B9) reduces to $2\delta_{11}$ and we obtain a convergent answer.

APPENDIX C: NUMERICAL EVALUATION OF BOSE MATSUBARA SUMS

While the real frequency representation of Eq. (26) gives physical insight into the deviations away from mean-field theory, it is numerically simpler to do the calculation on the imaginary frequency axis. On the real axis one encounters principal part singularities analogous to the ones encountered, e.g., in the normal-state calculations of Ref. [46] but further complicated by the broken symmetry in the superfluid state.

If one wants to use Eq. (26) on the Matsubara axis, one needs to explicitly take into account the convergence factor $e^{+iq_l\tau}$ and take the limit $\tau\to 0^+$ at the end. Here we outline an alternative procedure which simplifies the numerics. Let us begin by looking at a part of $\mathbf{M}_{11}(\mathbf{q},z)$

$$\mathbf{M}_{11}^C(q) = \frac{1}{g}+\sum_{\mathbf{k}}\frac{u^2u'^2}{iq_l-E-E'} = \mathbf{M}_{22}^C(-q),$$

which has no singularities (poles, branch cuts) or zeros in the left-half plane ($\mathrm{Re}\, z<0$). Since we will use this to obtain convergent results we call it $\mathbf{M}_{11}^C$ and $\mathbf{M}_{22}^C$.

We may write the $\mathbf{M}_{11}$ piece of Eq. (B8) as

$$\sum_{iq_l} 2\ln \mathbf{M}_{11}e^{iq_l 0^+} = \sum_{iq_l} 2[\ln(\mathbf{M}_{11}/\mathbf{M}_{11}^C)+\ln \mathbf{M}_{11}^C], \tag{C1}$$

where we drop $e^{iq_l 0^+}$ on the right because each term is convergent. The Matsubara sum of the second term is seen to be zero at $T=0$ by evaluating it as a standard contour integral and noting that $\ln \mathbf{M}_{11}^C$ has no singularities in the left-half plane. In fact, now we may write the above result in a more symmetrical form as $\Sigma_{iq_l}[\ln(\mathbf{M}_{22}/\mathbf{M}_{22}^C)+\ln(\mathbf{M}_{11}/\mathbf{M}_{11}^C)]$ and combine this with the second term of Eq. (B8) to obtain

$$\sum_q \ln\mathrm{Det}\,\mathbf{M}(q) \to \sum_q \ln\mathrm{Det}\left[\frac{\mathbf{M}(q)}{\mathbf{M}^C(q)}\right], \tag{C2}$$

where the matrix $\mathbf{M}^C(q)$ is a diagonal matrix with the entries $\mathbf{M}_{22}^C(q)$ and $\mathbf{M}_{11}^C(q)$. This expression leads to a rapidly convergent answer, which in the $T=0$ limit can be evaluated as an integral along the imaginary axis in the $iq_l\to z=(x+iy)$ plane with $\beta^{-1}\Sigma_{iq_l}\to\int dy/(2\pi)$.

APPENDIX D: FERMI-LIQUID CORRECTIONS FOR $k_F|a_s|\ll 1$ WITH $a_s<0$

Here we give some details of the argument that shows that the Gaussian corrections to the thermodynamic potential in the extreme BCS limit of the attractive Fermi gas have the same expression as the standard Galitskii and Huang-Lee-Yang theory [24–26] of the repulsive Fermi gases with a sign change in a_s. First we recall the usual Galitskii theory and discuss why it is not directly useful for $a_s<0$. Next, we describe how the BCS limit results of the superfluid state theory developed in the paper are related to those of normal state Galitskii theory.

In the Galitskii theory of the normal Fermi gas the thermodynamic potential Ω is written in terms of the two-particle propagator, which is the sum of particle-particle channel ladder diagrams of Fig. 10. For a repulsive interaction V_0, we find

$$\Omega = \Omega_{\mathrm{free}} + 2\sum_{\ell=1}^{\infty}(-1)^{\ell}\frac{V_0^{\ell}}{\ell}\sum_q\left(\sum_k G_0(-k)G_0(k+q)\right)^{\ell}, \tag{D1}$$

where G_0 is the noninteracting Green's function $G_0(k)=(ik_n-\epsilon_{\mathbf{k}}+\mu)^{-1}$. To make contact with results of our paper, it is useful to sum up the series and write it as

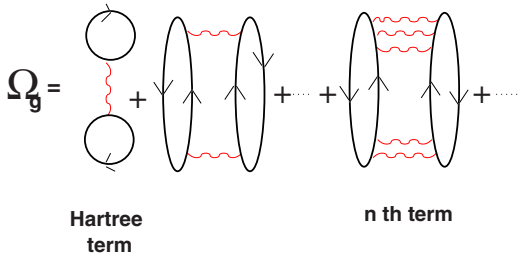

FIG. 10. (Color online) Diagrammatic representation of the Gaussian corrections to thermodynamic potential in the BCS limit. The full lines are fermion propagators and the wave lines represent the attractive interaction. The first diagram corresponds to the Hartree term.

$$\Omega = \Omega_{\text{free}} + 2\sum_q \ln\left(1 - V_0 \sum_k G_0(-k)G_0(k+q)\right). \quad \text{(D2)}$$

The repulsive V_0 can then be replaced by $a_s > 0$ in the usual way using $m/4\pi a_s = 1/V_0 + \Sigma_{\mathbf{q}}\, 1/2\epsilon_{\mathbf{q}}$.

It is well known that the pairing instability of the normal Fermi gas to attractive interactions implies that we *cannot* extend the Galitskii calculation directly to the case of attractive interactions $a_s < 0$. If we were to try and set $V_0 = -g$, the attraction of Eq. (2), we would find that, for small q, there is a pole on the imaginary axis in the *upper-half plane* in addition to a branch cut along the real axis $\omega \geqslant -2\mu + \epsilon_{\mathbf{q}}/2$, as shown in the top panel of Fig. 11. This pole, which occurs at $z \sim +i\epsilon_F \exp(-1/k_f|a_s|)$ for $\mathbf{q}=0$, is the signature of the Cooper pairing instability.

The superfluid state calculation for the attractive Fermi gas discussed in the text of this paper deals with the broken symmetry saddle point which is stable. The two particle propagator $\mathbf{M}^{-1}$ in the superfluid state has a very different analytical structure (lower panel of Fig. 11) compared with the unstable normal state just discussed (upper panel of Fig. 11). As described in Sec. IV below Eq. (26), $\mathbf{M}^{-1}$ has poles at the collective modes frequencies and branch cuts corresponding to the gapped two-particle continuum.

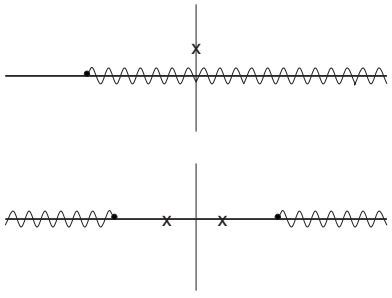

FIG. 11. Analytic structure of two-particle propagators for the attractive Fermi gas. The upper panel correspond to the unstable normal state which has a branch cut for $\omega \geqslant -2\mu + \epsilon_{\mathbf{q}}/2$, representing the continuum of excitations, and a pole on the imaginary axis in the upper-half plane, for small $\mathbf{q}$, which signals the BCS pairing instability. The lower panel shows the analytic structure of $\mathbf{M}^{-1}$ in the stable superfluid state with poles at $\pm\omega_0(\mathbf{q})$, the collective mode frequencies, and branch cuts beginning at $\pm\min(E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{q}})$.

In the BCS limit, $\Delta_0 \to 0$ and the contribution of the zero-point motion of the collective modes to Ω is utterly negligible for phase-space reasons, as discussed in Sec. VI. Thus the two-particle continuum dominates the Gaussian correction to Ω. In the limit $\Delta_0 \to 0$ the branch cut extends over the entire real line, although the appropriate limit of the u_k, v_k factors shows that the phase shift vanishes for $\omega < -2\mu + \epsilon_{\mathbf{q}}/2$. In this sense the continuum contribution to Ω given by $\int_{-\infty}^{-E_c(\mathbf{q})} d\omega \delta(\mathbf{q},\omega)$ may be simplified with the lower limit becoming $-2\mu + \epsilon_{\mathbf{q}}/2$ and the upper limit going to zero.

Now one can check that this continuum contribution is exactly the same as the corresponding continuum contribution of the normal state Galitskii theory, changing the sign of a_s. Note that the singular pole piece does *not* show up in this result. To see that the $\delta(\mathbf{q},\omega)$'s in the two theories are the same, start with the $\mathbf{M}$ matrix of the broken symmetry theory. As $\Delta_0 \to 0$, M_{12} vanishes and $\delta(\mathbf{q},\omega) \simeq 2\,\text{Im}\ln \mathbf{M}_{11} = 2\,\text{Im}\ln[1 - g\Sigma_k G_0(-k)G_0(k+q)]$, and we have used convergence factor tricks to obtain well-defined Matsubara sums. The last expression is the same as the phase shift obtained from the normal-state result above Eq. (D2) with $V_0 \to -g$. We thus conclude that in the $\Delta_0 \to 0$ limit of the superfluid state, the Gaussian correction to Ω is the same as the Galitskii and Huang-Lee-Yang result for the repulsive Fermi gas with sign of a_s changed to $a_s < 0$.

APPENDIX E: THERMODYNAMIC POTENTIAL IN THE BEC LIMIT

Here we briefly sketch how we arrive at the leading-order correction to the thermodynamic potential in the BEC limit, Eq. (36), starting with the results of Appendix C. In the BEC limit, $\mu < 0$ and approaches half the binding energy of the molecules $|\mu| = 1/(2ma_s^2)$. Thus $\Delta_0/|\mu| \ll 1$ and can be used as an expansion parameter. Then one can write $u_{\mathbf{k}}^2 = 1 - \Delta_0{}^2/4\xi_{\mathbf{k}}^2$, $v_{\mathbf{k}}^2 = \Delta_0{}^2/4\xi_{\mathbf{k}}^2$, and $E_{\mathbf{k}} = \xi_{\mathbf{k}} + \Delta_0{}^2/2\xi_{\mathbf{k}}$ with $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} + |\mu|$ to leading order in $\Delta_0/|\mu|$.

Now writing $\mathbf{M}_{11} = \mathbf{M}_{11}^C + \delta\mathbf{M}_{11}$, where $\mathbf{M}_{11}^C$ is defined in Eq. (C1) and

$$\delta\mathbf{M}_{11}(q) = -\sum_{\mathbf{k}} \frac{v^2 v'^2}{iq_l + E + E'} \quad \text{(E1)}$$

one can easily see that $\delta\mathbf{M}_{11} \sim \Delta_0{}^4$, while $\mathbf{M}_{12} \sim \Delta_0{}^2$. Then, to order $\sim\Delta_0{}^4$, the expression in Eq. (C2) gives

$$\Omega_g = \sum_q \text{Re}\left(\frac{\delta\mathbf{M}_{11}}{\mathbf{M}_{11}^C}\right) - \frac{\mathbf{M}_{12}^2}{2|\mathbf{M}_{11}^C|^2}. \quad \text{(E2)}$$

To leading order, $\delta\mathbf{M}_{11} = \Delta_0{}^4/|\mu|^{7/2} F(\mathbf{q}/\sqrt{2m|\mu|}, q_l/|\mu|)$, where $F(\mathbf{Q},Q_l)$ is a dimensionless function given by

$$F(\mathbf{Q},Q_l) = \frac{1}{16}\sum_{\mathbf{K}} \frac{1}{iQ_l + 2 + 2K^2 + Q^2/2} \times \frac{1}{[(\mathbf{K}+\mathbf{Q}/2)^2 + 1]^2[(\mathbf{K}-\mathbf{Q}/2)^2 + 1]^2}. \quad \text{(E3)}$$

Here we use capital letters for dimensionless variables

$\mathbf{Q}=\mathbf{q}/\sqrt{2m|\mu|}$ and $Q_l=q_l/|\mu|$. $\mathbf{M}_{12}=\Delta_0{}^2/|\mu|^{3/2}I(\mathbf{q}/\sqrt{2m|\mu|},q_l/|\mu|)$, where $I(\mathbf{Q},Q_l)$ is a dimensionless function given by

$$I(\mathbf{Q},Q_l)=-\frac{1}{4}\sum_{\mathbf{K}}\frac{2+2K^2+Q^2/2}{Q_l^2+(2+2K^2+Q^2/2)^2}\times\frac{1}{[(\mathbf{K}+\mathbf{Q}/2)^2+1][(\mathbf{K}-\mathbf{Q}/2)^2+1]} \tag{E4}$$

and $\mathbf{M}_{11}^C=\sqrt{|\mu|}H(\mathbf{q}/\sqrt{|\mu|},q_l/|\mu|)$ where $H(\mathbf{Q},Q_l)$ is a dimensionless function given by

$$H(\mathbf{Q},Q_l)=\frac{1}{8\pi}\left(\sqrt{-iQ_l/2+Q^2/4+1}-\frac{1}{\sqrt{2m}a_s\sqrt{|\mu|}}\right)\approx\frac{1}{8\pi}(\sqrt{-iQ_l/2+Q^2/4+1}-1). \tag{E5}$$

Putting all these together, we obtain

$$\Omega_g=\frac{(2m)^{3/2}\Delta_0^4}{4\pi^3|\mu|^{3/2}}\int d^3\mathbf{Q}\int dQ_l\times\left\{\mathrm{Re}\left[\frac{F(\mathbf{Q},Q_l)}{H(\mathbf{Q},Q_l)}\right]-\frac{[I(\mathbf{Q},Q_l)]^2}{2|H(\mathbf{Q},Q_l)|^2}\right\}. \tag{E6}$$

Numerical evaluation of the integral gives $\Omega_g=-\alpha(2m)^{3/2}\Delta_0{}^4/|\mu|^{3/2}/(256\pi)$ with $\alpha=2.61$.

APPENDIX F: THE AMPLITUDE-PHASE ACTION

Starting with $\Delta(x)=\Delta_0[1+\lambda(x)]e^{i\theta(x)}$ [see Eq. (49)] we transform to a gauge where $\Delta(x)$ is real. We transform the fermion fields

$$\tilde{\psi}(x)=\mathbf{U}(x)\psi(x) \tag{F1}$$

with

$$\mathbf{U}(x)=\begin{pmatrix}e^{-i\theta(x)/2} & 0\\ 0 & e^{i\theta(x)/2}\end{pmatrix} \tag{F2}$$

so that the action (7) now reads

$$S_{\tilde{\psi},\Delta}=\int dx\frac{1}{g}|\Delta(x)|^2-\tilde{\psi}^\dagger(x)\tilde{\mathbf{G}}^{-1}(x,x')\tilde{\psi}(x'), \tag{F3}$$

where $\tilde{\mathbf{G}}^{-1}=\mathbf{U}G\mathbf{U}^\dagger$.

We can now write $\tilde{\mathbf{G}}^{-1}=\mathbf{G}_0^{-1}+\tilde{\mathbf{K}}$, where $\mathbf{G}_0^{-1}$ is the (inverse) Nambu Green's function defined by Eq. (8) in $k=(\mathbf{k},ik_n)$ space. The matrix $\tilde{\mathbf{K}}$ is

$$\tilde{\mathbf{K}}(x,x')=\left[\Delta_0\lambda(x)\sigma_1+\frac{i}{2m}\left(\nabla\theta(x)\cdot\nabla+\frac{1}{2}\nabla^2\theta(x)\right)-\left(\frac{i}{2}\partial_\tau\theta(x)+\frac{1}{8m}|\nabla\theta(x)|^2\right)\sigma_3\right]\delta(x-x'), \tag{F4}$$

whose Fourier transform is

$$\tilde{\mathbf{K}}(k',k)=\left[\Delta_0\lambda_q\sigma_1+\frac{i}{2}(iq_l\sigma_3-\delta\xi)\theta_q\right]\delta(k-k'+q)+\frac{1}{8m}\sum_{q_1q_2}q_1\cdot q_2\theta_{q_1}\theta_{q_2}\sigma_3\delta(k-k'-q_1-q_2) \tag{F5}$$

with $\delta\xi=\xi_{\mathbf{k}+\mathbf{q}}-\xi_{\mathbf{k}}$.

Integrating out the fermion fields $\tilde{\psi}$ we obtain the functional integral (50) with the action $S_{\Delta_0,\lambda,\theta}=S_0+\tilde{S}_g$ of Eq. (51). The S_0 piece, defined in Eq. (12), comes from the $\mathbf{G}_0^{-1}$ term; for the J term in (51) see (52). The Gaussian piece, arising from $\tilde{\mathbf{K}}$, is given by

$$\tilde{S}_g=\frac{\Delta_0^2}{g}\lambda_q\lambda_{-q}-\mathrm{Tr}\,\mathbf{G}_0(k)\tilde{\mathbf{K}}(k,k)+\frac{1}{2}\mathrm{Tr}\,\mathbf{G}_0(k)\tilde{\mathbf{K}}(k,k+q)\mathbf{G}_0(k+q)\tilde{\mathbf{K}}(k+q,k). \tag{F6}$$

The Gaussian action of Eq. (53) follows immediately from Eqs. (F5) and (F6), with the $\mathbf{D}$ matrix given by Eq. (54). Our next task is to derive the equivalent expression for the $\mathbf{D}$ matrix (55) which is written purely in terms of $\mathbf{G}^0$, without any $iq_l\sigma_3-\delta\xi$ factors. The case of $\mathbf{D}_{11}$ is simple; there are no such factors to begin with and we only need to evaluate the Nambu trace in Eq. (54) to obtain Eq. (55). In what follows, we use the notation $\mathbf{G}=\mathbf{G}_0(k)$ and $\mathbf{G}'=\mathbf{G}_0(k+q)$, and drop the subscript 0 for notational convenience.

In order to write $\mathbf{D}_{12}$ and $\mathbf{D}_{22}$ in terms of the Green's functions, one needs to express the vertex $iq_l\sigma_3-\delta\xi$ in terms of matrix elements of $\mathbf{G}^{-1}$. It is easy to see that the vertex can be written as

$$iq_l\sigma_3-\delta\xi=\mathbf{V}=\begin{pmatrix}\delta_{11} & 0\\ 0 & -\delta_{22}\end{pmatrix},$$

where $\delta_{11}=\mathbf{G}_{11}'^{-1}-\mathbf{G}_{11}^{-1}$ and $\delta_{22}=\mathbf{G}_{22}'^{-1}-\mathbf{G}_{22}^{-1}$. We will also use the following identities:

$$\mathbf{G}_{22}\mathbf{G}_{22}^{-1}=1-\Delta_0\mathbf{G}_{12},\quad \mathbf{G}_{11}\mathbf{G}_{11}^{-1}=1-\Delta_0\mathbf{G}_{12},$$

$$\mathbf{G}_{12}\mathbf{G}_{22}^{-1}=-\Delta_0\mathbf{G}_{11},\quad \mathbf{G}_{12}\mathbf{G}_{11}^{-1}=-\Delta_0\mathbf{G}_{22}. \tag{F7}$$

By definition we have

$$\mathbf{D}_{12}=\Delta_0\frac{i}{4}\mathrm{Tr}\,\mathbf{G}_0(k+q)\mathbf{V}\mathbf{G}_0(k)\sigma_1=\frac{i\Delta_0}{4}\sum_k\delta_{11}(\mathbf{G}_{11}\mathbf{G}_{12}'+\mathbf{G}_{12}\mathbf{G}_{11}')-\delta_{22}(\mathbf{G}_{12}\mathbf{G}_{22}'+\mathbf{G}_{22}\mathbf{G}_{12}'). \tag{F8}$$

Now using the identities of Eq. (F7), we obtain $\Sigma_k\delta_{11}(\mathbf{G}_{11}\mathbf{G}_{12}'+\mathbf{G}_{12}\mathbf{G}_{11}')=\Sigma_k\Delta_0(\mathbf{G}_{22}\mathbf{G}_{11}'-\mathbf{G}_{11}\mathbf{G}_{22}')$ and a similar result holds for the δ_{22} piece. Adding both terms we obtain $\mathbf{D}_{12}$ of Eq. (55). For $\mathbf{D}_{22}$, one can write

$$\mathbf{D}_{22} = \frac{q^2}{8m}\sum_k (\mathbf{G}_{11} - \mathbf{G}_{22}) + \frac{1}{8}\mathrm{Tr}\,\mathbf{G}_0(k)\mathbf{V}\mathbf{G}_0(k+q)\mathbf{V}. \tag{F9}$$

The second term above can be written as

$$\frac{1}{8}\sum_k \delta_{11}^2\mathbf{G}_{11}\mathbf{G}'_{11} + \delta_{22}^2\mathbf{G}_{22}\mathbf{G}'_{22} - 2\delta_{11}\delta_{11}\mathbf{G}_{12}\mathbf{G}'_{12}.$$

Using the identities in Eq. (F7), we obtain

$$\sum_k \mathbf{G}_{11}\mathbf{G}'_{11}\delta_{11}^2 = \Delta_0^2\sum_k \mathbf{G}_{11}\mathbf{G}'_{22} + \mathbf{G}'_{11}\mathbf{G}_{22} - 2\mathbf{G}_{12}\mathbf{G}'_{12} + 2\Delta_0\sum_k (\mathbf{G}_{12} + \mathbf{G}'_{12}) + \sum_k \mathbf{G}_{11}\mathbf{G}'^{-1}_{11} + \mathbf{G}'_{11}\mathbf{G}^{-1}_{11} - 2$$

and a similar result holds for the δ_{22}^2 piece. For the last term we obtain

$$-2\sum_k \mathbf{G}_{12}\mathbf{G}'_{12}\delta_{11}\delta_{22} = 2\Delta_0^2\sum_k [\mathbf{G}_{11}\mathbf{G}'_{22} + \mathbf{G}'_{11}\mathbf{G}_{22} - 2\mathbf{G}_{12}\mathbf{G}'_{12}] + 2\Delta_0\sum_k (\mathbf{G}_{12} + \mathbf{G}'_{12}).$$

Adding all the terms we obtain

$$\frac{\Delta_0^2}{2}\sum_k \mathbf{G}_{22}\mathbf{G}'_{11} + \mathbf{G}'_{22}\mathbf{G}_{11} - 2\mathbf{G}_{12}\mathbf{G}'_{12} + \frac{3\Delta_0}{2}\sum_k \mathbf{G}_{12} + \frac{1}{8}\sum_k \mathbf{G}_{22}\mathbf{G}'^{-1}_{22} + \mathbf{G}'_{22}\mathbf{G}^{-1}_{22} + \mathbf{G}_{11}\mathbf{G}'^{-1}_{11} + \mathbf{G}'_{11}\mathbf{G}^{-1}_{11} - 4,$$

where we have used $\Sigma_k\mathbf{G}_{12}=\Sigma_k\mathbf{G}'_{12}$. We now use $\mathbf{G}'^{-1}_{11} = \mathbf{G}^{-1}_{11} + iq_l - \delta\xi$ and $\mathbf{G}'^{-1}_{22} = \mathbf{G}^{-1}_{22} + iq_l + \delta\xi$ to write the last term as $-\frac{1}{2}\Delta_0\Sigma_k\mathbf{G}_{12} + \frac{iq_l}{2}(\mathbf{G}_{11}+\mathbf{G}_{22}) - \frac{\delta\xi}{4}(\mathbf{G}_{11}-\mathbf{G}_{22}-\mathbf{G}'_{11}+\mathbf{G}'_{22})$, where we have used $\Sigma_k\mathbf{G}_{ij}=\Sigma_k\mathbf{G}'_{ij}$ to write this form. Now using proper convergence factors $\Sigma_k\mathbf{G}_{11}+\mathbf{G}_{22}=0$ and so the terms multiplying iq_l vanishes. In the last term, replace $\mathbf{k}\to\mathbf{k}+\mathbf{q}$ to show that this term is proportional to $\mathbf{q}^2/2m$ and it actually exactly cancels the similar term in $\mathbf{D}_{22}$ coming from the $(\mathbf{q}^2/2m)\mathrm{Tr}\,\mathbf{G}\sigma_3$ piece. Now $\Sigma_k\,\mathbf{G}_{12}=-\Delta_0\Sigma_k\,\mathrm{Det}\,\mathbf{G}$, and so combining everything we obtain the result for $\mathbf{D}_{22}$ in Eq. (55),

$$\mathbf{D}_{22} = \frac{\Delta_0^2}{2}\sum_k \mathbf{G}_{11}\mathbf{G}'_{22} + \mathbf{G}'_{11}\mathbf{G}_{22} - 2\mathbf{G}_{12}\mathbf{G}'_{12} - 2\,\mathrm{Det}\,\mathbf{G}. \tag{F10}$$

Going to the rescaled basis $(\tilde{\lambda},\tilde{\theta})$, we then have

$$\tilde{\mathbf{D}}_{11} = \frac{1}{g} + \frac{1}{2}\sum_k [\mathbf{G}_{22}\mathbf{G}'_{11} + \mathbf{G}_{11}\mathbf{G}'_{22} + 2\mathbf{G}_{12}\mathbf{G}'_{12}],$$

$$\tilde{\mathbf{D}}_{22} = \frac{1}{2}\sum_k [\mathbf{G}_{22}\mathbf{G}'_{11} + \mathbf{G}'_{22}\mathbf{G}_{11} - 2\mathbf{G}_{12}\mathbf{G}'_{12} - 2\,\mathrm{Det}\,\mathbf{G}],$$

$$\tilde{\mathbf{D}}_{12} = \frac{i}{2}\sum_k [\mathbf{G}_{22}\mathbf{G}'_{11} - \mathbf{G}_{11}\mathbf{G}'_{22}]. \tag{F11}$$

Just as in the case of the static saddle-point number equation, one runs into formally divergent quantities in evaluating the q sum to obtain the action. To fix these, one has to regularize using proper convergence factors. The D basis is not the basis of choice for fixing the convergence factors. Instead of the amplitude $\tilde{\lambda}$ and the phase $\tilde{\theta}$ we can work with the complex fluctuation fields defined in Eq. (56). In this basis the matrix $\mathbf{D}$ is transformed to

$$\mathbf{L} = \mathbf{W}\tilde{\mathbf{D}}\mathbf{W}^\dagger. \tag{F12}$$

Since this is an unitary transform $\mathrm{Det}\,\tilde{\mathbf{D}} = \mathrm{Det}\,\mathbf{L}$. Then we obtain

$$L_{11} = \frac{1}{g} + \sum_k \mathbf{G}_{22}\mathbf{G}'_{11} - \frac{X}{2} = \mathbf{M}_{11} - \frac{X}{2},$$

$$L_{12} = \sum_k \mathbf{G}_{12}\mathbf{G}'_{12} + \frac{X}{2} = \mathbf{M}_{12} + \frac{X}{2},$$

$$L_{22} = \frac{1}{g} + \sum_k \mathbf{G}_{11}\mathbf{G}'_{22} - \frac{X}{2} = \mathbf{M}_{22} - \frac{X}{2}, \tag{F13}$$

where $X = 1/g + \Sigma_k\,\mathrm{Det}\,\mathbf{G} = 1/g - \Sigma_\mathbf{k} 1/(2E_\mathbf{k})$ is the left-hand side of the mean-field gap equation and $\mathbf{L}_{12}=\mathbf{L}_{21}$.

Now we can fix convergence factors with $\ln\mathbf{L}_{11}$ carrying a convergence factor of $e^{+iq_l0^+}$ and $\ln\mathbf{L}_{22}$ carrying a convergence factor of $e^{-iq_l0^+}$. This can be seen by expanding the logarithm and remembering $\mathbf{G}_{22}$ carries a factor of $e^{-ik_n0^+}$, $\mathbf{G}'_{11}$ carries a factor of $e^{+i(k_n+q_l)0^+}$, and so on. The reasons for the convergence factors are related to taking the correct equal time limit and is discussed in detail in Appendixes A and B.

Remembering $\mathbf{L}_{11}(-q)=\mathbf{L}_{22}(q)$ one can take out $\ln\mathbf{L}_{11}+\ln\mathbf{L}_{22}$ from the $\ln\mathrm{Det}\,\mathbf{L}$ and then convert $\ln\mathbf{L}_{22}$ to $\ln\mathbf{L}_{11}$ using $q\to-q$. Now one can convert the Matsubara sums to real frequency integrals which are convergent. The resulting action is

$$S_g = \frac{1}{2}\sum_q \ln\left(\frac{\mathbf{L}_{11}}{\mathbf{L}_{22}}\,\mathrm{Det}\,L\right). \tag{F14}$$

One can then follow the asymptotic forms of the $\mathbf{M}$ matrix derived in Appendix E to obtain the large energy-short wavelength behavior of the $\mathbf{L}$ matrix. The asymptotic forms of $\mathbf{L}_{11}$ and $\mathbf{L}_{22}$ are the same as that of $\mathbf{M}_{11}$ and $\mathbf{M}_{22}$, with $m/4\pi a_s$ replaced by $m/4\pi a_s - X/2$. However the presence of the $X/2$ factor in $\mathbf{L}_{12}$ fundamentally changes its asymptotic behavior from $\omega^{-3/2}$ for the $\mathbf{M}$ matrix to a constant $(X/2)$. We can thus no longer neglect the $\mathbf{L}_{12}$ terms in the high-frequency limit and this leads to a divergent answer.

APPENDIX G: DILUTE BOSE GAS

In this appendix we show how the method of Gaussian fluctuations yields the correct answers in a somewhat differ-

ent problem, that of a dilute *Bose* gas with repulsive interactions. Although the results are standard [26], the method used here parallels that used in our paper, and serves to illustrate several technical points including (1) the role of convergence factors, (2) retaining the mean-field form of the saddle-point equation and including quantum fluctuations in the thermodynamic potential, and (3) taking into account the μ dependence of the saddle point in the number density equation.

The Hamiltonian for a repulsive ($g_0>0$) Bose gas is

$$H=\int d^3x\Phi^*(x)(-\nabla^2/2M-\mu)\Phi(x)+\frac{g_0}{2}\Phi^*(x)\Phi^*(x)\Phi(x)\Phi(x). \tag{G1}$$

Writing $\Phi(x)=\Phi_0+\zeta(x)$ the action is $S=S_0+S_g+\cdots$ where

$$S_0=\beta\left(-\mu\Phi_0^2+\frac{g_0}{2}\Phi_0^4\right) \tag{G2}$$

and the Gaussian part is given by

$$S_g=\frac{1}{2}\sum_{\mathbf{q},iq_l}(\zeta^*(q),\zeta(-q))\mathbf{A}(q)\begin{pmatrix}\zeta(q)\\ \zeta^*(-q)\end{pmatrix}. \tag{G3}$$

Here $\mathbf{A}_{11}(q)=\mathbf{A}_{22}(-q)=-iq_l+\epsilon_\mathbf{q}-\mu+2g_0\Phi_0^2$, with $\epsilon_\mathbf{q}=|\mathbf{q}|^2/2M$, and $\mathbf{A}_{12}(q)=\mathbf{A}_{21}(-q)=g_0\Phi_0^2$. Integrating out the ζ fields we obtain the thermodynamic potential

$$\Omega\simeq\Omega_0+(1/2\beta)\sum_{\mathbf{q},iq_l}\ln\mathrm{Det}\,\mathbf{A}(q), \tag{G4}$$

where $\Omega_0=S_0/\beta$. The Matsubara sum in the Gaussian piece is ill defined. We write $\ln\mathrm{Det}\,\mathbf{A}(q)=\ln\mathbf{A}_{11}+\ln\mathbf{A}_{22}+\ln(1-\mathbf{A}_{12}^2/\mathbf{A}_{22}\mathbf{A}_{11})$, introduce convergence factors of $\exp(iq_l0^+)$ with the $\mathbf{A}_{11}$ term (associated with $\zeta^*\zeta$), and $\exp(-iq_l0^+)$ with the $\mathbf{A}_{22}$ term (corresponding to $\zeta\zeta^*$) and use $q\to-q$ to write the $\mathbf{A}_{22}$ piece in terms of $\mathbf{A}_{11}$. At $T=0$ the sum $\beta^{-1}\Sigma_{iq_l}2\ln\mathbf{A}_{11}\exp(iq_l0^+)$ vanishes by contour integral methods since the integrand has no singularities in the left-half plane. The remaining sum can be explicitly done by contour methods to obtain

$$\Omega=\Omega_0+\frac{1}{2}\sum_\mathbf{q}(E_\mathbf{q}-\epsilon_\mathbf{q}+\mu-2g_0\Phi_0^2), \tag{G5}$$

where $E_\mathbf{q}=\sqrt{(\epsilon_\mathbf{q}-\mu+2g_0\Phi_0^2)^2-g_0^2\Phi_0^4}$ is the Bogoliubov dispersion. The quantum fluctuations are clearly seen to have the form of zero-point motion of the collective modes $E_\mathbf{q}/2$ with a "convergence factor" subtraction which eliminates the ultraviolet divergence by canceling out the contribution of the quadratic part of the Bogoliubov spectrum at large q.

The uniform, static saddle point is determined by $\delta S_0/\delta\Phi_0=0$, so that

$$\Phi_0^2=\mu/g_0, \tag{G6}$$

and this condition is again needed in order to satisfy that the excitation spectrum is gapless. We use $(\partial\Omega/\partial\mu)=-N$ to determine μ. In evaluating the thermodynamic derivative we *cannot* treat Φ_0 as a constant, and must keep track of the μ dependence of Φ_0 in Eq. (G6). We thus obtain $\Omega=-\mu^2/2g_0+\frac{1}{2}\Sigma_\mathbf{q}(E_\mathbf{q}-\epsilon_\mathbf{q}-\mu)$ with $E_\mathbf{q}=\sqrt{(\epsilon_\mathbf{q}+\mu)^2-\mu^2}$. Taking the derivative with respect to μ, we obtain $n=\mu/g_0+\frac{1}{2}\Sigma_\mathbf{q}(1-\epsilon_\mathbf{q}/E_\mathbf{q})$.

Now, using the relation between the bare repulsion g and the boson scattering length a_b given by $M/4\pi a_b=1/g_0+\Sigma_\mathbf{q}1/2\epsilon_\mathbf{q}$ we obtain

$$n=\mu M/4\pi a_b+\frac{1}{2}\sum_\mathbf{q}[1-(\epsilon_\mathbf{q}+\mu)/E_\mathbf{q}]+\frac{\mu}{2}\sum_\mathbf{q}(1/E_\mathbf{q}-1/\epsilon_\mathbf{q}), \tag{G7}$$

where we have added and subtracted $\mu/2E_\mathbf{q}$ to isolate the cancellation of divergences. The first integral is $-(1/3\pi^2)M^{3/2}\mu^{3/2}$ and the second one is $-M^{3/2}\mu^{3/2}/\pi^2$. So in all we obtain

$$n=\mu M/4\pi a_b-(4/3\pi^2)M^{3/2}\mu^{3/2}. \tag{G8}$$

We now solve this equation for $\mu(n)$ in powers of (na_b^3). To leading order $\mu=4\pi na_b/M$ and to the next order in a_b we obtain

$$\mu=4\pi na_b/M[1+32/3\pi^{-1/2}(na_b^3)^{1/2}]. \tag{G9}$$

This is the correct equation of state for a Bogoliubov dilute Bose gas, including the Lee-Yang correction.

We note that we *cannot* identify the saddle-point value of Φ_0^2 in Eq. (G6) with the condensate fraction, once quantum fluctuations are taken into account. This identification is usually made, together with the replacement $g_0\to4\pi a_b/M$. We note here that this identification makes Eq. (G5) divergent and is thus not well defined. To find the condensate fraction we use the expression for the $\mathbf{q}\neq\mathbf{0}$ momentum distribution,

$$n(\mathbf{q})=\frac{1}{\beta}\sum_{iq_l}e^{iq_l0^+}(\mathbf{A}^{-1})_{11}, \tag{G10}$$

to derive the well-known result

$$n(\mathbf{q})=\frac{1}{2}\left(\frac{\epsilon_\mathbf{q}+\mu}{E_\mathbf{q}}-1\right),\quad \mathbf{q}\neq\mathbf{0}. \tag{G11}$$

From the quantum depletion we can obtain the well-known result for the condensate fraction using $N_0=N-\Sigma_{\mathbf{q}\neq\mathbf{0}}n(\mathbf{q})=N[1-\frac{8}{3}\sqrt{(na_b)^3/\pi}]$.

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