Beyond Gaussian pair fluctuation theory for strongly interacting Fermi gases

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Interacting Fermi systems in the strongly correlated regime play a fundamental role in many areas of physics and are of particular interest to the condensed matter community. Though weakly interacting fermions are understood, strongly correlated fermions are difficult to describe theoretically as there is no small interaction parameter to expand about. Existing strong-coupling theories rely heavily on the so-called many-body $T$-matrix approximation that sums ladder-type Feynman diagrams. Here, by acknowledging the fact that the effective interparticle interaction (i.e., the vertex function) becomes smaller above three dimensions, we propose an alternative way to reorganize Feynman diagrams and develop a theoretical framework for interacting Fermi gases beyond the ladder approximation. As an application, we solve the equation of state for three- and two-dimensional strongly interacting fermions and find excellent agreement with experimental [M. J. H. Ku et al., Science 335, 563 (2012)] and other theoretical results above temperatures of $0.5T_F$.

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I. INTRODUCTION

Using Feshbach resonances to tune the $s$-wave scattering length of two-component atomic Fermi gases [1–3], the experimental exploration of the crossover from Bose-Einstein condensates (BECs) to Bardeen-Cooper-Schrieffer (BCS) superfluids in both three (3D) [4–7] and two dimensions (2D) [8–16] has attracted significant attention for understanding strongly interacting phenomena. This has offered insight to theorists as strongly correlated matter cannot be quantitatively described by a simple mean-field theory.

For strongly interacting systems, exact treatments only exist in some limiting situations; for example, Bethe ansatz solutions in one dimension [20], virial expansion at high temperature [21–24] and Tan relations at large momentum [25–28]. Numerically exact and sophisticated quantum Monte Carlo (QMC) simulations have also been developed [29–33]; however, these approaches have their own difficulty evaluating experimentally relevant observables. In addition to the exact techniques, there have been many attempts to solve strongly interacting fermions through approximate diagrammatic theories. A commonly used approximation is to sum over the complete geometric series of ladder diagrams, leading to the Gaussian pair fluctuation (GPF) theory [34–43]. Though the GPF theory seems to provide consistent predictions for recent experiments within certain errors [44–46], it is hard to evaluate its validity. Improvements through using a dressed Green’s function in the ladder diagrams, i.e., the partially self-consistent pseudogap theory [47] or fully self-consistent Luttinger-Ward (GW) theory [48–51], meet similar problems. To develop a better strong-coupling theory one needs to consider terms beyond GPF, which turns out to be notoriously difficult.

In this work, we attempt to tackle this daunting task and develop a beyond GPF theory, motivated through the dimensional $\epsilon$ expansion [52–56]. It was recognized that in the unitary regime [57]—where a bound state with zero energy appears—and near four dimensions ($d = 4 - \epsilon$), for small $\epsilon$, the two-component Fermi gas behaves like a system of noninteracting composite bosons. This is indicative of weaker effective interparticle interactions above three dimensions, as characterized by the particle-particle vertex function $\Gamma$. With such a re-interpretation of the small parameter in the dimensional expansion, i.e., the use of $\Gamma$ instead of $\epsilon$, we reorganize higher-order Feynman diagrams beyond GPF, within the functional path-integral approach. In principle, the resulting systematic expansion in terms of the vertex function is convergent for dimensions where $\epsilon < 1$, and may also asymptotically converge at three dimensions, where $\epsilon = 1$, following the extrapolation strategy in Ref. [31]. Building upon this generalization of the $\epsilon$ expansion, we examine the leading-order correction to the GPF.

The paper is organized as follows: in Sec. II we introduce the effective field theory and formalism for expanding the thermodynamic potential. In Sec. III we reinterpret the $\epsilon$ expansion in terms of the many-body formalism and comment on the convergence of the expansion. In Sec. IV we derive a methodology for calculating terms beyond the GPF in both the normal and superfluid state across the BEC-BCS crossover. As a test, in Sec. V, we apply our theory to 3D and 2D strongly interacting systems, finding excellent agreement with experimental benchmarks and other theoretical techniques within a certain temperature window. Finally, in Sec. VI we summarize our findings and comment on further work to be completed.

II. EFFECTIVE FIELD THEORY

We consider the thermodynamic potential, $\Omega = -k_B T \ln Z$, at a given temperature $T$ using the functional path-integral formulation, which has been extensively adopted in both 3D and 2D [35,39,42,43]. The partition function, $Z = \int D[\psi, \bar{\psi}] e^{-S[\psi, \bar{\psi}]}$, where $\psi$ and $\bar{\psi}$ are independent Grassmann fields, is defined through the action

$$S[\psi, \bar{\psi}] = \int_0^{\hbar \beta} d\tau \int d\mathbf{r} \left[ \sum_\sigma \bar{\psi}_\sigma(x) \partial_\tau \psi_\sigma(x) + H \right].$$ (1)
where the single-channel model Hamiltonian is
\[ H = \sum_x \psi_x^a(x)K\psi_x^b(x) + U_0\psi_x^a(x)\psi_x^b(x)\psi_x^a(x)\psi_x^b(x), \]
\[ K = -\hbar^2\nabla^2/(2m) - \mu, \quad \beta = (k_BT)^{-1}, \quad m \text{ is the mass of a fermion}, \]
\[ \mu \text{ is the chemical potential}, \quad \text{and throughout we shall use the notation } x = (x, \tau). \]
We take a contact attractive interaction, \( U_0 < 0 \), which has known divergences and must be fixed [45]. We will write most of the equations detailed in this work using the bare interaction, dealing with the divergences where necessary. Using the Hubbard-Stratonovich transformation to write the action in terms of a bosonic field, \( \Delta(q) \), and expanding about its saddle point \( \Delta_0 \), \( \Delta(q) = \Delta_0 + \phi_q \), we take a perturbative expansion of the bosonic action in orders of the fluctuation contribution is \( S_{\text{MF}} + S_{\text{GF}} + S^{(5)} + S^{(4)} + \cdots \), where \( S_{\text{MF}} \) is the mean-field contribution and the higher orders are
\[ S_{\text{GF}}^{(2)} = \frac{1}{2} \sum_q (\psi_q^a, \phi_{-q}) \left[ -\Gamma^{-1}(q) \right] (\psi_q^a, \phi_{-q}), \]
\[ S^{(n)} = \frac{1}{n!} \text{Tr}[(G_0(\mu)\Lambda(k))^n]. \]
Here we define \( G_0\Lambda = G_0\psi_q^a + G_0\phi_{-q}^a\), where
\[ G_0 = \begin{pmatrix} i\nu_{m} + \xi_k - \Delta_0 & -\Delta_0 \\ -\Delta_0 & i\nu_{m} + \xi_k \end{pmatrix}^{-1}, \]
\[ \xi_k = \epsilon_k - \mu \quad \text{and} \quad \epsilon_k = \hbar^2k^2/(2m), \]
and \( \sigma^z = \frac{1}{2}(\sigma_1^\pm i\sigma_2) \) are the Pauli matrices. The trace in Eq. (5) is over all space and spin indices and we have used the summation convention \( \sum_k = (k_BT/V, i\nu_m) \sum_{k,i\nu_m} \) and \( \sum_q = (k_BT/V, \sum_{q,i\nu_q}, \) where \( i\nu_{m} \) and \( i\nu_{m} \) are bosonic and fermionic Matsubara frequencies, respectively. The second-order Gaussian fluctuation term, \( S_{\text{GF}}^{(2)} \), is the repeated scattering of two opposite spin fermions, and the elements of the vertex function, \( \Gamma(q) \), are given by
\[ \Gamma_1(q) = 1/U_0 + \sum_k G_{11}^{(0)}(q - k)G_{11}^{(0)}(k), \]
\[ \Gamma_2(q) = \sum_k G_{12}^{(0)}(q - k)G_{12}^{(0)}(k). \]
\[ \Gamma_2(q) = \Gamma_1(q), \quad \text{and} \quad \Gamma_3(q) = \Gamma_1(-q). \]
In the normal phase where there is no superfluid order parameter, \( \Delta_0 = 0 \), the vertex function is given by \( \Gamma^{-1}(q) = 1/U_0 + \sum_k G_0(q - k)G_0(k) \). In the original Gaussian fluctuation theory (known alternatively as the NSR theory) [34], terms beyond \( S_{\text{GF}}^{(2)} \) are simply discarded and the bosonic fields are integrated out, giving \( \Omega = \Omega_0 + \Omega_{\text{GF}}^{(2)} \), where \( \Omega_0 \) is the thermodynamic potential for a noninteracting Fermi gas and the Gaussian fluctuation contribution is \( \Omega_{\text{GF}}^{(2)} = \sum_q \ln[-\Gamma^{-1}(q)] \). The number equation, \( n = -\partial \Omega /\partial \mu \), should be satisfied by adjusting the chemical potential for a given reduced temperature, \( T/T_F \), and the equation of state can then be found. The higher-order terms, \( S^{(n)} \), contain beyond Gaussian contributions of the bosonic fluctuation, \( \phi_q \), and the treatment of these terms in the literature is sparse [58–60].

III. REINTERPRETATION OF THE \( \epsilon \) EXPANSION

To calculate the beyond Gaussian contribution, we tie the GPF theory to the dimensional \( \epsilon \) expansion by clarifying the structure of the vertex function, \( \Gamma(q) \), near four dimensions (further results can be found in Appendix A). We split the normal-state vertex function into its two- and many-body parts, \( \Gamma^{-1}(q) = \Gamma^{-1}_{\text{GF}}(q) + \Gamma^{-1}_{\text{mb}}(q) \), where
\[ \Gamma^{-1}_{\text{GF}}(q) = \Gamma^{-1}_{\text{GF}}(q), \]
\[ \Gamma^{-1}_{\text{mb}}(q) = \sum_k \frac{f(q_k/2 - k) + f(q_k/2 + k)}{i\nu_m - q_k/2 - 2\epsilon_k - 2\mu}. \]
For small \( \epsilon = 4 - d \) and in the unitary limit, the two-body part of the vertex function, \( \Gamma^{-1}_{\text{GF}}(q) \), has a pole and dominates the inverse vertex function,
\[ \Gamma^{-1}_{\text{GF}} \approx \frac{m^2}{8\pi^2\hbar^2}\epsilon(i\nu_m - q_k/2 + 2\mu) = \frac{1}{g^2D^2}\epsilon \]
where we define \( g^2 = (8\pi^2\hbar^2/m^2)\epsilon \) and the bosonic propagator \( \Delta(q) = (i\nu_m - q_k + 2\mu)^{-1} \). Thus, we see that the vertex function, \( \Gamma(q) \), within the ladder approximation has the leading contribution of \( O(\epsilon) \) near four dimensions in the unitary regime. This is visualized in Fig. 1, where we show the contribution of the two-body scattering near four dimensions.

In the \( \epsilon \) expansion, the series is arranged according to orders of \( \epsilon \), or equivalently \( \Gamma_{\text{GF}}^{(2)} \). While such an arrangement is convenient to analytically calculate the next-to-leading order (NLO) [53] or next-to-next-to-leading order (NNLO) of the expansion [56], it was known that one may encounter a convergence problem in dealing with some dangerous higher-order terms that contribute like \( O(n!\epsilon^n) \) due to the exponentially large prefactor \( n! \) [62]. These terms are contributions from the many-body part of the vertex function, \( \Gamma_{\text{mb}} \), to the Gaussian fluctuation part of the thermodynamic potential, \( \Omega_{\text{GF}}^{(2)} \). The summation of these terms is given by \( \sum_{n=1,q}(-1)^{n+1} \Gamma_{\text{GF}}^{(2)}(\Gamma_{\text{GF}}^{(2)}(q_n)^n/n) = \sum_q \ln[1 - \Gamma_{\text{GF}}^{(2)}(\Gamma_{\text{GF}}^{(2)}(q_n)^n/n)] \) (Appendix A), and combining this with the two-body part, \( \sum_q \ln[-\Gamma^{-1}_{\text{GF}}(q)] \), we recover \( \Omega_{\text{GF}}^{(2)} \). Therefore, since \( \Omega_{\text{GF}}^{(2)} \) contains one power of the vertex function, which is \( O(\epsilon) \) at the NLO, the \( \epsilon \) expansion can be understood from the framework of the GPF theory. This re-interpretation suggests that it might be more useful to make an expansion in terms of the vertex function, \( \Gamma(q) \), instead of \( \epsilon \).

IV. BEYOND GPF

As previously noted, we have the effective bosonic action, \( S_{\text{eff}} \), and it is not possible to integrate out the bosonic fluctuations for orders beyond \( n = 2 \) without significant approximations. Using the reinterpretation of the the \( \epsilon \)
expansion, we expand the higher-order action terms and use the vertex function as a perturbation parameter. The higher-order contributions to the action $S_{\text{eff}}$ will contain multiple orders of the vertex function, $\Gamma(q)$, and contribute beyond $O(\epsilon)$ near four dimensions. In these cases we may treat the terms $S^{(n>2)}$ as perturbative terms with respect to $S_{\text{GF}}^{(2)}$ and take them into account order by order, using a standard diagrammatic approach and the physical motivation of the dimensional expansion in the unitary limit. That is, by denoting, $\hat{V} = S^{(3)} + S^{(4)} + \cdots$, we have for the partition function

$$Z = e^{-S_{\text{eff}}^{(0)}} \int \mathcal{D}[\Delta, \Delta^*] e^{-S_{\text{GF}}^{(2)}} = e^{-S_{\text{eff}}^{(0)}} \int \mathcal{D}[\Delta, \Delta^*] e^{-S_{\text{GF}}^{(2)}} \sum_{n=0}^{\infty} \frac{(-\epsilon)^n}{n!} \langle \hat{V}_1 \hat{V}_2 \cdots \hat{V}_n \rangle, \quad (10)$$

where we have inserted a normalization term and defined, for any observable (operator) $\hat{A}$,

$$\langle \hat{A} \rangle = \frac{\int \mathcal{D}[\Delta, \Delta^*] \hat{A} e^{-S_{\text{GF}}^{(2)}}}{\int \mathcal{D}[\Delta, \Delta^*] e^{-S_{\text{GF}}^{(2)}}}. \quad (11)$$

Using the linked cluster expansion, we may write

$$Z = e^{-S_{\text{eff}}^{(0)}} \int \mathcal{D}[\Delta, \Delta^*] e^{-S_{\text{GF}}^{(2)}} \exp \left( \sum_{l=1}^{\infty} U_l \right). \quad (12)$$

where the only contribution to the partition function is from the differently connected diagrams,

$$U_l = \frac{(-\epsilon)^{l+1}}{l} \langle \hat{V}_1 \hat{V}_2 \cdots \hat{V}_l \rangle_{\text{dc}}. \quad (13)$$

The expansion of the thermodynamic potential is then given by

$$\Omega = \Omega_{\text{MF}}^{(0)} + \Omega_{\text{GF}}^{(2)} + \frac{1}{\beta V} \sum_{l=1}^{\infty} \frac{(-\epsilon)^{l+1}}{l} \langle \hat{V}_1 \hat{V}_2 \cdots \hat{V}_l \rangle_{\text{dc}}. \quad (14)$$

where $\Omega_{\text{MF}}^{(0)}$ is the mean-field contribution, $\Omega_{\text{GF}}^{(2)}$ is the Gaussian fluctuation, the final term is the contribution from beyond the Gaussian effective action, and $\hat{V}$ are the higher-order effective terms. The expansion should converge near four dimensions, where $\Gamma(q)$ is small. Therefore, to select the important diagrams in the calculation of the thermodynamic potential for 3D or 2D, we choose the leading diagrams in orders of $\epsilon$ near four dimensions.

In order to determine the contribution of the higher orders, it is most convenient to calculate expectation values by adding to the action, or partition function, an external source $J_q$. Within the framework of the Gaussian pair fluctuation theory we have

$$S_{\text{GF}}^{(2)}[J] = \frac{1}{2} \sum_q \langle \psi_q^* \varphi_{-q} \rangle \left[ -\Gamma^{-1}(q) \right] \left( \psi_q^* \varphi_{-q} \right)$$

$$- \langle \varphi_q^* \varphi_{-q} \rangle \left( J_q^* J_{-q} - J_q J_{-q} \right) \left( \psi_q^* \varphi_{-q} \right). \quad (15)$$

Using the standard result of integrating out bosonic fields leads to [61–63]

$$\int \mathcal{D}[\Delta^*, \Delta] e^{-S_{\text{GF}}^{(2)}[J]} = \int \mathcal{D}[\Delta^*, \Delta] e^{-S_{\text{GF}}^{(2)}[J=0]} B[J, J^*], \quad (16)$$

where

$$B[J, J^*] = \exp \left[ \sum_q \frac{1}{2} \left( J_q^* J_{-q} \right) \Gamma(q) \left( J_q J_{-q} \right) \right]. \quad (17)$$

We use this definition to find expectation values; for example, a pair propagator in the normal state is defined as

$$\langle \psi_q^* \varphi_{q'} \rangle = \frac{\delta^2 \int \mathcal{D}[\Delta^*, \Delta] e^{-S_{\text{GF}}^{(2)}[J]}/\delta \Delta_{q}^* \delta \Delta_{q'} \rangle}{\int \mathcal{D}[\Delta^*, \Delta] e^{-S_{\text{GF}}^{(2)}[J]}/\delta \Delta_{q}^* \delta \Delta_{q'} \rangle} \approx \Gamma(q) \delta_{qq'}. \quad (18)$$

With the methodology of finding the expectation values we can calculate the contributions to the thermodynamic potential. The simplest term we can calculate in the beyond Gaussian expansion is the first connected diagram, $\hat{V} = S^{(4)}$. In the normal state, where the superfluid parameter is zero, $\Delta_0 = 0$, we have

$$\frac{S^{(4)}}{\beta V} = \frac{1}{2} \sum_{k, q_1, q_2, q_3} \delta_{q_1+q_2+q_3+k} G_0(k) G_0(q_1-k) G_0(q_2-k) G_0(q_3-k) \varphi_{q_1}^* \varphi_{q_2} \varphi_{q_3}^* \varphi_{q_4}. \quad (19)$$

From this term we wish to find the time-ordered product, or expectation value, through Wick’s theorem, and with the use of Eq. (18) we can write for the bosonic fields

$$\langle \psi_q^* \varphi_{q'}^* \varphi_q \varphi_{q''} \rangle = \delta_{q+q', q+q''} \Gamma(q_1) \Gamma(q_2) + \delta_{q+q', q+q''} \Gamma(q_1) \Gamma(q_2). \quad (20)$$

The contribution to the thermodynamic potential is then given by

$$\frac{1}{\beta V} \langle S^{(4)} \rangle = \sum_k \langle G_0(k) \Sigma_0(k) \rangle^2. \quad (21)$$

where $\Sigma_0(k) = \sum_q G_0(k-q-k) \Gamma_0(q)$ is the self-energy and we find these terms by analytically continuing to real frequencies, $i\omega_{\nu} = \omega + i\theta$. This procedure has advantages over the full numerical calculation [41] and is significantly simpler to implement than the self-consistent GG calculations. Details about the calculation can be found in Appendix B. As we can see, $\langle S^{(4)} \rangle$ contains two $\Gamma(q)$ vertex functions and near four dimensions the NNLO, $O(\epsilon^3)$ contribution. In other words, if we calculate $\langle S^{(4)} \rangle$ in $d = 4-\epsilon$ dimensions and numerically extract the coefficients at $O(\epsilon^2)$, we are able to recover the NNLO $\epsilon$ expansion [56]. Higher-order contributions to the $\epsilon$ expansion can be obtained as we go further beyond GPF.

The NNLO contribution to the superfluid phase can also be calculated with the same method used in the normal state calculation. The $S^{(4)}$ term is the next order to contribute beyond
the GPF theory, giving
\[
\frac{S^{(4)}}{\beta V} = \frac{1}{4} \sum_{kq_1q_2q_3q_4} \text{Tr}_c G_{0}(k) \left( \begin{array}{cc}
0 & \varphi_{q_1} \\
\varphi_{-q_1} & 0
\end{array} \right) \times G_{0}(k - q_1) \left( \begin{array}{cc}
0 & \varphi_{q_2} \\
\varphi_{-q_2} & 0
\end{array} \right) \times G_{0}(\tilde{k}) \left( \begin{array}{cc}
0 & \varphi_{q_3} \\
\varphi_{-q_3} & 0
\end{array} \right),
\]
where \( q_1 + q_2 = q_3 + q_4 \) and \( \tilde{k} = k - q_1 + q_2 \). Expanding this out, there are 16 terms in total, and using Wick’s theorem we expand each of the 16 terms find the total contribution. We find terms of the form
\[
\langle \varphi_{q_1} \varphi_{-q_1} \varphi_{q_2} \varphi_{-q_2} \rangle = \delta_{q_1,q_2} \delta_{q_3,q_4} \Gamma_{12}(q_1) \Gamma_{12}(q_3) + \delta_{q_1,-q_2} \delta_{q_3,-q_4} \Gamma_{12}(q_1) \Gamma_{12}(q_2) + \delta_{q_1,q_2} \delta_{q_3,q_4} \Gamma_{11}(q_1) \Gamma_{12}(q_2),
\]
and using the fact that \( \Gamma_{11} \sim \epsilon \) and \( \Gamma_{12} \sim \epsilon^2 \) we can make several approximations, giving the three leading contributions
\[
\frac{1}{\beta V} \langle S^{(4)} \rangle = \Omega^{(a)} + \Omega^{(b)} + \Omega^{(c)},
\]
where
\[
\Omega^{(a)} = \sum_{k} G_{11}^{(0)}(k) G_{11}^{(0)}(k) \Sigma_{11}^{(0)}(k) \Sigma_{11}^{(0)}(k),
\]
\[
\Omega^{(b)} = \sum_{k} G_{12}^{(0)}(k) G_{12}^{(0)}(k) \Sigma_{11}^{(0)}(k) \Sigma_{22}^{(0)}(k),
\]
\[
\Omega^{(c)} = \sum_{k} G_{12}^{(0)}(k) G_{12}^{(0)}(k - q_1) G_{12}^{(0)}(k - q_1 + q_2)
\times G_{22}^{(0)}(k + q_2) \Gamma_{11}(q_1) \Gamma_{12}(q_2).
\]

V. EQUATION OF STATE

As an application of our beyond GPF theory, we determine the equation of state of above-threshold strongly interacting Fermi gases in both 3D and 2D through solving the number equation for the thermodynamic potential, \( \Omega = \Omega^{(a)}_{\text{MF}} + \Omega^{(b)}_{G} + (\beta V)^{-1} \langle S^{(4)} \rangle \). We use \( \langle S^{(4)} \rangle \) as the shorthand notation for our beyond GPF theory in the normal state.

In Fig. 2, we report the chemical potential of a 3D unitary Fermi gas as a function of reduced temperature, \( T/T_F \), predicted from the \( \langle S^{(4)} \rangle \), NSR [34], and self-consistent \( GG \) theories [48], and measured by the MIT experiment [7]. Here, we find that the \( \langle S^{(4)} \rangle \) prediction is in excellent agreement with the experimental data up to temperatures of \( T \simeq 0.5T_F \), below which our prediction begins to diverge away from the NSR solution and pairing fluctuations in \( \langle S^{(4)} \rangle \) start to dominate. This is because, as the temperature becomes lower, the effective interaction and fluctuation between pairs become stronger and the NSR approximation itself [37,38,44] and leading-order correction beyond GPF are no longer controllable. Thus, in this work we do not attempt to make a comparison of the transition temperature, \( T_c \), and leave such a calculation for further work.

A further comparison is given in Fig. 3, where we plot the density equation of state, \( n/n_0 \), as a function of \( \beta \mu \), normalized by the ideal gas result at the same temperature \( T \) and chemical potential \( \mu \). We find again excellent agreement between the \( \langle S^{(4)} \rangle \) prediction and experimental data up to values of \( \beta \mu \simeq 0 \), as seen clearly in the inset of Fig. 3 for high temperatures. The \( \langle S^{(4)} \rangle \) prediction agrees well with the exact virial expansion (orange dot-dashed) for high temperatures, and we see that the beyond GPF theory is an improvement on the self-consistent \( GG \) theory and comparable to bold-diagrammatic QMC [31], up to slightly below the Fermi degeneracy temperature. This is significant, as the computational intensity of the beyond
GPF calculation is considerably less than the self-consistent methodologies. The \(\langle S^{(4)} \rangle\) theory breaks down at lower temperatures, \(\beta \mu \simeq 1\), and as mentioned earlier this is due to the unphysical pair fluctuations dominating as we only calculate the leading term. Our calculations are not stable towards the experimentally measured critical temperature. To understand the superfluid transition using our beyond GPF theory, a below-\(T_c\) calculation with the inclusion of a superfluid order parameter will need to be implemented and this will be reported later in a more detailed publication.

Encouraged by the excellent agreement between the beyond GPF theory and experiment in 3D, we now turn to consider the density equation of state for a 2D system, where pair fluctuations are believed to become larger, applying the same density equation of state for a 2D system, where pair fluctuations are more significant, and have shown that our theory significantly improves the NSR calculation and captures the high-temperature behavior for strong interactions.

Our theory for the normal state breaks down before the superfluid transition in both 3D and 2D as the NSR theory itself breaks down \([37,38]\), and we expect that the addition of more terms will lower the temperature range of validity. At zero temperature, where the GPF theory is more reliable \([36,39,42]\), we anticipate our theory \([i.e., Eqs. (25)]\) will provide quantitatively accurate predictions for strongly interacting Fermi gases.

\section{VI. CONCLUSIONS}

We have extended the many-body strong-coupling theory beyond the commonly used Gaussian fluctuation approximation \((i.e., the NSR \([34]\) or GPF theory \([36]\)). Inspired by the dimensional expansion near four dimensions \([53]\) and using the functional path-integral formulation of the thermodynamic potential \([35]\), we artificially treat a strongly interacting Fermi gas as a system of weakly interacting Cooper pairs and use the vertex function summed over the ladder-type diagrams as a small parameter. This treatment is well justified near four dimensions, where the vertex function is indeed small \([53]\). Following this generalization of the dimensional expansion, we reorganize the Feynman diagrams and determine the leading correction term to the Gaussian fluctuations. Applying such a beyond Gaussian fluctuation theory to the three-dimensional strongly interacting unitary Fermi gas in its normal state, we have calculated the equation of state and compared the prediction with the latest experimental data \([7]\) and other theoretical results \([34,48]\). We have found a sizable improvement on previous many-body calculations down to temperatures of 0.5\(T_F\). To further examine the advantage of the theory, we have considered a strongly interacting two-dimensional Fermi gas, for which the pair fluctuations are more significant, and have shown that our theory significantly improves the NSR calculation and captures the high-temperature behavior for strong interactions.

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\section{APPENDIX A: DANGEROUS TERMS IN THE \(\epsilon\) EXPANSION}

In the \(\epsilon\) expansion approach developed by Nishida and Son \([53]\), it was noted that there are a class of dangerous
higher-order diagrams, which contribute $O(n! \epsilon^n)$ [52]. The contribution of such a diagram is illustrated in Fig. 5. Due to the exponentially large prefactor $n!$, it is not clear whether these contributions will survive and dominate the large order behavior of the $\epsilon$ expansion. It is anticipated that possibly there might be cancellations with other $n$th-order diagrams and/or with subleading contributions from lower-order diagrams [52].

Here, we show that indeed there is a cancellation among diagrams. Actually, by using the finite-temperature Green’s function, we may write down the following contribution of the dangerous $n$th-order diagram to the pressure ($P = -\Omega$):

$$P_n = -\frac{(-y)^n}{n} \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \left[ \Gamma_{2b}(\mathbf{q}, i\nu_n) \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n) \right]^n.$$  \hspace{1cm} (A1)

This expression is identical to Eq. (A.1) in Nishida’s Ph.D. thesis [52]. Though Eq. (A.1) is a zero temperature equation (using real frequency), its finite temperature version is easy to obtain:

$$-V_n = \frac{1}{\beta n} \sum_{\mathbf{q}, i\nu_n} \left[ \mathcal{D}(\mathbf{q}, i\nu_n) [\Pi_a(\mathbf{q}, i\nu_n) + \Pi_0(\mathbf{q}, i\nu_n)] \right]^n.$$  \hspace{1cm} (A2)

Here $\Pi_a$ and $\Pi_0$ are defined in Eqs. (3.10) and (3.17) in Nishida’s thesis, and are given by $\Pi_0(\mathbf{q}, i\nu_n) = D^{-1}(\mathbf{q}, i\nu_n) = g^2 \Gamma_{2b}^{-1}(\mathbf{q}, i\nu_n)$ and $\Pi_a(\mathbf{q}, i\nu_n) = -g^2 \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n)$. Then, we find immediately

$$\Pi_a(\mathbf{q}, i\nu_n) + \Pi_0(\mathbf{q}, i\nu_n) = -g^2 \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n).$$  \hspace{1cm} (A3)

Plugging this expression into Eq. (A2), we obtain Eq. (A1). We note that, when $n = 1$, we have $(\sum_{i\nu_n} 1 = 0)$

$$-\frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \Gamma_{2b}(\mathbf{q}, i\nu_n) \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n) = -\frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \Gamma_{2b}(\mathbf{q}, i\nu_n) \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n)$$
\[
\approx -g^2 \frac{1}{\beta^2} \sum_{\mathbf{q}, i\nu_n} \sum_{\mathbf{k}, i\omega_m} \mathcal{D}(\mathbf{q}, i\nu_n) G_0 \left( \frac{\mathbf{q}}{2} - \mathbf{k}, i\nu_n - i\omega_m \right) G_0 \left( \frac{\mathbf{q}}{2} + \mathbf{k}, i\omega_m \right),
\]
\[
= g^2 \frac{1}{\beta^2} \sum_{\mathbf{q}, i\nu_n} \sum_{\mathbf{k}, i\omega_m} \mathcal{D}(\mathbf{q}, i\nu_n) G^{(0)}(\mathbf{q} - \mathbf{k}, i\nu_n - i\omega_m) G^{(0)}_{11} (\frac{\mathbf{q}}{2} - \mathbf{k}, i\nu_n - i\omega_m).
\]

This is precisely Eq. (63) in Nishida’s finite temperature paper [55] or Eq. (49) in Nishida’s zero temperature paper [54], which gives the next-to-leading order (NLO) contribution. The summation of all the terms with different orders in Eq. (A1) leads to

$$-\sum_{n=1}^{\infty} \left( \frac{-y}{n} \right)^n \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \left[ \Gamma_{2b}(\mathbf{q}, i\nu_n) \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n) \right]^n = -\frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \ln \left[ 1 + \Gamma_{2b}(\mathbf{q}, i\nu_n) \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n) \right].$$  \hspace{1cm} (A5)

Adding the zero-order contributions, we obtain the expression for the total pressure,

$$\mathcal{P} = \frac{2}{\beta} \sum_{i\nu_n} \ln(1 + e^{-\beta \epsilon_k}) - \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \ln \left[ -\Gamma_{2b}^{-1}(\mathbf{q}, i\nu_n) \right] - \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \ln \left[ 1 + \Gamma_{2b}(\mathbf{q}, i\nu_n) / \Gamma_{mb}(\mathbf{q}, i\nu_n) \right],$$
\[
= \frac{2}{\beta} \sum_{i\nu_n} \ln(1 + e^{-\beta \epsilon_k}) - \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \ln \left[ -\Gamma_{2b}(\mathbf{q}, i\nu_n) \right],
\]

which is precisely the pressure given by the Gaussian pair fluctuation approximation. Thus, we see the high-order diagrams cancel.

We now show explicitly that the summation of the terms in Eq. (A1) with $n > 2$ is at $O(\epsilon^2)$. For this purpose, we define

$$\delta \mathcal{P} = -\frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \ln \left[ 1 + \Gamma_{2b}(\mathbf{q}, i\nu_n) / \Gamma_{mb}(\mathbf{q}, i\nu_n) \right] + \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \Gamma_{2b}(\mathbf{q}, i\nu_n) / \Gamma_{mb}(\mathbf{q}, i\nu_n),$$  \hspace{1cm} (A7)

and wish to prove that $\delta \mathcal{P} = O(\epsilon^2)$. It is convenient to introduce

$$\Gamma_{2b} \Gamma_{mb}^{-1}(\mathbf{q}, i\nu_n) \rightarrow \Omega + i\nu_n \equiv \epsilon [A + iB].$$  \hspace{1cm} (A8)
Then, we may write
\[
\delta \mathcal{P} = \frac{1}{\pi} \sum_q \int \frac{d\Omega}{e^{\beta \Omega} - 1} [- \text{Im} \ln (1 + \epsilon A + i \epsilon B) + \epsilon B],
\]
\[
= \frac{1}{\pi} \sum_q \int \frac{d\Omega}{e^{\beta \Omega} - 1} \left[ - \frac{i \epsilon B}{1 + \epsilon A} + \epsilon B \right],
\]
\[
= \frac{1}{\pi} \sum_q \int \frac{d\Omega}{e^{\beta \Omega} - 1} [AB \epsilon^2 + O(\epsilon^3)]. \tag{A9}
\]
It is readily seen that \( \delta \mathcal{P} = O(\epsilon^2) \). The relation between the \( \epsilon \) expansion and the NSR theory discussed in this section is of great interest. It suggests a new way to determine higher-order \( \epsilon \) expansion coefficients, which has been shown to be a challenging task by Arnold, Drut, and Son [56].

**APPENDIX B: CALCULATION DETAILS IN THE NORMAL STATE**

In order to determine the contribution to the thermodynamic potential from Eq. (21), we analytically continue the functions
\[
\Gamma(q, i\nu_n) = \int_{-\infty}^{\infty} \frac{d\omega}{i\nu_n - \Omega} \int \frac{d\omega}{i\omega_m - \omega}, \tag{B1}
\]
\[
\Sigma_0(q, i\omega_m) = \int_{-\infty}^{\infty} \frac{d\omega}{i\omega_m - \omega}, \tag{B2}
\]
to the real axis, where the spectral representations
\[
\mathcal{B}(q, \Omega) = -\frac{1}{\pi} \text{Im} \Gamma(q, i\nu_n \rightarrow \Omega + i0^+), \tag{B3}
\]
\[
\mathcal{C}(q, \omega) = -\frac{1}{\pi} \text{Im} \Sigma(q, i\omega_m \rightarrow \omega + i0^+) \tag{B4}
\]
are the imaginary parts of the vertex function and self-energy, respectively. We then expand out the self-energy and find its spectral representation [64],
\[
\Sigma_0(k) = \frac{1}{\beta V} \sum_{q,i\nu_n} \frac{1}{(i\nu_n - i\omega_m) - \xi_k^2} \int_{-\infty}^{\infty} d\Omega \frac{B(q, \Omega)}{i\nu_n - \Omega},
\]
\[
= \frac{1}{\beta V} \sum_{q} \int_{-\infty}^{\infty} d\Omega \frac{B(q + k, \Omega)}{i\omega_m + \xi_k^2 - \Omega} [f(\xi_q) + f_B(\Omega)],
\tag{B5}
\]
where \( f_B(\Omega) \) is the bosonic distribution, giving
\[
\mathcal{C}(k, \omega) = \frac{1}{\beta V} \sum_{q} B(q + k, \omega + \xi_k^2) [f(\xi_q) + f_B(\omega + \xi_k^2)].
\tag{B6}
\]
The real frequency formulation allows us to calculate \( \mathcal{C}(k, \omega) \) exactly and in the numerical calculations offers high accuracy. Finally, we calculate the total \( \langle S^{(4)} \rangle \) term, giving
\[
\langle S^{(4)} \rangle = \beta V \sum_k [G_0(k) \Sigma_0(k)]^2 = \sum_k \int_{-\infty}^{\infty} d\omega d\omega' \mathcal{C}(k, \omega) \mathcal{C}(k, \omega') \times \sum_{i\omega_m} \frac{1}{(i\omega_m - \xi_k^2)(i\omega_m - \omega)(i\omega_m - \omega')}, \tag{B7}
\]
where the sum over the Matsubara frequencies can be easily performed. The number equation, \( n = -\partial \Omega / \partial \mu \), is then determined and converged for a given temperature, \( T \), in both three and two dimensions.
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