

# Low-momentum interactions for ultracold Fermi gases

M. Urban<sup>✉\*</sup>

*Université Paris-Saclay, CNRS-IN2P3, IJCLab, 91405 Orsay, France*

S. Ramanan<sup>†</sup>

*Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India*



(Received 6 April 2021; accepted 28 May 2021; published 14 June 2021)

We consider a two-component Fermi gas with a contact interaction from the BCS regime to the unitary limit. Starting from the idea that many-body effects should not depend on short-distance or high-momentum physics which is encoded in the  $s$ -wave scattering length, but only on momentum scales of the order of the Fermi momentum, we build effective low-momentum interactions that reproduce the scattering phase shifts of the contact interaction below some momentum cutoff. Inspired by recent successes of this method in nuclear structure theory, we use these interactions to describe the equation of state of the Fermi gas in the framework of Hartree-Fock-Bogoliubov theory with perturbative corrections. In the BCS regime, there is a range of cutoffs where we obtain fully converged results. Near unitarity, convergence is not yet reached, but we obtain promising results for the ground-state energies close to the experimental ones. Limitations and possible extensions of the approach are discussed.

DOI: [10.1103/PhysRevA.103.063306](https://doi.org/10.1103/PhysRevA.103.063306)

## I. INTRODUCTION

The study of ultracold Fermi gases opens new and exciting avenues into the rich physics of fermions, where one can observe the effects of quantum degeneracy and interactions and explore regions of strong correlations, for example, the crossover from the BCS to the BEC state, including the unitary limit, where the scattering length diverges [1]. The progress made in the theoretical understanding has been intimately coupled to the experimental observation of these phenomena using advanced trapping and cooling techniques and the possibility to tune the interaction between alkali atoms such as  $^6\text{Li}$  or  $^{40}\text{K}$  via Feshbach resonances.

In nuclear physics, it is well known that the  $s$ -wave scattering length between two nucleons in the spin-singlet channel is very large compared to the range of the interaction. Furthermore, in neutron stars, the neutrons in the inner layers of the crust are in a strongly correlated (almost) unitary regime. Therefore, much can be gleaned by the connection between cold Fermi gases near the unitary limit and low-energy nucleons.

Since in the case of ultracold atoms the range of the interaction is about four orders of magnitude smaller than the typical interparticle spacing, the interaction between two fermions has been usually modeled as a contact interaction with a coupling constant  $g$ . This simplifies the many-body calculations, as the interactions get restricted to the  $s$  wave. The use of this so-called single-channel model is valid in the case of a broad Feshbach resonance [2]. However, such an interaction has to

be regularized, which can be done by choosing a momentum cutoff  $\Lambda$ . Fixing the coupling constant for a given cutoff by the requirement that it should reproduce the physical scattering length  $a$ , one gets [3]

$$\frac{1}{g} = \frac{m}{4\pi a} - \frac{m\Lambda}{2\pi^2}, \quad (1)$$

where  $m$  is the atom mass. This shows that the coupling constant vanishes when  $\Lambda \rightarrow \infty$  and hence particle-particle ladders have to be resummed in order to get a nonvanishing contribution [4]. However, for a realistic description of the atom-atom interaction, the limit  $\Lambda \rightarrow \infty$  must be taken, since otherwise the finite cutoff results in an effective range of the interaction,  $r_{\text{eff}} = 4/(\pi\Lambda)$ .

In nuclear structure theory, the idea of using renormalization group (RG) approaches to get low-momentum effective interactions has allowed for major advances over the past two decades [5]. In the two-body sector, starting with the  $s$ -wave  $T$ -matrix equation,

$$T_0(k, k'; E) = V_0(k, k') + \frac{2}{\pi} \int_0^\Lambda dq q^2 \frac{V_0(k, q) T_0(q, k'; E)}{E - q^2/m}, \quad (2)$$

where  $V_0$  denotes the interaction in the  $s$  wave,  $E$  is the total energy of the pair, and  $k$  and  $k'$  are the incoming and outgoing momenta in the center of mass frame, the intermediate states are cut off at  $\Lambda$ . The requirement that the two-body observables (bound states and phase shifts at momenta below the cutoff) must be independent of the cutoff leads to a  $\Lambda$ -dependent effective low-momentum interaction called  $V_{\text{low-}k}$ . Therefore, contrary to what is done in cold-atom physics, the cutoff  $\Lambda$  for the low-momentum interaction is

\*urban@ijclab.in2p3.fr

†suna@physics.iitm.ac.in

not only finite but typically lowered as much as possible to include just the relevant momentum scales of the problem. Such low-momentum interactions are “soft” and hence have the advantage that many-body calculations become more perturbative.

To give an example, using RG softened interactions derived from chiral perturbation theory, including the three-body force, one gets bound nuclei already at the Hartree-Fock (HF) [6] or Hartree-Fock-Bogoliubov (HFB)<sup>1</sup> [7] level and obtains satisfactory results for ground-state energies if one includes perturbatively corrections to the HF(B) ground state. As another example, we mention our recent work on screening of the pairing interaction in neutron matter [8], where the use of a small cutoff allowed us to retrieve the Gorkov-Melik-Barkhudarov result [9] in the low-density limit without the resummation of ladder diagrams in the (three-particle-one-hole and one-particle-three-hole) vertices.

The aim of this paper is to try this strategy, which is very successful in nuclear physics, in the case of ultracold Fermi gases in the BCS-BEC crossover. On the one hand, the situation is more favorable in the case of cold atoms, namely in what concerns the three-body force. While the  $\Lambda$  dependence of  $V_{\text{low-}k}$  completely accounts for the effects of the intermediate states beyond  $\Lambda$  in the two-body sector, this is not true in the many-body sector. There, the RG running generates  $\Lambda$ -dependent three- and higher body forces [10–12]. The leading three-body term is of the form  $(\psi^\dagger \psi)^3$ , where  $\psi$  is the field operator. Because of the Pauli principle, this term can only contribute if  $\psi$  has at least three components, which is the case in nuclear physics (neutrons and protons with spin  $\uparrow$  and  $\downarrow$ ), but not in ultracold atoms with only two spin states. On the other hand, the pairing correlations can become much more important in ultracold atoms than in nuclei, especially near unitarity and on the BEC side ( $a > 0$ ). Far on the BEC side, the lowest excitations are molecules out of the condensate, which clearly require a nonperturbative resummation of ladder diagrams. Therefore, we will limit ourselves in the present work to the BCS side ( $a < 0$ ) of the crossover, up to the unitary limit.

The paper is organized as follows. In Sec. II, we set up a separable interaction which exactly reproduces the two-body scattering phase shifts of a contact interaction up to the cutoff. The elements of HFB and the Bogoliubov many-body perturbation theory (BMBPT) are set up in Secs. III and IV. We present our results in Sec. V and our conclusions in Sec. VI, where we discuss perspectives for future work. Some technical details and lengthy equations are relegated to the Appendixes. Throughout the paper, we use units with  $\hbar = 1$ , where  $\hbar$  is the reduced Planck constant.

## II. SEPARABLE FORM OF A CONTACT INTERACTION

The scattering phase shifts of two particles, 1 and 2, with opposite spins,  $\uparrow$  and  $\downarrow$ , interacting via a contact interaction

with  $s$ -wave scattering length  $a$ , are given by

$$\delta(q) = \text{arccot}\left(-\frac{1}{qa}\right), \quad (3)$$

where  $q = q'$  is the momentum in the center of mass frame, i.e.,  $\mathbf{q} = (\mathbf{p}_1 - \mathbf{p}_2)/2$  and  $\mathbf{q}' = (\mathbf{p}'_1 - \mathbf{p}'_2)/2$ , if in- and outgoing momenta of the two particles are denoted  $\mathbf{p}_{1,2}$  and  $\mathbf{p}'_{1,2}$ , respectively.

We want to describe the system with a Hamiltonian written in second quantization as

$$\hat{H} = \sum_{\mathbf{p}\sigma} \frac{p^2}{2m} a_{\sigma\mathbf{p}}^\dagger a_{\sigma\mathbf{p}} + \sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}'_1\mathbf{p}'_2} V_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}'_1\mathbf{p}'_2} a_{\mathbf{p}_1\uparrow}^\dagger a_{\mathbf{p}_2\downarrow}^\dagger a_{\mathbf{p}'_2\downarrow} a_{\mathbf{p}'_1\uparrow}. \quad (4)$$

This form is written for a finite volume  $\mathcal{V}$ , but as usual, in the limit of a large system, the summations over momenta will be replaced by integrals:

$$\sum_{\mathbf{p}} \cdots \rightarrow \frac{\mathcal{V}}{(2\pi)^3} \int d^3p \cdots. \quad (5)$$

Since a contact interaction acts only in the  $s$  wave ( $l = 0$ ), we write it in the conventions that are common if one works in a partial-wave basis as

$$V_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}'_1\mathbf{p}'_2} = \frac{1}{\mathcal{V}} 4\pi V_0(q, q') \delta_{\mathbf{Q}, \mathbf{Q}'}, \quad (6)$$

where  $\mathbf{Q} = \mathbf{p}_1 + \mathbf{p}_2$  and  $\mathbf{Q}' = \mathbf{p}'_1 + \mathbf{p}'_2$  are the incoming and outgoing total momenta. The factor  $1/\mathcal{V}$  in Eq. (6) ensures that  $V_0(q, q')$  (having dimension energy times volume) is independent of  $\mathcal{V}$ .

Our aim is to construct a separable interaction of the form

$$V_0(q, q') = g_0 F(q) F(q'), \quad (7)$$

which reproduces the phase shifts (3) below some cutoff  $\Lambda$  but tends toward zero above this cutoff. In Eq. (7),  $g_0$  denotes the coupling constant and  $F(q)$  is the form factor [normalized to  $F(0) = 1$ ]. If the interaction tends to zero at high momenta, this implies that the phase shifts also tend to zero.

Rather than determining  $F(q)$  from the RG evolution as is done for  $V_{\text{low-}k}$ , we find it easier to impose the behavior of the phase shifts as follows:

$$\delta(q) = R\left(\frac{q}{\Lambda}\right) \text{arccot}\left(-\frac{1}{qa}\right), \quad (8)$$

where  $R(x)$  is a regulator function. This approach was also followed in Refs. [13–16], where the authors used a sharp regulator  $\theta(1 - x)$ . However, for better numerical convergence near  $q = \Lambda$ , we prefer an exponential regulator of the form  $R(x) = \exp(-x^{2n})$ , where  $n$  is a parameter that determines how smoothly  $R(x)$  drops from 1 to 0 near  $x = 1$ . The phase shifts of a contact interaction (black solid line) and examples of phase shifts cut off at different  $\Lambda$  (dashed lines) are displayed in the upper panel of Fig. 1 for the case  $n = 10$ . One sees that in practice the regulator can be set to zero beyond some momentum  $\Lambda'$ , where the ratio  $\Lambda'/\Lambda > 1$  depends on the smoothness parameter  $n$ . In our calculations, we choose

<sup>1</sup>In Ref. [7], the interaction was softened by the similarity renormalization group (SRG) instead of  $V_{\text{low-}k}$ .

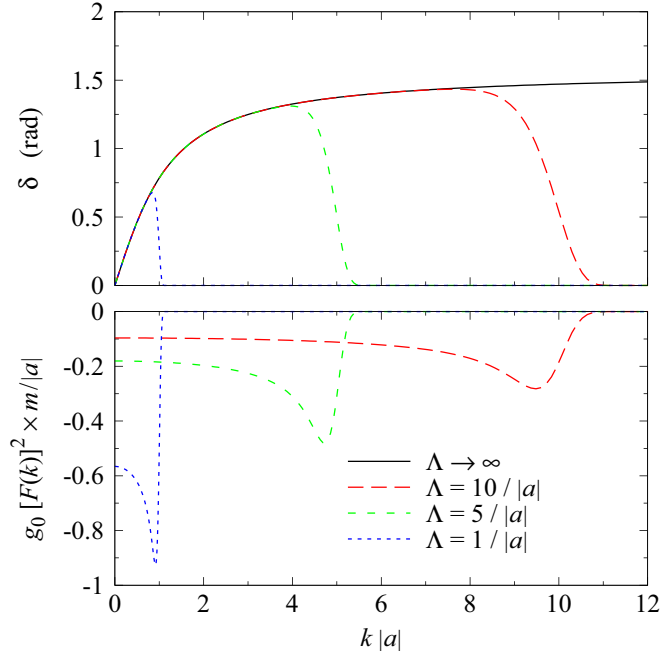


FIG. 1. Momentum dependence of the phase shifts multiplied by the regulator, and of the corresponding diagonal matrix elements of the potential, for different cutoffs (quantities made dimensionless by multiplication with the appropriate powers of  $|a|$  and  $m$ ).

$\Lambda'$  such that  $R(\Lambda'/\Lambda) = 10^{-10}$  which in the case  $n = 10$  gives  $\Lambda' \approx 1.17 \Lambda$ .

The problem of finding the separable interaction corresponding to given phase shifts  $\delta(q)$  was solved long ago by Tabakin [17]: The diagonal elements of the interaction, for particles of mass  $m$ , can be computed with a principal-value integral as

$$V_0(q, q) = -\frac{\sin \delta(q)}{mq} \exp\left(\frac{2}{\pi} \mathcal{P} \int_0^\infty dq' \frac{q' \delta(q')}{q^2 - q'^2}\right), \quad (9)$$

from which follow the coupling constant and form factor

$$g_0 = V_0(0, 0), \quad F(q) = \sqrt{V_0(q, q)/g_0}. \quad (10)$$

In the case  $a > 0$ , when the potential has a bound state with binding energy  $1/(ma^2)$ , the right-hand side of Eq. (9) gets an additional factor  $1 + 1/(qa)^2$  [17, 18]. Equation (9) was used in Refs. [13] and [16] to derive an analytical expression for the separable interaction in the unitary limit with a sharp cutoff.

As an illustration, we display in the lower panel of Fig. 1 the diagonal matrix elements of the potential corresponding to the phase shifts with different cutoffs shown in the upper panel. The coupling constant increases when the cutoff is lowered, thereby compensating the missing contribution from intermediate states which are cut off by the regulator. Nevertheless, the procedure explained here is not equivalent to the simpler prescription (1), corresponding to  $g_0 = g/(4\pi)$  and  $F(q) = \theta(\Lambda - q)$ , preserving only the scattering length  $a$  but not the momentum dependence of the phase shifts up to the cutoff. In the present case, the form factor  $F(q)$  is a nontrivial function of momentum, which ensures that not only the scattering length  $a$  but the entire momentum dependence of the phase shifts remains cutoff independent, as is the case

with  $V_{\text{low-}k}$ . Actually,  $V_{\text{low-}k}$  for the neutron-neutron interaction in the  $s$  wave resembles very much our separable interaction if  $\Lambda \ll 1/r_{\text{eff}}$ , as shown in Fig. 11 of Ref. [8].

### III. HARTREE-FOCK-BOGOLIUBOV

It is well known that BCS mean-field theory can qualitatively describe the BCS-BEC crossover. In the cold-atom literature, this theory is usually defined by the gap and number equations [Eqs. (21) and (25) below] with a contact interaction regularized according to Eq. (1) in the limit  $\Lambda \rightarrow \infty$ . However, in the weak-coupling regime (i.e.,  $1/(\beta_F a) \ll -1$ , where  $k_F$  is the Fermi momentum), the gap is exponentially suppressed and the dominant energy correction compared to the ideal gas comes from the normal part of the self-energy (i.e., the diagonal part in Nambu-Gorkov formalism). In the limit  $\Lambda \rightarrow \infty$ , the calculation of this self-energy requires the resummation of ladder diagrams as done, e.g., in Ref. [4], whereas in the present framework, we obtain it already at the HF level. The mean-field theory including both the HF self-energy and the pairing gap is called HFB theory.

Following Ref. [19], we start by defining the quasiparticle operators<sup>2</sup>

$$\beta_{\mathbf{k}\uparrow} = u_{\mathbf{k}} a_{\mathbf{k}\uparrow} - v_{\mathbf{k}} a_{-\mathbf{k}\downarrow}^\dagger, \quad \beta_{\mathbf{k}\downarrow} = u_{\mathbf{k}} a_{\mathbf{k}\downarrow} + v_{\mathbf{k}} a_{-\mathbf{k}\uparrow}^\dagger \quad (11)$$

with  $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ . This Bogoliubov transformation can be inverted to rewrite the creation and annihilation operators  $a_{\mathbf{k}\sigma}^\dagger$  and  $a_{\mathbf{k}\sigma}$  in terms of the quasiparticle creation and annihilation operators  $\beta_{\mathbf{k}\sigma}^\dagger$  and  $\beta_{\mathbf{k}\sigma}$ . For example, the annihilation operators can be expressed as

$$a_{\mathbf{k}\uparrow} = u_{\mathbf{k}} \beta_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \beta_{-\mathbf{k}\downarrow}^\dagger, \quad a_{\mathbf{k}\downarrow} = u_{\mathbf{k}} \beta_{\mathbf{k}\downarrow} - v_{\mathbf{k}} \beta_{-\mathbf{k}\uparrow}^\dagger. \quad (12)$$

Let us now consider the operator

$$\hat{K} = \hat{H} - \mu \hat{N} \quad (13)$$

with  $\hat{H}$  being the Hamiltonian defined in Eq. (4),  $\hat{N}$  being the particle-number operator

$$\hat{N} = \sum_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}, \quad (14)$$

and  $\mu$  being the chemical potential. Following the usual procedure [19], one obtains the expressions for the  $u$  and  $v$  factors:

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2} + \frac{\xi_{\mathbf{k}}}{2E_{\mathbf{k}}}}, \quad v_{\mathbf{k}} = \sqrt{\frac{1}{2} - \frac{\xi_{\mathbf{k}}}{2E_{\mathbf{k}}}}, \quad (15)$$

where

$$\xi_{\mathbf{k}} = \frac{k^2}{2m} + U_{\mathbf{k}} - \mu, \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}, \quad (16)$$

with a HF-like mean field  $U_{\mathbf{k}}$  and the gap  $\Delta_{\mathbf{k}}$ .

The gap equation reads

$$\Delta_{\mathbf{k}} = -\frac{2}{\pi} \int_0^{\Lambda'} dp p^2 V_0(k, p) \frac{\Delta_p}{2E_p}. \quad (17)$$

<sup>2</sup>In the notation of Ref. [19], our operators  $\beta_{\mathbf{k}\uparrow}$  and  $\beta_{\mathbf{k}\downarrow}$  correspond to the operators  $\alpha_{\mathbf{k}}$  and  $\beta_{\mathbf{k}}$ , respectively.

Because of the separable form of the interaction, it is evident that the momentum dependence of the gap  $\Delta_k$  is given by

$$\Delta_k = \Delta_0 F(k), \quad (18)$$

and solving the gap equation amounts to simply finding the number  $\Delta_0$  for which the following equation is satisfied:

$$\frac{1}{g_0} = -\frac{2}{\pi} \int_0^{\Lambda'} dp p^2 \frac{[F(p)]^2}{2E_p}, \quad (19)$$

with  $E_p = \sqrt{\xi_p^2 + [\Delta_0 F(p)]^2}$ . Using the relationship between  $g_0$  and the scattering length  $a$  in free space,

$$\frac{1}{a} = \frac{1}{mg_0} + \frac{2}{\pi} \int_0^{\Lambda'} dp [F(p)]^2, \quad (20)$$

one can rewrite Eq. (19) in the form

$$\frac{1}{a} = -\frac{2}{\pi} \int_0^{\Lambda'} dp [F(p)]^2 \left( \frac{p^2}{2mE_p} - 1 \right), \quad (21)$$

which has the advantage that the integrand tends toward zero more smoothly, already before  $p$  approaches the cutoff  $\Lambda'$ , and one can see that the gap equation remains well defined in the limit  $\Lambda \rightarrow \infty$ .

So far, we have only discussed the gap but not the mean field  $U_k$ . In the literature on ultracold atoms, the latter is usually not taken into account, because it vanishes in the limit  $\Lambda \rightarrow \infty$  [4]. It is given by

$$U_k = \int \frac{d^3p}{(2\pi)^3} \left( \frac{1}{2} - \frac{\xi_p}{2E_p} \right) 4\pi V_0 \left( \frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{p}-\mathbf{k}}{2} \right). \quad (22)$$

For the numerical calculation of  $U_k$ , it is useful to define an interaction that is averaged over the angle  $\theta$  between  $\mathbf{k}$  and  $\mathbf{p}$  as follows:

$$\bar{V}_0(k, p) = \frac{1}{2} \int_{-1}^1 d \cos \theta V_0 \left( \frac{\mathbf{p}-\mathbf{k}}{2}, \frac{\mathbf{p}-\mathbf{k}}{2} \right). \quad (23)$$

In terms of this angle-averaged interaction, the mean field can now be written as

$$U_k = \frac{1}{\pi} \int_0^{\Lambda'} dp p^2 \left( 1 - \frac{\xi_p}{E_p} \right) \bar{V}_0(k, p). \quad (24)$$

It turns out that  $U_k = 0$  for  $k > 3\Lambda'$ .

For a given chemical potential  $\mu$ , the HFB density reads

$$n_{\text{HFB}} = \frac{N_{\text{HFB}}}{\mathcal{V}} = \frac{1}{2\pi^2} \int_0^{\Lambda'} dk k^2 \left( 1 - \frac{\xi_k}{E_k} \right). \quad (25)$$

Therefore, if one wants to obtain results for a given density  $n$  and not for a given chemical potential  $\mu$ , one has to determine  $\mu$  by solving the equation  $n = n_{\text{HFB}}(\mu)$  simultaneously with the gap equation.

Finally, the ground-state energy density is given by

$$\frac{\mathcal{E}_{\text{HFB}}}{\mathcal{V}} = \frac{1}{4\pi^2} \int_0^{\Lambda'} dk k^2 \left[ \left( 1 - \frac{\xi_k}{E_k} \right) \left( \frac{k^2}{m} + U_k \right) - \frac{\Delta_k^2}{E_k} \right]. \quad (26)$$

## IV. BOGOLIUBOV MANY-BODY PERTURBATION THEORY

### A. Perturbative corrections to the HFB ground-state energy

The HFB theory may be a good starting point, but generally corrections to it are needed. In particular, the energy shift due to the HF field that we have just discussed is roughly proportional to the coupling constant  $g_0$  and hence strongly dependent on the choice of the cutoff  $\Lambda$ , whereas physical results should be of course cutoff independent. We therefore expect that, by including higher order corrections, if these converge to the exact value of the ground-state energy, the cutoff dependence should cancel out.

Expressing in  $\hat{K}$  the operators  $a^\dagger$  and  $a$  in terms of quasi-particle operators  $\beta^\dagger$  and  $\beta$ , and normal ordering with respect to these (i.e., putting all  $\beta^\dagger$  operators to the left of the  $\beta$  operators), one can write  $\hat{K}$  in the form

$$\hat{K} = K_{00} + \hat{K}_{11} + \hat{K}_{40} + \hat{K}_{31} + \hat{K}_{22} + \hat{K}_{13} + \hat{K}_{04}, \quad (27)$$

where  $\hat{K}_{ij}$  represents the terms having products of  $i$  quasi-particle creation operators  $\beta^\dagger$  followed by  $j$  quasiparticle annihilation operators  $\beta$ . Notice that there are no terms  $\hat{K}_{20}$  and  $\hat{K}_{02}$  with two  $\beta^\dagger$  or two  $\beta$  operators, because these terms vanish if the  $u$  and  $v$  factors are determined according to Eq. (15). The first term,  $K_{00}$ , is just a  $c$ -number and obviously it corresponds to the expectation value of  $\hat{K}$  in the state that has no quasiparticles, i.e., in the HFB ground state:

$$K_{00} = \mathcal{E}_{\text{HFB}} - \mu N_{\text{HFB}}. \quad (28)$$

The second term,  $\hat{K}_{11}$ , has the simple form

$$\hat{K}_{11} = \sum_{\mathbf{k}\sigma} E_k \beta_{\mathbf{k}\sigma}^\dagger \beta_{\mathbf{k}\sigma}. \quad (29)$$

Hence, the eigenstates and eigenvalues of

$$\hat{K}_0 = K_{00} + \hat{K}_{11} \quad (30)$$

are simple and known: Its ground state is the HFB state  $|0^{(0)}\rangle = |\text{HFB}\rangle$  with eigenvalue  $\Omega_0^{(0)} = K_{00}$ , the lowest excited states are one-quasiparticle (1qp) states  $|(\mathbf{k}\sigma)^{(0)}\rangle = \beta_{\mathbf{k}\sigma}^\dagger |\text{HFB}\rangle$  with eigenvalues  $\Omega_{\mathbf{k}\sigma}^{(0)} = K_{00} + E_k$ , followed by the two-quasiparticle (2qp) states  $|(\mathbf{k}_1\sigma_1\mathbf{k}_2\sigma_2)^{(0)}\rangle = \beta_{\mathbf{k}_1\sigma_1}^\dagger \beta_{\mathbf{k}_2\sigma_2}^\dagger |\text{HFB}\rangle$  with eigenvalues  $\Omega_{\mathbf{k}_1\sigma_1\mathbf{k}_2\sigma_2}^{(0)} = K_{00} + E_{k_1} + E_{k_2}$ , and so on.

We will denote the remaining terms of  $\hat{K}$  as

$$\hat{W} = \hat{K}_{40} + \hat{K}_{31} + \hat{K}_{22} + \hat{K}_{13} + \hat{K}_{04} \quad (31)$$

and introduce a formal parameter  $\lambda$  (where the physical situation corresponds to  $\lambda = 1$ ) to write

$$\hat{K} = \hat{K}_0 + \lambda \hat{W}. \quad (32)$$

Following, e.g., the book by Sakurai [20], we can now apply time-independent perturbation theory, i.e., an expansion of the eigenstates and eigenvalues of  $\hat{K}$  in powers of  $\lambda$ , where  $\hat{K}_0$ ,  $\hat{W}$ , and  $\Omega_\mu^{(0)}$  play the roles of the unperturbed Hamiltonian  $H_0$ , the perturbation  $V$ , and the unperturbed energies  $E_\mu^{(0)}$ , respectively. This is exactly what was done in Ref. [7] and called there Bogoliubov many-body perturbation theory (BMBPT), generalizing the usual many-body perturbation theory (MBPT) on top of HF to the case with pairing. To



fix our notations, which are slightly different from those of Ref. [7], we write the expansion of the ground state  $|0\rangle$  up to some order  $n$  and the corresponding eigenvalue  $\Omega_0$  as

$$|0\rangle \approx \sum_{i=0}^n \lambda^i |0^{(i)}\rangle, \quad \Omega_0 \approx \sum_{i=0}^{n+1} \lambda^i \Omega_0^{(i)}. \quad (33)$$

The leading ( $i = 0$ ) contributions correspond to the HFB result. The first corrections to the ground state are given by

$$|0^{(1)}\rangle = \sum_{\mu \neq 0} |\mu^{(0)}\rangle \frac{\langle \mu^{(0)} | \hat{W} | 0^{(0)} \rangle}{\Omega_0^{(0)} - \Omega_\mu^{(0)}}, \quad (34)$$

$$|0^{(2)}\rangle = \sum_{\mu \nu \neq 0} |\nu^{(0)}\rangle \frac{\langle \nu^{(0)} | \hat{W} | \mu^{(0)} \rangle \langle \mu^{(0)} | \hat{W} | 0^{(0)} \rangle}{(\Omega_0^{(0)} - \Omega_\nu^{(0)})(\Omega_0^{(0)} - \Omega_\mu^{(0)})}, \quad (35)$$

where we have used the fact that  $\Omega_0^{(1)} = \langle 0^{(0)} | \hat{W} | 0^{(0)} \rangle = 0$ . The corresponding corrections to  $\Omega_0$  are

$$\Omega_0^{(2)} = \sum_{\mu \neq 0} \frac{\langle 0^{(0)} | \hat{W} | \mu^{(0)} \rangle \langle \mu^{(0)} | \hat{W} | 0^{(0)} \rangle}{\Omega_0^{(0)} - \Omega_\mu^{(0)}}, \quad (36)$$

$$\Omega_0^{(3)} = \sum_{\mu \nu \neq 0} \frac{\langle 0^{(0)} | \hat{W} | \nu^{(0)} \rangle \langle \nu^{(0)} | \hat{W} | \mu^{(0)} \rangle \langle \mu^{(0)} | \hat{W} | 0^{(0)} \rangle}{(\Omega_0^{(0)} - \Omega_\nu^{(0)})(\Omega_0^{(0)} - \Omega_\mu^{(0)})}. \quad (37)$$

At higher orders, there are “disconnected diagrams,” which have to be discarded [21], but this does not yet happen at the second and third orders considered here. In practice, since the only part of  $\hat{W}$  that gives a nonvanishing result when acting on  $|0^{(0)}\rangle$  is  $\hat{K}_{40}$ , the index  $\mu$  runs only over 4qp states with two  $\uparrow$  and two  $\downarrow$  quasiparticles. The same is true for the index  $\nu$  in Eq. (37) for  $\Omega_0^{(3)}$ , where the operator that acts on  $\langle 0^{(0)} |$  to the left must be  $\hat{K}_{04}$ . Consequently, in this equation, the  $\hat{W}$  operator in the middle must not change the number of quasiparticles, and therefore it must be  $\hat{K}_{22}$ . The situation is more difficult in Eq. (35) for the state  $|0^{(2)}\rangle$ , where the sum over  $\nu$  has to include also 2qp and 6qp states, which are generated when  $\hat{K}_{13}$  and  $\hat{K}_{31}$  act on the 4qp state  $|\mu^{(0)}\rangle$ .

From now on, since we are only interested in the ground state, we will simply write  $\Omega$  instead of  $\Omega_0$  for the lowest eigenvalue.

The question arises of how one can compute, e.g., the energy  $\mathcal{E}$  as a function of the density  $n = N/V$ . The problem is that  $\hat{N}$  does not commute with  $\hat{K}_0$ , although it commutes of course with  $\hat{K}$ . Therefore, as it is well known in HFB theory, the eigenstates of  $\hat{K}_0$  are not eigenstates of  $\hat{N}$ , and one may wonder what value one should use for  $N$ . Interestingly, one can show that up to order  $\lambda^3$ , the energy  $\mathcal{E}$  as a function of the density  $n = N/V$  can be immediately obtained from the expansion of the grand potential  $\Omega$  as follows:

$$\mathcal{E}(n_{\text{HFB}}(\mu)) = \mathcal{E}_{\text{HFB}}(\mu) + \lambda^2 \Omega^{(2)}(\mu) + \lambda^3 \Omega^{(3)}(\mu) + O(\lambda^4). \quad (38)$$

where  $\Omega^{(2)}$  and  $\Omega^{(3)}$  are second- and third-order corrections. These are explicitly computed in the following two subsections.

## B. Second-order BMBPT correction

As mentioned before, the second-order correction (36) requires us to sum over 4qp states having two  $\uparrow$  and two  $\downarrow$  quasiparticles and zero total momentum ( $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4 = 0$ )

$$|\mu^{(0)}\rangle = \beta_{\mathbf{k}_1\uparrow}^\dagger \beta_{\mathbf{k}_2\downarrow}^\dagger \beta_{\mathbf{k}_3\uparrow}^\dagger \beta_{\mathbf{k}_4\downarrow}^\dagger |0^{(0)}\rangle \quad (39)$$

with energies

$$\Omega_\mu^{(0)} = \Omega_0^{(0)} + E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}. \quad (40)$$

Notice that permutations of  $\mathbf{k}_1$  and  $\mathbf{k}_3$  or of  $\mathbf{k}_2$  and  $\mathbf{k}_4$  do not generate a different state, so when integrating over all momenta one has to divide by 4. Therefore, Eq. (36) becomes

$$\Omega^{(2)} = -\frac{1}{4} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} \frac{|\langle 0^{(0)} | \hat{K}_{04} \beta_{\mathbf{k}_1\uparrow}^\dagger \beta_{\mathbf{k}_2\downarrow}^\dagger \beta_{\mathbf{k}_3\uparrow}^\dagger \beta_{\mathbf{k}_4\downarrow}^\dagger | 0^{(0)} \rangle|^2}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}, \quad (41)$$

with  $\mathbf{k}_4 = -\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3$ . The explicit form of  $\hat{K}_{04}$  is obtained by inserting Eq. (12) into Eq. (4) with Eq. (6) and keeping only the term with four  $\beta$  operators

$$\begin{aligned} \hat{K}_{04} = & -\frac{4\pi}{V} \sum_{\mathbf{p}_1 \dots \mathbf{p}_4} V_0(q_{12}, q_{34}) \delta_{\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3 + \mathbf{p}_4, 0} \\ & \times u_{p_1} u_{p_2} v_{p_3} v_{p_4} \beta_{\mathbf{p}_4\downarrow} \beta_{\mathbf{p}_3\uparrow} \beta_{\mathbf{p}_2\downarrow} \beta_{\mathbf{p}_1\uparrow}, \end{aligned} \quad (42)$$

where  $q_{ij} = |\mathbf{k}_i - \mathbf{k}_j|/2$ . For convenience, we have renamed the original momentum labels  $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}'_1, \mathbf{p}'_2$  of Eq. (4) into  $-\mathbf{p}_4, -\mathbf{p}_3, \mathbf{p}_1, \mathbf{p}_2$  and we have used  $V_0(q, q') = V_0(q', q)$ . It is straightforward to work out the matrix element in the numerator of Eq. (41):

$$\begin{aligned} & \langle 0^{(0)} | \hat{K}_{04} \beta_{\mathbf{k}_1\uparrow}^\dagger \beta_{\mathbf{k}_2\downarrow}^\dagger \beta_{\mathbf{k}_3\uparrow}^\dagger \beta_{\mathbf{k}_4\downarrow}^\dagger | 0^{(0)} \rangle \\ & = -\frac{4\pi}{V} [V_0(q_{12}, q_{34})(u_1 u_2 v_3 v_4 + v_1 v_2 u_3 u_4) \\ & \quad - V_0(q_{14}, q_{32})(v_1 u_2 u_3 v_4 + u_1 v_2 v_3 u_4)], \end{aligned} \quad (43)$$

where  $u_{k_i}$  and  $v_{k_i}$  are denoted as  $u_i$  and  $v_i$  for better readability. The square of this expression gives 10 terms, which after a suitable relabeling of the momenta [leaving the denominator of Eq. (41) unchanged] can be grouped together into three terms. The final expression reads

$$\Omega^{(2)} = -\frac{(4\pi)^2}{V^2} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} \frac{A + B + C}{E_1 + E_2 + E_3 + E_4}, \quad (44)$$

$$A = v_1^2 v_2^2 u_3^2 u_4^2 [V_0(q_{12}, q_{34})]^2, \quad (45)$$

$$B = u_1 v_1 u_2 v_2 u_3 v_3 u_4 v_4 [V_0(q_{12}, q_{34})]^2, \quad (46)$$

$$C = -2 u_1 v_1 v_2^2 u_3 v_3 u_4^2 V_0(q_{12}, q_{34}) V_0(q_{14}, q_{23}), \quad (47)$$

where  $E_i = E_{k_i}$ . These three terms can be interpreted diagrammatically as the three Goldstone-like diagrams shown in Fig. 2.

Notice that, in the limit of no pairing ( $\Delta_k = 0$ ), where  $u_k^2 = \theta(k - k_F)$ ,  $v_k^2 = \theta(k_F - k)$ , and  $u_k v_k = 0$ , only the term  $A$  contributes while the terms  $B$  and  $C$  vanish. Then the energy denominator becomes  $\xi_3 + \xi_4 - \xi_1 - \xi_2$ , and we recover the usual second-order correction to the HF energy.

In practice, the sums over the  $\mathbf{k}_i$  are replaced by integrals according to Eq. (5), so that  $\Omega^{(2)}$  becomes proportional to the

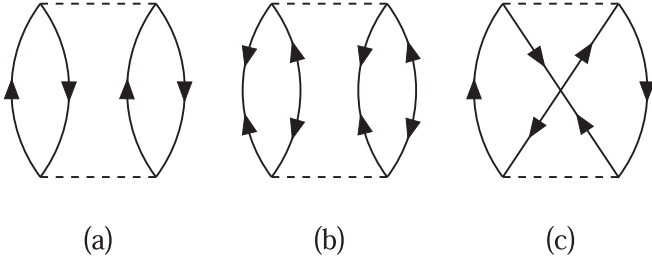


FIG. 2. Goldstone-like diagrams corresponding to the three terms in the second-order BMBPT contribution to the ground-state energy. Lines with upward-pointing arrows represent particles (factor  $u^2$ ), lines with downward-pointing arrows represent holes (factor  $v^2$ ), and lines with two opposite arrows represent anomalous propagators (factor  $uv$ ). The dashed lines represent the interaction. Diagram (a) is the only one that exists in the limit of no pairing.

volume  $\mathcal{V}$  as it should be, since  $\Omega$  is related to the pressure  $P$  by  $\Omega = -P\mathcal{V}$ .

The integrations are done with Monte Carlo sampling. Notice that for each integration variable  $\mathbf{k}_i$ , the integral can be written in the form  $\int d^3k_i w(k_i) f(k_i, \theta_i, \phi_i)$ , where  $w(k)$  is one of the functions  $v_k^2$ ,  $u_k v_k$ , or  $u_k^2$ , and all the angle dependence is in the remaining function  $f$ . If the integrand contains a factor of  $v_k^2$  or  $u_k v_k$ , the integration region is automatically limited to  $k < \Lambda'$ , because  $v_k = 0$  for  $k > \Lambda'$ . However, if the integrand contains a factor of  $u_k^2$ , as it is the case for the  $\mathbf{k}_3$  integration in term A, it is only cut off through the interaction term  $[V_0(q_{12}, q_{34})]^2$  contained in the function  $f$ , which vanishes for  $q_{34} > \Lambda'$ . In this case, combining the constraints  $k_1, k_2, q_{34} < \Lambda'$  and momentum conservation  $\mathbf{k}_3 = (2\mathbf{q}_{34} - \mathbf{k}_1 - \mathbf{k}_2)/2$ , one sees that  $k_3$  is limited to the region  $k_3 < 2\Lambda'$ . We implement importance sampling to efficiently distribute the integration points along  $k_i$ , according to the weights  $k_i^2 w(k_i)$  by introducing three transformations of variables. For each function  $w(k)$ , we define a function

$$x_w(p) = \int_0^p dk k^2 w(k). \quad (48)$$

We also define the corresponding inverse functions  $p_w(x)$  such that  $p_w(x_w(p)) = p$ . Hence, we can write

$$\begin{aligned} & \int d^3k_i w(k_i) f(k_i, \theta_i, \phi_i) \\ &= \int_0^{x_w(k_{i\max})} dx_i \int_{-1}^1 d \cos \theta_i \int_0^{2\pi} d\phi_i f(p_w(x_i), \theta_i, \phi_i), \end{aligned} \quad (49)$$

with  $k_{i\max} = \Lambda'$  or  $2\Lambda'$ , respectively, as discussed above. The advantage of these transformations is that now uniformly distributed random variables  $x_i$  correspond to momenta  $k_i = p_w(x_i)$  whose distributions automatically account for the factors  $k_i^2 w(k_i)$  in the integrand.

Finally, because of rotational invariance, the integrand depends only on relative angles. Therefore, we may choose without any loss of generality  $\mathbf{k}_1$  in  $z$  direction and  $\mathbf{k}_2$  in the  $xz$  plane, so that the integrations over  $\cos \theta_1$ ,  $\phi_1$ , and  $\phi_2$  become trivial.

### C. Third-order BMBPT correction

According to Eq. (37) and the discussion below that equation, the third-order correction is given by

$$\begin{aligned} \Omega_0^{(3)} &= \frac{1}{16} \sum_{\mathbf{k}_1 \dots \mathbf{k}_8} \frac{1}{E_{1,2,3,4} E_{5,6,7,8}} \\ &\times \langle 0^{(0)} | \hat{K}_{04} \beta_{\mathbf{k}_1 \uparrow}^\dagger \beta_{\mathbf{k}_2 \downarrow}^\dagger \beta_{\mathbf{k}_3 \uparrow}^\dagger \beta_{\mathbf{k}_4 \downarrow}^\dagger | 0^{(0)} \rangle \\ &\times \langle 0^{(0)} | \beta_{\mathbf{k}_4 \downarrow} \beta_{\mathbf{k}_3 \uparrow} \beta_{\mathbf{k}_2 \downarrow} \beta_{\mathbf{k}_1 \uparrow} \hat{K}_{22} \beta_{\mathbf{k}_5 \uparrow}^\dagger \beta_{\mathbf{k}_6 \downarrow}^\dagger \beta_{\mathbf{k}_7 \uparrow}^\dagger \beta_{\mathbf{k}_8 \downarrow}^\dagger | 0^{(0)} \rangle \\ &\times \langle 0^{(0)} | \beta_{\mathbf{k}_8 \downarrow} \beta_{\mathbf{k}_7 \uparrow} \beta_{\mathbf{k}_6 \downarrow} \beta_{\mathbf{k}_5 \uparrow} \hat{K}_{40} | 0^{(0)} \rangle, \end{aligned} \quad (50)$$

with the abbreviations

$$E_{1,2,3,4} = E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4} \quad (51)$$

and so on. Analogous to the factor  $1/4$  in Eq. (41), the factor  $1/16$  in Eq. (50) takes into account that permutations  $\mathbf{k}_1 \leftrightarrow \mathbf{k}_3$ ,  $\mathbf{k}_2 \leftrightarrow \mathbf{k}_4$ , etc., describe the same state and therefore must be counted only once. Momentum conservation in  $\hat{K}_{04}$  and  $\hat{K}_{40}$  require that  $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4 = \mathbf{k}_5 + \mathbf{k}_6 + \mathbf{k}_7 + \mathbf{k}_8 = 0$ . The explicit expression of  $\hat{K}_{22}$  reads

$$\begin{aligned} \hat{K}_{22} &= \frac{4\pi}{\mathcal{V}} \sum_{\mathbf{p}_1 \dots \mathbf{p}_4} \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}_3 + \mathbf{p}_4} \left\{ \left[ V_0 \left( \frac{|\mathbf{p}_1 - \mathbf{p}_2|}{2}, \frac{|\mathbf{p}_3 - \mathbf{p}_4|}{2} \right) (u_{p_1} u_{p_2} u_{p_3} u_{p_4} + v_{p_1} v_{p_2} v_{p_3} v_{p_4}) \right. \right. \\ &+ V_0 \left( \frac{|\mathbf{p}_1 + \mathbf{p}_3|}{2}, \frac{|\mathbf{p}_2 + \mathbf{p}_4|}{2} \right) (u_{p_1} v_{p_2} v_{p_3} u_{p_4} + v_{p_1} u_{p_2} u_{p_3} v_{p_4}) \left. \beta_{\mathbf{p}_1 \uparrow}^\dagger \beta_{\mathbf{p}_2 \downarrow}^\dagger \beta_{\mathbf{p}_4 \downarrow} \beta_{\mathbf{p}_3 \uparrow} \right. \\ &\left. \left. - V_0 \left( \frac{|\mathbf{p}_1 + \mathbf{p}_4|}{2}, \frac{|\mathbf{p}_2 + \mathbf{p}_3|}{2} \right) [u_{p_1} v_{p_2} u_{p_3} v_{p_4} \beta_{\mathbf{p}_1 \uparrow}^\dagger \beta_{\mathbf{p}_2 \uparrow}^\dagger \beta_{\mathbf{p}_4 \uparrow} \beta_{\mathbf{p}_3 \uparrow} + v_{p_1} u_{p_2} v_{p_3} u_{p_4} \beta_{\mathbf{p}_1 \downarrow}^\dagger \beta_{\mathbf{p}_2 \downarrow}^\dagger \beta_{\mathbf{p}_4 \downarrow} \beta_{\mathbf{p}_3 \downarrow}] \right] \right\}. \end{aligned} \quad (52)$$

One can easily see that  $\hat{K}_{22}$  changes only two out of the four quasiparticle momenta in Eq. (50). So, finally, there are only four independent momenta over which we have to integrate. Like the second-order correction, the third-order correction can again be interpreted in terms of Goldstone-like diagrams. Some examples for such diagrams are shown in Fig. 3. By relabeling the momenta and combining terms with the same weight functions, one

obtains finally an expression which is suitable for numerical integration using the importance-sampling method given in Eq. (49). The explicit formula is given in Appendix B.

As was the case for the second-order correction, the third-order correlation energy without pairing can be obtained by setting in this expression  $\Delta_k = 0$ ,  $v_k^2 = \theta(k_F - k)$ ,  $u_k^2 = \theta(k - k_F)$ , and  $u_k v_k = 0$ .

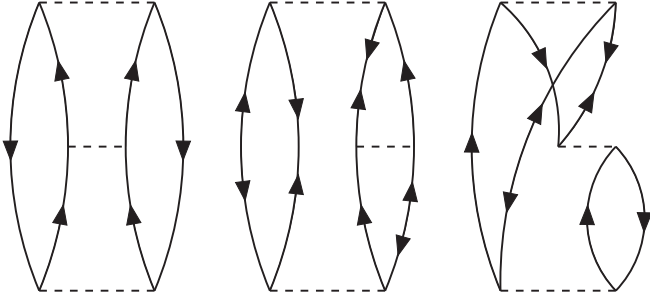


FIG. 3. Three examples out of the 27 distinct Goldstone-like diagrams for the third-order BMBPT correction to the ground-state energy.

## V. RESULTS

For a given interaction, the equation of state is given by the energy density  $\mathcal{E}/\mathcal{V}$  as a function of the density  $n = N/\mathcal{V}$ . In the case of a contact interaction, which is determined by the scattering length  $a$ , it can be reduced to a dimensionless function  $\mathcal{E}/\mathcal{E}_0$ , depending on one dimensionless parameter  $1/(k_F a)$ , where  $k_F = (3\pi^2 n)^{1/3}$  is the Fermi momentum and  $\mathcal{E}_0/\mathcal{V} = k_F^5/(10\pi^2 m)$  is the energy density of the ideal Fermi gas.

In our case, a complication arises from the cutoff  $\Lambda$ , leading to an additional dependence on the dimensionless parameter  $\Lambda/k_F$ . Ideally, the results should be independent of this unphysical parameter, but of course the cutoff must be always large enough to include all relevant degrees of freedom, i.e., at least  $\Lambda > k_F$ . Figure 4 shows the cutoff dependence of the ground-state energy  $\mathcal{E}$  in units of  $\mathcal{E}_0$ , obtained according

to Eq. (38), for different values of the parameter  $1/(k_F a)$ . The thick lines are the HFB (+ BMBPT) results, while the thin lines are HF (+ MBPT) results.

Let us start our discussion with the first two panels,  $1/(k_F a) = -5$  and  $-2$ , corresponding to the weak-coupling regime. In this regime, the pairing gap is so small that the thick and thin lines practically coincide, and the dominant contribution comes from the HF self-energy. Since the HF contribution is proportional to the coupling constant  $g_0$ , which tends toward zero for  $\Lambda \rightarrow \infty$ , it is not surprising that the HF(B) result (short blue dashes) shows a strong cutoff dependence. However, the situation improves once the perturbative corrections are included (green long dashes and red solid lines). In some range of not too large cutoffs ( $\Lambda/k_F \lesssim 2.5$ ), the cutoff dependence of the HF(B) energy is compensated by the cutoff dependence of the perturbative corrections already at third order. Furthermore, in this range of cutoffs, the perturbation expansion of the energy converges to the energy obtained in Ref. [23] from an expansion in powers of  $k_F a$  up to fourth order (purple dots).

When the interaction strength increases, the pairing gaps get bigger. Therefore, in the range  $-1 \leq 1/(k_F a) \leq 0$ , where the gas is strongly correlated, the HFB + BMBPT results markedly differ from the HF + MBPT ones. In particular, only when starting from HFB, one obtains a finite correction to the energy in the limit  $\Lambda \rightarrow \infty$ . As  $1/(k_F a)$  approaches 0, which is the unitary limit, the results are always cutoff dependent. However, it is worth noting that with the HFB + BMBPT, the cutoff dependence between the different orders of the perturbation theory is less compared to the HF + MBPT results. In the HFB + BMBPT case, we observe that, as a function of the cutoff, the energy has a minimum around  $\Lambda/k_F \approx 1.5$ .

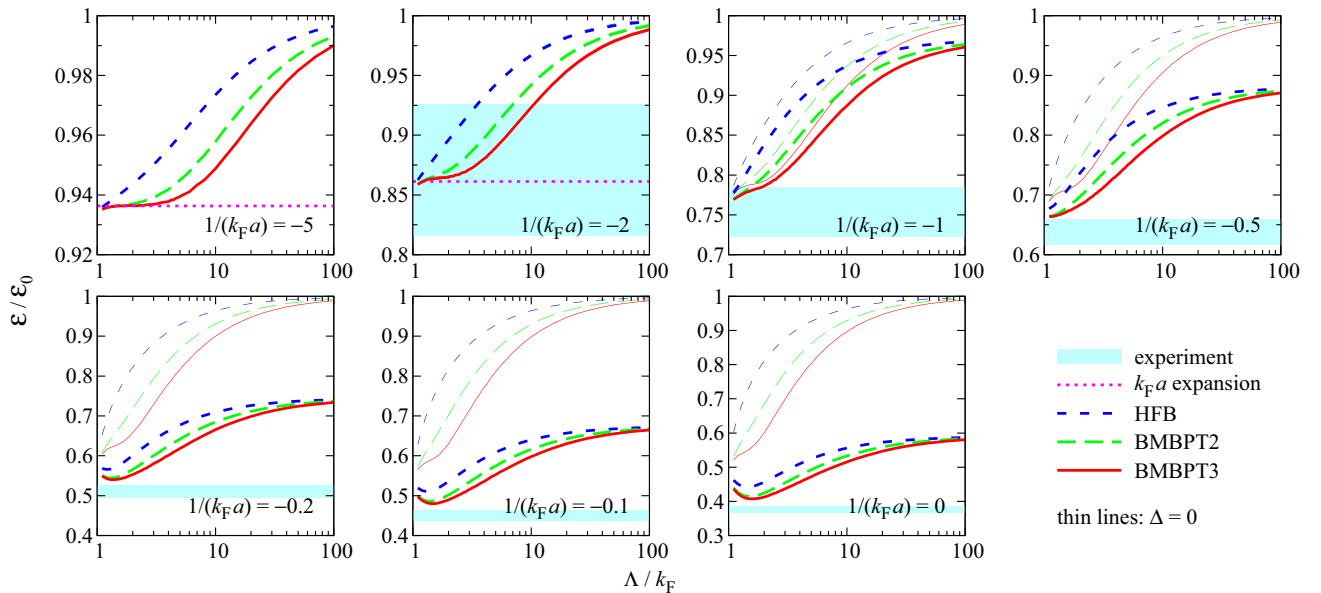


FIG. 4. Cutoff dependence of the computed ground-state energy  $\mathcal{E}$  in units of the energy of an ideal Fermi gas,  $\mathcal{E}_0$ , for seven values of the interaction parameter  $1/(k_F a)$  at different levels of approximation. Thick lines start from the HFB ground state,  $\mathcal{E}_{\text{HFB}}$  (blue short dashes),  $\mathcal{E}_{\text{BMBPT2}} = \mathcal{E}_{\text{HFB}} + \Omega^{(2)}$  (green long dashes), and  $\mathcal{E}_{\text{BMBPT3}} = \mathcal{E}_{\text{HFB}} + \Omega^{(2)} + \Omega^{(3)}$  (red solid line), while the corresponding thin lines are obtained without pairing, i.e., starting from HF instead of HFB. For comparison, the light blue areas are the experimental results of Ref. [22] and the purple dots in the first two panels are obtained from the  $k_F a$  expansion up to order  $(k_F a)^4$  of Ref. [23].

Various thermodynamic quantities for the homogenous one-component Fermi gas from the BCS regime to the unitary limit were recently determined in Ref. [22] using  $^6\text{Li}$  atoms in a hybrid trap. The results for the energy with their error bands are shown in Fig. 4 by the light blue regions. Our minimum energies agree rather well with these experimental results. Although we do not see true convergence as in the weakly interacting case, one may argue that these minimum energies can be considered our best estimates because the third-order change is much smaller than the second-order one, and also there is at least local cutoff independence. However, as one approaches the unitary limit, the best estimate from HFB + BMBPT is still somewhat higher than the experimentally determined value of the energy. The ratio of  $\mathcal{E}/\mathcal{E}_0$  in the unitary limit is called the Bertsch parameter  $\xi$ . At the respective minima, we find  $\xi_{\text{HFB}} = 0.442$ ,  $\xi_{\text{BMBPT2}} = 0.414$ , and  $\xi_{\text{BMBPT3}} = 0.407$ , while the most precise experimental value is  $\xi = 0.370 \pm 0.005$  [24], which lies inside the error band of Ref. [22] shown in our figure and agrees also very well with the quantum Monte Carlo results  $\xi = 0.372 \pm 0.005$  [25] and  $\xi = 0.366^{+0.016}_{-0.011}$  [26]. Comparing the HFB and BMBPT energies, we observe that the minima get broader at higher orders of perturbation theory. This might indicate the onset of convergence, which should eventually lead to cutoff independence at least in some range of cutoffs, as discussed above for the weakly interacting case.

## VI. CONCLUSION AND OPEN QUESTIONS

Inspired by the  $V_{\text{low-}k}$  interactions used in nuclear physics, we have constructed effective interactions which tend to zero above some momentum cutoff  $\Lambda$  but preserve exactly the scattering phase shifts of the contact interaction below that cutoff. Since the phase shifts do not change sign, one can obtain rank-1 separable interactions with these properties using the inverse-scattering formula of Tabakin [17], without solving explicitly the RG evolution equation.

Using these separable interactions, we have calculated the equation of state of the zero-temperature Fermi gas within the HFB + BMBPT approach. In the weak-coupling BCS regime, where the HF term is much more important than pairing, we find that, for  $\Lambda/k_F \lesssim 2.5$ , the BMBPT converges quickly to the correct result. At stronger coupling, we do not yet find convergence but nevertheless the results are encouraging and our best estimate for the Bertsch parameter in the unitary limit,  $\xi = 0.407$ , is not very far from the experimental value  $\xi = 0.370 \pm 0.005$  [24].

An obvious problem of the approach is the cutoff dependence of the results. For observables that are insensitive to the short-range scales, the fact that the interaction gives by construction cutoff independent results in the two-body sector (phase shifts) at low momentum implies that any cutoff dependence in the many-body sector is indicative of missing contributions. These missing contributions can be higher order corrections in the perturbative expansion or missing three- and higher body interactions.

Even if the simplest three-body interaction of the form  $(\psi^\dagger \psi)^3$  is absent in the limit  $\Lambda \rightarrow \infty$  because it is forbidden by the Pauli principle for a two-component Fermi system, more complicated terms involving derivatives, i.e., momenta,

would be generated in the RG evolution when the cutoff is lowered [10–12]. These terms should be either included explicitly or, in an approximate way, in the form of a density-dependent two-body interaction.

Concerning the perturbation expansion in BMBPT, it is well known from nuclear structure theory that this can only work if the interactions are soft enough. This means that, while the cutoff must be larger than  $k_F$  to describe the interactions among the particles in the Fermi sea, it should not be too large compared to  $k_F$ . If the cutoff is too large, e.g., in the limit  $\Lambda \rightarrow \infty$ , nonperturbative resummations (ladder diagrams) are necessary even in the weakly coupled regime. In order to see in which range of  $\Lambda/k_F$  and  $1/(k_F a)$  the BMBPT expansion converges, it would be desirable to push it to higher orders. This necessitates, however, the development of tools that can compute these corrections automatically, as was done for nuclear-structure theory [27]. Once the equations have been derived, their numerical computation using Monte Carlo integration would not be any more difficult than the third order that we have done here. As usual with Monte Carlo integration, the computation time depends on the precision that one asks for. Let us mention that a completely different strategy to sum the perturbative corrections to much higher orders is the diagrammatic Monte Carlo method [28].

In the strongly coupled regime, it may be necessary to resum ladder-like diagrams even in the case of small cutoffs, for the following reason. The BMBPT expansion as explained in Sec. IV is based on excited states built out of fermionic quasiparticle excitations. But on the BEC ( $a > 0$ ) side of the crossover, it is clear that the most relevant excitations are bosonic ones. Therefore, it is possible that bosonic excitations, namely, the Bogoliubov-Anderson (BA) phonon, play also some role at unitarity and for  $a < 0$  [4]. This collective mode is described in the superfluid version of the random-phase approximation (RPA) [29] (called quasiparticle RPA in the nuclear-physics literature), corresponding to particle-particle and particle-hole ladder diagrams which are coupled to one another due to the anomalous propagators. For a regularized contact interaction in the limit  $\Lambda \rightarrow \infty$ , the effect of the BA mode on the ground state was included in Ref. [4]. Recently, it was also studied in Ref. [30] for the case of dilute neutron matter with a separable interaction, but without the HF field.

In such  $T$ -matrix approaches, the use of a finite cutoff would have some advantages compared to the limit  $\Lambda \rightarrow \infty$ . At weak coupling, one gets the right result almost for free (at the HF level) with low-momentum interactions, whereas for  $\Lambda \rightarrow \infty$  one has to use at least partially self-consistent versions of the  $T$ -matrix theory [31] such as the extended  $T$ -matrix approximation [32] or fully self-consistent Green's functions [33]. In addition, low-momentum interactions may simplify the numerical implementation of these approaches because a smaller grid in momentum space is required. The price to pay are uncertainties due to the unknown many-body interactions that are in principle induced when one lowers the cutoff.

Furthermore, one might wonder whether the HFB ground state is the best starting point for the perturbative expansion, although it is known that the gap is reduced due to “screening” of the interaction by the surrounding medium [9]. We leave all these open questions for future work.



## ACKNOWLEDGMENTS

We thank T. Duguet for discussions and H. Tajima for sending us the data of Ref. [22]. We acknowledge support from the Collaborative Research Program of IFPCAR/CEFIPRA, Project No. 6304-4.

## APPENDIX A: DETAILS OF THE COMPUTATION OF THE SEPARABLE INTERACTION

Let us first consider the case  $a < 0$ . When solving the inverse scattering problem, Eqs. (9) and (10), it is helpful to determine the coupling constant  $g_0$  by considering Eq. (9) in the limit  $q \rightarrow 0$ :

$$g_0 = \frac{a}{m} \exp\left(-\frac{2}{\pi} \int_0^{\Lambda'} dq' \frac{\delta(q')}{q'}\right). \quad (\text{A1})$$

Then the form factor is given by

$$F(q) = \sqrt{\frac{V_0(q, q)}{g_0}} = \sqrt{\frac{\sin \delta(q)}{-qa}} \exp\left(-\frac{x(q)}{2\pi}\right), \quad (\text{A2})$$

with

$$x(q) = 2q \int_0^{\Lambda'} dq' \frac{q\delta(q') - q'\delta(q)}{q'(q'^2 - q^2)} + \delta(q) \ln \frac{\Lambda' - q}{\Lambda' + q} \quad (\text{A3})$$

for  $0 < q < \Lambda'$ . Furthermore,  $F(0) = 1$  and we set  $F(q \geq \Lambda') = 0$  since it is negligible by the definition of  $\Lambda'$ .

Let us now consider the unitary limit,  $a \rightarrow \infty$ . In this case, the coupling constant can be written as

$$g_0 = -\frac{1}{m\Lambda'} \exp\left(-\frac{2}{\pi} \int_0^{\Lambda'} dq' \frac{\tilde{\delta}(q')}{q'}\right), \quad (\text{A4})$$

with

$$\tilde{\delta}(q') = \delta(q') - \delta(0), \quad (\text{A5})$$

and the form factor for  $0 < q < \Lambda'$  is given by

$$F(q) = \sqrt{\frac{\sin \delta(q)}{\sqrt{1 - q^2/\Lambda'^2}}} \exp\left(-\frac{\tilde{x}(q)}{2\pi}\right), \quad (\text{A6})$$

where  $\tilde{x}(q)$  is defined analogously to Eq. (A3) with  $\delta(q')$  replaced by  $\tilde{\delta}(q') = \delta(q') - \pi/2$ .

Finally, let us consider the case  $a > 0$ . Then the potential has a bound state with binding energy  $1/(ma^2)$  and the phase shift fulfils  $\delta(0) = \pi$ . In this case, the coupling constant can be written as

$$g_0 = -\frac{1}{m\Lambda'^2 a} \exp\left(-\frac{2}{\pi} \int_0^{\Lambda'} dq' \frac{\tilde{\delta}(q')}{q'}\right), \quad (\text{A7})$$

and the form factor for  $0 < q < \Lambda'$  is given by

$$F(q) = \sqrt{\frac{1 + q^2 a^2}{1 - q^2/\Lambda'^2}} \frac{\sin \delta(q)}{qa} \exp\left(-\frac{\tilde{x}(q)}{2\pi}\right), \quad (\text{A8})$$

where  $\tilde{x}(q)$  is defined analogously to Eq. (A3) with  $\delta(q')$  replaced by  $\tilde{\delta}(q') = \delta(q') - \pi$ .

## APPENDIX B: EXPLICIT EXPRESSION OF THE THIRD-ORDER BMBPT CORRECTION

As explained in Sec. IV C, in each term of  $\Omega^{(3)}$ , we must integrate over four independent momentum vectors. We relabel in each term the indices in such a way that the independent integration variables are called  $\mathbf{k}_1 \dots \mathbf{k}_4$ . The remaining four momentum vectors are then given by various combinations of these integration variables, and we denote these combinations as

$$\begin{aligned} \mathbf{k}_5 &= -\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3, & \mathbf{k}_6 &= -\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_4, \\ \mathbf{k}_7 &= -\mathbf{k}_1 - \mathbf{k}_3 - \mathbf{k}_4, & \mathbf{k}_8 &= -\mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4, \\ \mathbf{k}_9 &= \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3, & \mathbf{k}_{10} &= \mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_2, \\ \mathbf{k}_{11} &= \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_4, & \mathbf{k}_{12} &= \mathbf{k}_1 + \mathbf{k}_4 - \mathbf{k}_2, \\ \mathbf{k}_{13} &= \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4. \end{aligned} \quad (\text{B1})$$

The interaction potential appears with various differences or sums of momenta and we define the notation

$$F_{i,j}^{\pm} = F(|\mathbf{k}_i \pm \mathbf{k}_j|/2). \quad (\text{B2})$$

Combining terms having the same weight functions, the third-order correction can be finally written as

$$\begin{aligned} \Omega^{(3)} &= \frac{(4\pi g_0)^3}{\mathcal{V}^3} \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} (u_1 v_1 u_2 v_2 u_3 v_3 u_4 v_4 A_1 \\ &+ u_1 v_1 u_2 v_2 u_3 v_3 v_4^2 A_2 + u_1 v_1 u_2 v_2 u_3 v_3 u_4^2 A_3 \\ &+ u_1 v_1 u_2 v_2 v_3^2 v_4^2 A_4 + u_1 v_1 u_2 v_2 v_3^2 u_4^2 A_5 \\ &+ v_1^2 v_2^2 v_3^2 u_4^2 A_6 + v_1^2 v_2^2 u_3^2 u_4^2 A_7), \end{aligned} \quad (\text{B3})$$

with

$$\begin{aligned} A_1 &= -\frac{4(u_{13}^2 u_5^2 + v_{13}^2 v_5^2) F_{2,3}^- F_{4,13}^- F_{2,3}^- F_{1,5}^- F_{1,4}^- F_{5,13}^-}{E_{1,13,4,5} E_{1,2,3,5}} \\ &+ \frac{4u_5 v_5 u_6 v_6 F_{1,3}^- F_{2,5}^- F_{1,4}^- F_{2,6}^- F_{3,4}^+ F_{5,6}^+}{E_{1,2,3,5} E_{1,2,4,6}} \\ &+ \frac{2u_5^2 u_6^2 F_{2,3}^- F_{1,5}^- F_{1,4}^- F_{2,6}^- F_{3,5}^- F_{4,6}^-}{E_{1,2,3,5} E_{1,2,4,6}} \\ &- \frac{4(u_5^2 v_{13}^2 + u_{13}^2 v_5^2) F_{1,3}^- F_{2,5}^- F_{3,13}^+ F_{2,4}^+ F_{4,13}^- F_{1,5}^-}{E_{1,13,4,5} E_{1,2,3,5}} \\ &+ \frac{4u_6^2 v_5^2 F_{1,2}^- F_{3,5}^- F_{1,2}^- F_{4,6}^- F_{3,4}^+ F_{5,6}^+}{E_{1,2,3,5} E_{1,2,4,6}} \\ &+ \frac{2v_5^2 v_6^2 F_{1,3}^- F_{2,5}^- F_{2,4}^- F_{1,6}^- F_{3,5}^- F_{4,6}^-}{E_{1,2,3,5} E_{1,2,4,6}}, \quad (\text{B4}) \\ A_2 &= -\frac{2u_6^2 u_9 v_9 F_{1,3}^+ F_{2,9}^- F_{2,4}^- F_{1,6}^- F_{3,4}^- F_{6,9}^-}{E_{1,2,4,6} E_{3,4,6,9}} \\ &- \frac{4u_6^2 u_5 v_5 F_{1,3}^- F_{2,5}^- F_{2,4}^- F_{1,6}^- F_{3,4}^+ F_{5,6}^+}{E_{1,2,3,5} E_{1,2,4,6}} \end{aligned}$$

$$\begin{aligned}
& + \frac{2u_5v_5v_6^2F_{1,2}^-F_{3,5}^-F_{1,2}^-F_{4,6}^-F_{3,5}^-F_{4,6}^-}{E_{1,2,3,5}E_{1,2,4,6}} \\
& + \frac{u_9v_9v_6^2F_{1,2}^-F_{4,6}^-F_{1,2}^-F_{3,9}^-F_{4,6}^-F_{3,9}^-}{E_{1,2,4,6}E_{3,4,6,9}}, \quad (B5)
\end{aligned}$$

$$\begin{aligned}
A_3 = & \frac{2u_6^2u_5v_5F_{1,2}^-F_{3,5}^-F_{1,2}^-F_{4,6}^-F_{3,5}^-F_{4,6}^-}{E_{1,2,3,5}E_{1,2,4,6}} \\
& + \frac{u_6^2u_9v_9F_{1,2}^-F_{4,6}^-F_{1,2}^-F_{3,9}^-F_{4,6}^-F_{3,9}^-}{E_{1,2,4,6}E_{3,4,6,9}}, \quad (B6)
\end{aligned}$$

$$\begin{aligned}
A_4 = & -\frac{4u_{13}^2u_5^2F_{2,3}^-F_{1,5}^-F_{3,13}^+F_{2,4}^+F_{1,4}^-F_{5,13}^-}{E_{1,13,4,5}E_{1,2,3,5}} \\
& + \frac{8u_{11}^2u_5^2F_{2,11}^+F_{1,4}^+F_{1,3}^-F_{2,5}^-F_{3,4}^-F_{5,11}^-}{E_{1,2,3,5}E_{11,3,4,5}} \\
& + \frac{4u_5^2u_6^2F_{2,3}^-F_{1,5}^-F_{1,4}^-F_{2,6}^-F_{4,5}^+F_{3,6}^+}{E_{1,2,3,5}E_{1,2,4,6}} \\
& - \frac{4u_5^2u_7^2F_{1,3}^-F_{2,5}^-F_{3,4}^-F_{1,7}^+F_{4,5}^+F_{2,7}^+}{E_{1,2,3,5}E_{1,3,4,7}} \\
& + \frac{2u_7^2u_8^2F_{3,4}^-F_{1,7}^-F_{3,4}^-F_{2,8}^+F_{2,7}^+F_{1,8}^+}{E_{1,3,4,7}E_{2,3,4,8}}
\end{aligned}$$

$$\begin{aligned}
& + \frac{2u_7^2v_{12}^2F_{2,12}^-F_{1,4}^-F_{3,12}^-F_{2,7}^-F_{3,4}^-F_{1,7}^-}{E_{1,3,4,7}E_{12,2,3,7}} \\
& - \frac{4u_5^2v_{13}^2F_{1,3}^-F_{2,5}^-F_{2,3}^-F_{4,13}^-F_{4,13}^-F_{1,5}^-}{E_{1,13,4,5}E_{1,2,3,5}}, \quad (B7)
\end{aligned}$$

$$\begin{aligned}
A_5 = & -\frac{4u_5^2u_7^2F_{1,3}^-F_{4,7}^-F_{2,3}^-F_{1,5}^-F_{2,5}^-F_{4,7}^-}{E_{1,2,3,5}E_{1,3,4,7}} \\
& + \frac{2u_7^2u_8^2F_{1,3}^-F_{4,7}^-F_{2,3}^-F_{4,8}^-F_{1,7}^-F_{2,8}^-}{E_{1,3,4,7}E_{2,3,4,8}} \\
& + \frac{2u_7^2v_{10}^2F_{1,10}^+F_{2,3}^+F_{2,10}^-F_{4,7}^-F_{1,3}^-F_{4,7}^-}{E_{1,3,4,7}E_{10,2,4,7}}, \quad (B8)
\end{aligned}$$

$$\begin{aligned}
A_6 = & -\frac{2u_6^2u_7^2F_{1,2}^-F_{4,6}^-F_{1,3}^-F_{4,7}^-F_{3,6}^+F_{2,7}^+}{E_{1,2,4,6}E_{1,3,4,7}} \\
& + \frac{u_6^2v_9^2F_{1,2}^-F_{4,6}^-F_{1,2}^-F_{3,9}^-F_{4,6}^-F_{3,9}^-}{E_{1,2,4,6}E_{3,4,6,9}}, \quad (B9)
\end{aligned}$$

$$A_7 = \frac{u_5^2u_6^2F_{1,2}^-F_{3,5}^-F_{1,2}^-F_{4,6}^-F_{3,5}^-F_{4,6}^-}{E_{1,2,3,5}E_{1,2,4,6}}. \quad (B10)$$

- 
- [1] G. C. Strinati, P. Pieri, G. Röpke, P. Schuck, and M. Urban, *Phys. Rept.* **738**, 1 (2018).
- [2] S. Simonucci, P. Pieri, and G. C. Strinati, *Europhys. Lett.* **69**, 713 (2005).
- [3] P. Pieri and G. C. Strinati, *Phys. Rev. B* **61**, 15370 (2000).
- [4] P. Pieri, L. Pisani, and G. C. Strinati, *Phys. Rev. B* **70**, 094508 (2004).
- [5] S. K. Bogner, R. J. Furnstahl, and A. Schwenk, *Prog. Part. Nucl. Phys.* **65**, 94 (2010).
- [6] L. Coraggio, N. Itaco, A. Covello, A. Gargano, and T. T. S. Kuo, *Phys. Rev. C* **68**, 034320 (2003).
- [7] A. Tichai, P. Arthuis, T. Duguet, H. Hergert, V. Somà, and R. Roth, *Phys. Lett. B* **786**, 195 (2018).
- [8] S. Ramanan and M. Urban, *Phys. Rev. C* **98**, 024314 (2018).
- [9] L. P. Gor'kov and T. K. Melik-Barkhudarov, *Sov. Phys. JETP* **13**, 1018 (1961) [*Zh. Eksp. Teor. Fiz.* **40**, 1452 (1961)].
- [10] L. Tolos, B. Friman, and A. Schwenk, *Nucl. Phys. A* **806**, 105 (2008).
- [11] K. Hebeler and A. Schwenk, *Phys. Rev. C* **82**, 014314 (2010).
- [12] H.-W. Hammer, A. Nogga, and A. Schwenk, *Rev. Mod. Phys.* **85**, 197 (2013).
- [13] H. S. Köhler, [arXiv:0705.0944](#).
- [14] H. S. Köhler, [arXiv:0801.1123](#).
- [15] H. S. Köhler, [arXiv:1008.3884](#).
- [16] E. Ruiz Arriola, S. Szpigel, and V. S. Timóteo, [arXiv:1712.05931](#).
- [17] F. Tabakin, *Phys. Rev.* **177**, 1443 (1969).
- [18] S. K. Bogner, R. J. Furnstahl, S. Ramanan, and A. Schwenk, *Nucl. Phys. A* **773**, 203 (2006).
- [19] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
- [20] J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, Reading, MA, 1994).
- [21] I. Shavitt and R. Bartlett, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory* (Cambridge University Press, Cambridge, UK, 2009).
- [22] M. Horikoshi, M. Koashi, H. Tajima, Y. Ohashi, and M. Kuwata-Gonokami, *Phys. Rev. X* **7**, 041004 (2017).
- [23] C. Wellenhofer, C. Drischler, and A. Schwenk, [arXiv:2102.05966](#).
- [24] M. J. H. Ku, A. T. Sommer, L. W. Cheuk, and M. W. Zwierlein, *Science* **335**, 563 (2012).
- [25] J. Carlson, S. Gandolfi, K. E. Schmidt, and S. Zhang, *Phys. Rev. A* **84**, 061602(R) (2011).
- [26] M. G. Endres, D. B. Kaplan, J.-W. Lee, and A. N. Nicholson, *Phys. Rev. A* **87**, 023615 (2013).
- [27] P. Arthuis, T. Duguet, A. Tichai, R.-D. Lasserri, and J.-P. Ebran, *Comp. Phys. Comm.* **240**, 202 (2019).
- [28] G. Spada, R. Rossi, F. Šimkovic, R. Garioud, M. Ferrero, K. Van Houcke, and F. Werner, [arXiv:2103.12038](#).
- [29] R. Combescot, M. Y. Kagan, and S. Stringari, *Phys. Rev. A* **74**, 042717 (2006).
- [30] D. Inotani, S. Yasui, and M. Nitta, *Phys. Rev. C* **102**, 065802 (2020).
- [31] M. Pini, P. Pieri, and G. Calvanese Strinati, *Phys. Rev. B* **99**, 094502 (2019).
- [32] T. Kashimura, R. Watanabe, and Y. Ohashi, *Phys. Rev. A* **86**, 043622 (2012).
- [33] R. Haussmann, *Phys. Rev. B* **49**, 12975 (1994).