Effective contact pairing forces from realistic calculations in infinite homogeneous nuclear matter

N. Chamel
Institut d'Astronomie et d'Astrophysique, CP-226, Université Libre de Bruxelles, B-1050 Brussels, Belgium
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Nonempirical effective contact pairing forces to be used in self-consistent mean-field calculations are presented. These pairing forces, constructed so as to reproduce exactly any given microscopic pairing gaps in infinite homogeneous nuclear matter for any isospin asymmetry, are given in analytical form. As a by-product, this work provides an analytical solution of the BCS gap equations which could be applied to describe various many-body systems.

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I. INTRODUCTION

Self-consistent mean-field calculations using effective interactions have been very successful in describing the properties and the dynamics of a wide range of nuclei [1]. One of the most popular effective interactions are zero-range interactions of the Skyrme type because of the fast numerical computations which can thus be performed [2]. Even though Negele and Vautherin [3] showed a long time ago how to obtain effective interactions using nuclear many-body methods, a more empirical approach has usually been followed. A specific parametric form of the effective interaction is postulated and the unknown parameters are determined *a posteriori* so as to reproduce a set of nuclear data selected according to a specific purpose. The nonuniqueness of the fitting procedure has thus led to a large number of different parametrizations. Some of them may yield very different predictions when applied outside the domain where they were fitted [4].

This situation is particularly unsatisfactory for nuclear astrophysical applications which require the knowledge of nuclear masses for nuclei so neutron rich that there is no hope of measuring them in the foreseeable future; such nuclei play a vital role in the r process of nucleosynthesis [5] and are also found in the outer crust of neutron stars [6]. Extrapolations far beyond the neutron drip line are required for the description of the inner crust of neutron stars where nuclear clusters are embedded in a sea of superfluid neutrons [7]. Such environments cannot be reproduced in the laboratory. However, many astrophysical phenomena observed in neutron stars are precisely related to the physics of these outer layers [8]. The need for more reliable extrapolations of these nuclear models has motivated recent efforts to construct nonempirical effective interactions and more generally microscopic nuclear energy density functionals [9]. Unfortunately, such *ab initio* nuclear energy density functionals able to reproduce existing experimental nuclear data with the same degree of accuracy as phenomenological interactions are not yet available.

For the time being, a reasonable approach is to fit these phenomenological interactions with as many available nuclear data as possible, not only from experiments but also from realistic calculations in infinite homogeneous nuclear matter. Very accurate nuclear mass models based on the Hartree-Fock-Bogoliubov (HFB) method with zero- and finite-range effective forces have thus been recently developed [10,11]. In particular, in our model HFB-17 [12,13], we have achieved our best fit ever to essentially all the available experimental mass data, the rms deviation for the set of 2149 measured masses of nuclei with N and $Z \geqslant 8$ [14] being only 0.581 MeV. Significant improvements compared to our previous models have been made possible by a better treatment of pairing correlations first introduced in Ref. [15] and extended in Refs. [12,13]. The effective interaction used in the pairing channel was constrained to reproduce the $^1S_0$ pairing gaps as obtained by microscopic calculations using realistic nucleon-nucleon interactions. We have recently applied these effective forces to study the properties of the neutron superfluid phase in the inner crust of neutron stars [16].

The effective pairing interaction associated with our nuclear mass models requires the evaluation of one-dimensional integrals. Although its numerical implementation is straightforward, using such interaction could become computationally costly for large-scale calculations such as the determination of fission barriers. In this article, a more tractable expression of the pairing interaction is presented by calculating the underlying integrals analytically. We consider effective interactions of the Skyrme type in the particle-hole channel. However, results can be easily generalized to other kinds of interactions.

II. EFFECTIVE DENSITY-DEPENDENT CONTACT PAIRING FORCE

The pairing interaction that we consider here acts only between nucleons of the same charge state q ($q = n$ or p for neutron or proton, respectively) and is given by

$$v^{\text{pair}}(\boldsymbol{r}_i, \boldsymbol{r}_j) = \tfrac{1}{2}(1 - P_\sigma) v^{\pi q}[\rho_n(\boldsymbol{r}), \rho_p(\boldsymbol{r})]\delta(\boldsymbol{r}_{ij}), \qquad (1)$$

where P_σ is the two-body spin-exchange operator, $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, and $\boldsymbol{r} = (\boldsymbol{r}_i + \boldsymbol{r}_j)/2$. Owing to the zero range of this interaction, a cutoff has to be introduced in the gap equations to avoid divergences (for a review of the various prescriptions, see, for instance, Ref. [17]). In this work we include all single-particle states whose energy lies below $\lambda_q + \varepsilon_\Lambda$, where λ_q is the chemical potential and ε_Λ is an energy cutoff. Although microscopic calculations in semi-infinite nuclear matter suggest that pairing in nuclei is a surface phenomenon [18], the density dependence of the pairing force is still poorly known. It is generally assumed that $v^{\pi q}[\rho_n, \rho_p]$ depends only

on the isoscalar density $\rho = \rho_n + \rho_p$ and is often parametrized as [19]

$$v^{\pi q}[\rho_n, \rho_p] = V^{\Lambda}_{\pi q}\left[1 - \eta_q \left(\frac{\rho}{\rho_0}\right)^{\alpha_q}\right], \tag{2}$$

where ρ_0 is the nuclear saturation density while $V^{\Lambda}_{\pi q}$, η_q, and α_q are adjustable parameters. The superscript Λ on $V^{\Lambda}_{\pi q}$ is a reminder that the pairing strength depends very strongly on the cutoff used in the gap equations (in principle, changing the cutoff modifies also the other parameters but the effects are usually ignored). Effective interactions with $\eta_q = 0$ ($\eta_q = 1$) have been traditionally referred to as volume (surface) pairing. The parameters in Eq. (2) are usually fitted directly to experimental data. The standard prescription is to adjust the value of the pairing strength $V^{\Lambda}_{\pi q}$ to the average gap in ^{120}Sn [20]. However, this does not allow an unambiguous determination of the remaining parameters η_q and α_q. Systematic studies of nuclei seem to favor a so-called mixed pairing with $\eta_q \sim 0.5$ and $1/2 \lesssim \alpha_q \lesssim 1$ [21,22].

Even though such forces have been widely applied in nuclear structure calculations with some success, they lack a direct connection with realistic nucleon-nucleon forces. The reliability of these forces far beyond the domain where they were fitted is therefore not guaranteed. In particular, pairing forces fitted only to finite nuclei generally yield unrealistic pairing gaps in infinite nuclear matter [15,23], thus rendering their application to neutron-star crusts unreliable. Garrido *et al.* [24] proposed to determine the parameters of the pairing interaction in Eq. (2) by fitting the $^1S_0$ pairing gaps in infinite symmetric nuclear matter as obtained by the realistic Paris potential in the BCS approximation. The parametric form Eq. (2) has been recently extended by Margueron *et al.* [25], who introduced an isospin dependence in the pairing strength to reproduce the $^1S_0$ pairing gaps in both symmetric nuclear matter and pure neutron matter as obtained from Brueckner calculations [26]. This approach assumes that the pairing *interaction* between two nucleons inside a nucleus is locally the same as the pairing interaction between two nucleons in infinite uniform matter. This should not be confused with the so-called "local density approximation," which supposes that the pairing *field* $\Delta(\boldsymbol{r})$ appearing in the HFB equations (see, for instance, Appendix A of Ref. [15]) is locally the same in finite nuclei and in infinite nuclear matter. Even though the coupling to surface vibrations is expected to contribute to pairing [27], a local pairing theory seems a reasonable first step [28,29]. Finite size effects can be subsequently taken into account by introducing density gradient terms in the expression of the effective pairing force, as suggested in Ref. [30] in the general framework of the density functional theory. Effective pairing forces with density gradients have been implemented in Ref. [31].

The drawback of using a phenomenological pairing force to fit microscopic pairing gaps in infinite uniform matter is that the functional form of the associated pairing strength is not *a priori* known. In particular, different pairing gaps require different expressions of $v^{\pi q}[\rho_n, \rho_p]$, which can hardly be guessed owing to the highly nonlinear character of pairing correlations [32,33]. It should also be remarked that the parameters of the pairing force depend on the effective interaction used in the particle-hole channel because effective masses appear in the gap equations. Fitting the parameters of the effective interaction to essentially all experimental nuclear masses in both the particle-hole and the particle-particle channels while simultaneously reproducing microscopic pairing gaps in infinite uniform matter would thus be an extremely onerous numerical task.

III. MICROSCOPICALLY DEDUCED CONTACT PAIRING FORCE

Actually, as shown in Refs. [12,13,15], the density and isospin dependence of the pairing strength can be calculated exactly for any given $^1S_0$ pairing-gap function $\Delta_q[\rho_n, \rho_p]$ by solving directly the HFB equations in infinite uniform matter, yielding

$$v^{\pi q}[\rho_n, \rho_p] = -\frac{8\pi^2}{I_q(\rho_n, \rho_p)}\left(\frac{\hbar^2}{2M^*_q(\rho_n, \rho_p)}\right)^{3/2}, \tag{3}$$

where $M^*_q(\rho_n, \rho_p)$ is the nucleon effective mass and

$$I_q(\rho_n, \rho_p) = \int_0^{\mu_q + \varepsilon_\Lambda} \mathrm{d}\xi \, \frac{\sqrt{\xi}}{\sqrt{(\xi - \mu_q)^2 + \Delta_q(\rho_n, \rho_p)^2}}. \tag{4}$$

The expression of $M^*_q(\rho_n, \rho_p)$ for Skyrme forces can be found, for instance, in Appendix A of Ref. [15]. In Eq. (4), $\mu_q = \lambda_q - U_q$ is a reduced chemical potential (U_q being the mean field potential) which can be obtained by imposing the conservation of the nucleon particle number density

$$\rho_q = \left(\frac{2M^*_q}{\hbar^2}\right)^{3/2} \int_0^{+\infty} \frac{d\xi}{4\pi^2}\sqrt{\xi}\left(1 - \frac{\xi - \mu_q}{\sqrt{(\xi - \mu_q)^2 + \Delta_q^2}}\right). \tag{5}$$

However, it is usually a very good approximation to replace μ_q in Eq. (4) with the Fermi energy

$$\varepsilon^{(q)}_{\mathrm{F}} = \frac{\hbar^2 k^2_{\mathrm{F}q}}{2M^*_q}, \tag{6}$$

where $k_{\mathrm{F}q} = (3\pi^2\rho_q)^{1/3}$ is the Fermi wave number. The approximation $\mu_q \simeq \varepsilon^{(q)}_{\mathrm{F}}$ holds provided $\Delta_q \ll \varepsilon^{(q)}_{\mathrm{F}}$, which is typically the case [34].

Using Eq. (3) instead of a phenomenological expression such as Eq. (2) guarantees that in infinite uniform matter the microscopic pairing gaps $\Delta_q(\rho_n, \rho_p)$ will be exactly reproduced. It also ensures that the pairing strength is suitably renormalized for any change in the energy cutoff. The price to be paid is the evaluation of the one-dimensional integral [Eq. (4)], for the neutron density $\rho_n(\boldsymbol{r})$ and proton density $\rho_p(\boldsymbol{r})$ at all points inside the nucleus. The computational cost becomes significant in fully self-consistent 2D and 3D calculations [6]. However, we will now show that these numerical integrations can be avoided by making use of the weak-coupling approximation.

The integrand in Eq. (4) is all the more peaked around $\xi = \mu_q \simeq \varepsilon^{(q)}_{\mathrm{F}}$ because Δ_q is small compared to $\varepsilon^{(q)}_{\mathrm{F}}$. This

suggests to expand the integrand in powers of $\Delta_q/\varepsilon_{\rm F}^{(q)}$, leading to

$$I_q = \sqrt{\varepsilon_{\rm F}^{(q)}} \sum_{n=0}^{+\infty} \tilde{I}_q^{(n)}, \tag{7}$$

where the dimensionless coefficients $\tilde{I}_q^{(n)}$ are defined by

$$\tilde{I}_q^{(n)} = \frac{(2n)!}{(1-2n)(n!)^2} \left(\frac{-\Delta_q}{4\varepsilon_{\rm F}^{(q)}}\right)^n \int_{-\varepsilon_{\rm F}^{(q)}/\Delta_q}^{\varepsilon_\Lambda/\Delta_q} \frac{x^n dx}{\sqrt{1+x^2}}. \tag{8}$$

In the weak-coupling approximation $\Delta_q \ll \varepsilon_{\rm F}^{(q)}$ and $\Delta_q \ll \varepsilon_\Lambda$, only the first coefficient in Eq. (7) is usually retained, that is, $I_q \simeq \sqrt{\varepsilon_{\rm F}^{(q)}}\,\tilde{I}_q^{(0)}$. This approximation is equivalent in taking a constant density of single-particle states in the gap equations. Calculating the integral $\tilde{I}_q^{(0)}$ and keeping lowest-order terms in $\Delta_q/\varepsilon_{\rm F}^{(q)}$ and $\Delta_q/\varepsilon_\Lambda$, Eq. (8) thus yields

$$\tilde{I}_q^{(0)} \simeq \ln\left(\frac{4\varepsilon_{\rm F}^{(q)}\varepsilon_\Lambda}{\Delta_q^2}\right). \tag{9}$$

Inserting Eq. (9) in Eq. (3) and solving for Δ_q leads to the familiar expression (note that $v^{\pi q} < 0$)

$$\Delta_q^{(0)} = 2\sqrt{\varepsilon_{\rm F}^{(q)}\varepsilon_\Lambda}\,\exp\left(\frac{2\pi^2\hbar^2}{v^{\pi q} M_q^* k_{{\rm F}q}}\right). \tag{10}$$

Even though the weak-coupling approximation provides good results in the case of conventional BCS superconductivity [35], it is less accurate in the nuclear context because of the large number of states involved in the pairing mechanism. Nevertheless, the higher-order coefficients in Eq. (8) can be easily evaluated. Calculating the integrals $\tilde{I}_q^{(n)}$, keeping as before lowest-order terms in $\Delta_q/\varepsilon_{\rm F}^{(q)}$ and $\Delta_q/\varepsilon_\Lambda$, and summing all coefficients, we find

$$\sum_{n=1}^{+\infty} \tilde{I}_q^{(n)} \simeq 2\sqrt{1+y} - 2\ln\left[\frac{1}{4}(1+\sqrt{1+y})\right] - 4, \tag{11}$$

where $y = \varepsilon_\Lambda/\varepsilon_{\rm F}^{(q)}$. Adding Eqs. (9) and (11) in Eq. (7) leads to

$$I_q = \sqrt{\varepsilon_{\rm F}^{(q)}}\left[2\ln\left(\frac{2\varepsilon_{\rm F}^{(q)}}{\Delta_q}\right) + \Lambda\left(\frac{\varepsilon_\Lambda}{\varepsilon_{\rm F}^{(q)}}\right)\right], \tag{12}$$

with

$$\Lambda(x) = \ln(16x) + 2\sqrt{1+x} - 2\ln(1+\sqrt{1+x}) - 4. \tag{13}$$

The highly nonlinear character of the pairing phenomenon is evident in Eqs. (3) and (12). These equations also show that the density dependence of the pairing strength is intimately related to the choice of the pairing cutoff. The contribution of the latter is entirely contained in the function $\Lambda(x)$. It can also be seen from Eqs. (3) and (12) that the pairing strength vanishes whenever the pairing gap Δ_q goes to zero at *finite* density, as expected.

Note that as a by-product we have also obtained a more accurate expression of the pairing gap. Substituting Eq. (12) in Eq. (3) yields

$$\Delta_q = \Delta_q^{(0)} \exp\left(\tfrac{1}{2}\Lambda(y)\right) y^{-1/2}, \tag{14}$$

where $y = \varepsilon_\Lambda/\varepsilon_{\rm F}^{(q)}$.

We have tested the validity of the analytical expression given by Eq. (12) as compared to the numerical integration of Eq. (4) using the effective interactions underlying our HFB-17 nuclear mass model [12,13]. The pairing force used in this model was adjusted so as to reproduce the $^1S_0$ pairing gaps in both symmetric nuclear matter and pure neutron matter as obtained from Brueckner calculations using the Argonne $V18$ nucleon-nucleon potential [26]. The pairing cutoff was fixed at $\varepsilon_\Lambda = 16$ MeV. As can be seen in Figs. 1 and 2, Eqs. (3) and (12) provide a very good estimate of the pairing strength for all densities and different isospin asymmetries. The figures also show that keeping only the first term in Eq. (7) with $\tilde{I}_q^{(0)}$ given by Eq. (9) leads to fairly good results except at low densities.

At very low densities $\rho \to 0$, both the pairing gap Δ_q and the chemical potential vanish so that the integral I_q is then

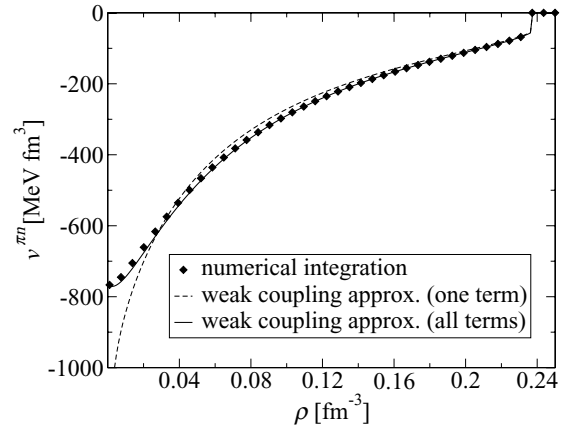

FIG. 1. Neutron pairing strength $v^{\pi n}[\rho_n, \rho_p]$, as defined by Eq. (3), vs nucleon number density ρ in symmetric nuclear matter using the effective interaction underlying the nuclear mass model HFB-17 [12,13]. The symbols are the results of numerically integrating Eq. (4). The dashed and solid lines were obtained using Eqs. (9) (12), respectively.

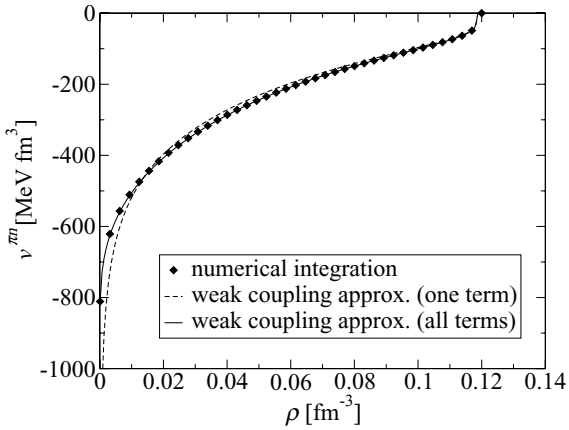

FIG. 2. Same as Fig. 1 but for pure neutron matter.

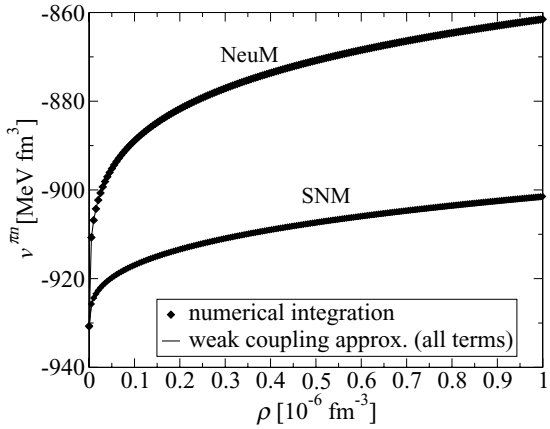

FIG. 3. Neutron pairing strength $v^{\pi n}[\rho_n, \rho_p]$, as defined by Eq. (3), vs nucleon number density ρ in symmetric nuclear matter (SNM) and pure neutron matter (NeuM) using the effective interaction underlying the nuclear mass model HFB-17 [12,13]. The symbols are the results of numerically integrating Eq. (4) and the solid line was obtained from Eq. (12).

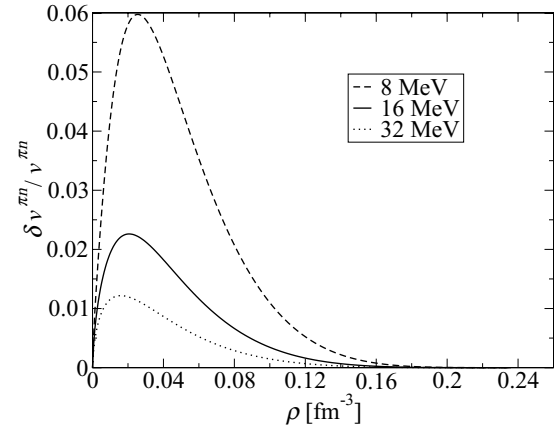

FIG. 4. Relative error between the neutron pairing strength $v^{\pi n}[\rho_n, \rho_p]$ calculated numerically and that obtained from the weak-coupling approximation vs nucleon number density ρ. The different curves correspond to different values of the pairing cutoff ε_Λ indicated in the plot. Calculations were carried out in symmetric nuclear matter using the effective interaction underlying the nuclear mass model HFB-17 [12,13].

simply given by $2\sqrt{\varepsilon_\Lambda}$. It is easily seen from Eq. (3) that the pairing strength remains finite in this limit and is given by

$$v^{\pi q}[\rho \to 0] = -\frac{4\pi^2}{\sqrt{\varepsilon_\Lambda}} \left(\frac{\hbar^2}{2M_q}\right)^{3/2}, \qquad (15)$$

assuming that $M_q^*(\rho \to 0) = M_q$. The weak-coupling expression, given by Eqs. (3) and (12), tends to the exact limit as shown in Fig. 3, whereas Eq. (9) leads to a divergence (the corresponding pairing strength lies far below the range shown in Fig. 3). The reason for this discrepancy lies in the underlying assumption of a constant density of single-particle states, which is strongly violated at low energies ε where the density of states decreases as $\sqrt{\varepsilon}$.

The value of the pairing cutoff ε_Λ can be *a priori* arbitrarily chosen. However, it has been argued [24,36] that in the limit $\rho \to 0$, the pairing strength should coincide with the bare force in the $^1S_0$ channel, which in turn is determined by the experimental $^1S_0$ nucleon-nucleon phase shifts. According to Eq. (15), specifying $v^{\pi q}[\rho \to 0]$ is equivalent to specifying the pairing cutoff ε_Λ. As shown in Fig. 1 of Ref. [36], the optimal value of the cutoff is $\varepsilon_\Lambda \sim 7 - 8$ MeV (note that ε_Λ is half the cutoff used in Ref. [36]). Using the experimental phase shifts would thus remove the only free remaining parameter. However, choosing such a low cutoff can deteriorate the precision of the weak-coupling approximation, because Eq. (12) was obtained assuming $\Delta_q \ll \varepsilon_\Lambda$. We have therefore calculated the relative error between the pairing strength calculated numerically and that obtained from Eqs. (3) and (12) for different values of the pairing cutoff. Results are shown in Figs. 4 and 5 for symmetric nuclear and pure neutron matter, respectively. We have verified that the differences come solely from the weak-coupling approximation and not from the numerical method used to solve Eq. (4). It can be seen that for the effective interactions underlying our HFB-17 nuclear mass model [12,13], the weak-coupling approximation is quite accurate because the largest relative error is of a few percent only for $\varepsilon_\Lambda = 8$ MeV. The precision is higher in neutron matter than in symmetric matter because the $^1S_0$ pairing gap of neutron matter is smaller than that of symmetric matter. Note that the pairing gaps we adopted in our HFB-17 mass model are rather large [the maximum of the gap function $\Delta_q(\rho_n, \rho_p)$ is about 4.8 MeV in symmetric matter and 2.6 MeV in neutron matter]. These gaps were obtained from Brueckner calculations including medium polarization effects but without self-energy corrections [26]. When both effects are taken into account, the maximum pairing gaps are much lower [26]. The precision of the weak-coupling approximation would thus be even better with such gaps. In any case, if the constraint of reproducing the $^1S_0$ nucleon-nucleon phase shifts is released, one is free to adjust the cutoff so as to achieve a better precision, as illustrated in Figs. 4 and 5.

In the more general context of the nuclear energy density functional theory, the HFB equations can be obtained by minimizing the energy with respect to the normal and pairing density matrices for a fixed average number of neutrons and protons [37] (the link between different formulations of the

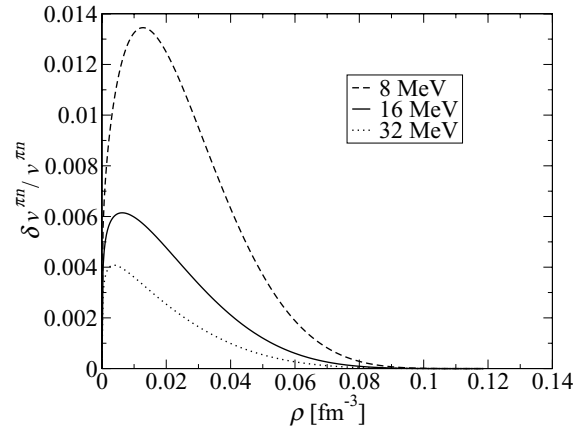

FIG. 5. Same as Fig. 4 but in neutron matter.

HFB equations is discussed for instance in Ref. [15]). All that is needed is therefore the specification of the nuclear energy density functional. The pairing energy density associated with an effective pairing force defined by Eq. (1) is given by

$$\mathcal{E}_{\text{pair}}(\boldsymbol{r}) = \frac{1}{4} \sum_{q=n,p} v^{\pi q}[\rho_n(\boldsymbol{r}), \rho_p(\boldsymbol{r})]\tilde{\rho}_q(\boldsymbol{r})^2, \tag{16}$$

where $\tilde{\rho}_q(\boldsymbol{r})$ is the so-called local pairing density. The pairing field appearing in the HFB equations is then defined by

$$\Delta_q(\boldsymbol{r}) \equiv \frac{\partial \mathcal{E}_{\text{pair}}(\boldsymbol{r})}{\partial \tilde{\rho}_q(\boldsymbol{r})}. \tag{17}$$

Because $\mathcal{E}_{\text{pair}}(\boldsymbol{r})$ depends on the nucleon densities, it contributes also to the mean-field potentials (see, for instance, Appendix A of Ref. [15]). Local pairing functionals can be constructed from infinite nuclear-matter calculations using Eqs. (3), (12), and (13). The construction of nonempirical (and nonlocal) pairing functionals using realistic nucleon-nucleon interactions has been discussed in Ref. [38] (see also Ref. [9] for a review).

IV. CONCLUSIONS

In conclusion, we have shown how to construct nonempirical effective contact pairing forces (or equivalently local nuclear pairing energy density functionals) using any given $^1S_0$ pairing-gap functions $\Delta_q(\rho_n, \rho_p)$ obtained from microscopic calculations in infinite uniform nuclear matter with realistic nucleon-nucleon potentials. The resulting parameter-free pairing forces, embodied in Eqs. (3), (12), and (13), can be easily implemented in nuclear-structure calculations. These forces could be helpful for understanding the origin of pairing in finite nuclei and could be used to estimate the importance of bulk contribution as compared to finite-size effects. Alternatively, the analytical solution of the BCS gap equations which we have obtained in Eq. (14), can be applied to calculate the pairing gaps in nuclear matter for any given contact pairing force (provided the conditions for the weak-coupling approximation remain valid). Even though we have been interested in nuclear pairing, the present results could be easily adapted to other contexts.

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