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LOCAL ENERGY-DENSITY FUNCTIONAL AND DENSITY-DEPENDENT PAIRING IN NUCLEAR SYSTEMS

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An approach based on the local energy-density functional method for describing the ground-state properties of superfluid nuclei is presented. The generalized variational principle is formulated which corresponds, in the weak pairing approximation, to a full treatment of the Hartree–Fock–Bogoliubov problem with an effective contact pairing interaction. The Gor'kov equations for generalized Green's functions are treated exactly in the coordinate-space representation. The method is used to calculate the differential observables including odd-even mass differences and odd-even effects in charge radii which occur to be very sensitive to the density dependence of the effective pairing force. A better knowledge of this density dependence allows one to make predictions for the pairing gap at the Fermi surface as a function of nuclear matter density.

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The study of pairing correlations is currently one central issue in nuclear structure physics and nuclear astrophysics. For example, the superfluidity of neutron matter is expected to play an essential role in the neutron stars [1], while pairing in neutron-rich nuclei is of importance in a domain close to the drip line [2] and also in the light halo nuclei [3]. The effective nucleon-nucleon interaction in the pairing channel suitable for the nuclear structure calculations and for obtaining an accurate value of the pairing energy gap in infinite matter is not yet well established. The major difficulties are connected with the consistent account for the in-medium renormalizations [4, 5] and, particularly in nonuniform systems, for the finite-range and nonlocal effects [6] which should be calculated in a reliable way to elucidate the proper dependence of the effective force on the density ρ and its gradients. At present the pairing gap can not be obtained on a satisfactory level from first-principle approaches with a bare NN interaction. The empirical information gained from the studies of laboratory nuclei seems to be indispensable in this respect. The presently most successful *simultaneous* description of the *bulk* nuclear properties, such as binding energies and radii, is achieved with phenomenological ρ-dependent forces (e.g. [7, 8]) and thus the density dependence of the effective interaction in the particle-hole channel is now established fairly well. In other words, the Hartree-Fock (HF) part of the energy-density functional (EDF) is more or less known, though, as one may notice, considerable effort is still continuing to optimize this part [9]. On the same ground, one may expect that *simultaneous* description of the *differential* observables, such as odd-even effects in masses and radii, would shed light on the ρ-dependence of the effective interaction in the particle-particle (pp) channel and on the pairing part of the EDF.

To reveal the form of Δ as a function of ρ through the ρ-dependence of the underlying effective pairing force, the observed changes of geometrical characterstics of nuclei, first

of all the odd-even staggering in *charge radii*, should be analysed [10]. This point may be illustrated by considering how the density changes when the pairing gap appears in nuclear matter [11]. It occured that the density is sensitive to the derivative $d\Delta/dx$ near the saturation point $\rho \approx 0.16$ fm^{-3}. A negative slope in Δ causes a decrease of ρ, i.e. an expansion of the system. In finite systems this effect leads to the increase of radii as was confirmed by self-consistent EDF calculations [11 – 13]. Amplified ρ-dependent variations of Δ in odd systems through supression of anomalous density by the blocking effect causes an enhancement of the odd-even staggering in radii [10].

Here we present an EDF approach based on the general variational principle applied to the EDF with a fixed energy cutoff $\epsilon_c > \epsilon_F$ (ϵ_F is the Fermi energy). It involves an integration of the Green's functions, obtained by solving the coordinate-space Gor'kov equations exactly, in the complex energy plane. This technique is appropriate for the correct treatment of the coupling with particle continuum, especially in weakly bound nuclei [14]. We extend such an approach also for the systems with odd particle number by using the uniform filling approximation. Compared to refs. [11, 12, 15] where the calculations were done mostly in the HF+Bardeen–Cooper–Schrieffer (HF+BCS) framework, the approach formulated here corresponds to a full treatment of the Hartree–Fock–Bogoliubov (HFB) problem and permits direct comparison of the pairing gap extracted from the analysis of nuclear data with nuclear matter calculations.

The energy E of a superfluid nucleus is given by a functional of the generalized density matrix $\widehat{R}$ containing both normal, $\hat{\rho}$, and anomalous, $\hat{\nu}$, components:

$$E[\widehat{R}] = E_{kin}[\hat{\rho}] + E_{int}[\hat{\rho}, \hat{\nu}]\,, \tag{1}$$

where $E_{kin}[\hat{\rho}] = \mathrm{Tr}(t\hat{\rho})$, and $E_{int}[\hat{\rho}, \hat{\nu}] = E_{int(normal)}[\hat{\rho}] + E_{anomal}[\hat{\rho}, \hat{\nu}]$. The anomalous energy E_{anomal} is chosen such that it vanishes in the limit $\nu \to 0$. The weak-pairing approximation $|\bar{\Delta}| \ll \epsilon_F$ is assumed which is generally the case for nuclear systems. That means we need to retain only the first-order term $\sim \nu^2$ in the anomalous part of the EDF:

$$E_{anomal}[\hat{\rho}, \hat{\nu}] = \frac{1}{4}\left(\hat{\nu}^\dagger \hat{\mathcal{F}}_a^{pp}[\hat{\rho}]\hat{\nu}\right)\,, \tag{2}$$

where $\hat{\mathcal{F}}_a^{pp}$ is an antisymmetrized effective interaction in the pp channel and the round brackets imply integration and summation over all variables. To calculate the ground state properties, one can now use the general variational principle with two contraints,

$$\langle \mathrm{HFB}|\hat{N}(\mu)|\mathrm{HFB}\rangle \equiv N(\mu) = N\,, \quad \widehat{R}^2 = \widehat{R}\,, \tag{3}$$

leading to the variational functional of the form

$$I[\widehat{R}] = E[\widehat{R}] - \mu N(\mu) - \mathrm{Tr}\hat{\Lambda}(\widehat{R} - \widehat{R}^2)\,, \tag{4}$$

where N is the particle number, μ the chemical potential, and $\hat{\Lambda}$ the matrix of Lagrange parameters (see e.g. [16]).

The anomalous energy (2) can be calculated if one knows a solution of the gap equation for the pairing field $\hat{\Delta}$ and the anomalous density matrix $\hat{\nu}$. In general, the gap equation is nonlocal and its solution (starting, for example, from a realistic bare NN interaction [6, 5]) poses serious problems. It can be shown that, in the case of weak pairing $|\bar{\Delta}| \ll \epsilon_F$, the EDF method and the general variational principle can be used with an effective contact density-dependent pairing interaction. The formal development by using the Green's function formalism is described in detail in our forthcoming paper [17]. Here we give only a brief account of the main issues.

We introduce an arbitrary cutoff ϵ_c in the energy space, but such that $\epsilon_c > \epsilon_F$, and split the generalized density matrix into two parts, $\widehat{R} = \widehat{R}_c + \delta_c\widehat{R}$ where $\delta_c\widehat{R}$ is related to the integration over energies $|\epsilon| > \epsilon_c$. The gap equation is renormalized to yield

$$\hat{\Delta} = \frac{1}{2}\hat{\mathcal{F}}^{\xi}_{a}\hat{\nu}_c\,, \tag{5}$$

where $\hat{\nu}_c$ is the cutoff anomalous density matrix and $\hat{\mathcal{F}}^{\xi}_{a}$ is the effective antisymmetrized pairing interaction in which the contribution coming from the energy region $|\epsilon| > \epsilon_c$ is included by renormalization.

For homogeneous infinite matter it is shown that the variational function $E - \mu N$ does not change in first order in $\hat{\Delta}^2$ upon variation with respect to $\delta_c\widehat{R}$. The total energy of the system and the chemical potential also remain the same if one imposes the particle number constraint (3) for the cutoff functional. To a good approximation, as discussed in [17], this should be also valid for finite nuclei.

Such an outcome may be understood by noting that the major pairing effects are developed near the Fermi surface and the pairing energy is defined by a sum concentrated near the Fermi surface (e.g. [16]). In infinite matter the pairing energy per particle is $E_{pair}/N = -3\Delta^2(k_F)/8\epsilon_F$. It follows that, with cutoff EDF, this leading pairing contribution to the energy of the system is exactly accounted for. Thus the nuclear ground state properties can be described by applying the general variational principle to minimize the cutoff functional which has exactly the same form as (4) with the constraint (3) but with $\widehat{R}$ replaced by $\widehat{R}_c$. Recalling now the Hohenberg–Kohn theorem [18], we specify that the EDF can be chosen to be of a local form, i.e. dependent on the normal and anomalous local real densities $\rho(\mathbf{r})$ and $\nu_c(\mathbf{r})$. Then anomalous energy acquires the simple form

$$E^{c}_{anomal}[\rho_c, \nu_c] = \int d\mathbf{r}\nu^{*}_{c}(\mathbf{r})\mathcal{F}^{\xi}(\mathbf{r}; [\rho_c])\nu_c(\mathbf{r})\,. \tag{6}$$

That corresponds to the multiplicative gap equation

$$\Delta(\mathbf{r}) = \mathcal{F}^{\xi}(\mathbf{r}; [\rho_c])\nu_c(\mathbf{r})\,. \tag{7}$$

Having found the pairing field $\Delta(\mathbf{r})$, and the mean-field potential $U(\mathbf{r})$, the Gor'kov equations may be solved exactly by using the coordinate-space technique. The generalized Green's function obtained this way can be integrated over energy up to ϵ_c to yield both the normal and anomalous densities ρ_c and ν_c which are used then to compute the energy of the system. We stress that our approach does not imply a cutoff of the basis since the general variational principle is formulated with a "cutoff" local functional from which the ground state characteristics of a superfluid system may be calculated by using the generalized Green's function expressed through the solutions of the Bogoliubov equations at the stationary point. To construct the normal and anomalous densities, entering this local functional, only those solutions from the whole set are needed which corresponds to the eigenenergies E_α of the HFB hamiltonian, which is a matrix of the first variational derivatives of the EDF, up to the cutoff $\epsilon_c > \epsilon_F$. In contrast to the BCS-like methods in which the presence of an unphysical "particle gas" is almost unavoidable the coordinate-space Gor'kov (or HFB) equations [14] for finite systems naturally give a localized wave function with correct asymptotics for the normal and anomalous densities [19, 20].

From the Gor'kov equations, after separating angular variables, for the generalized radial Green's function $\hat{g}_{jl}$ one gets the equation

$$\begin{pmatrix} \epsilon - h_{jl} + \mu & -\Delta \\ -\Delta & \epsilon + h_{jl} - \mu \end{pmatrix} \hat{g}_{jl}(r_1, r_2; \epsilon) = \begin{pmatrix} \delta(r_1 - r_2) & 0 \\ 0 & \delta(r_1 - r_2) \end{pmatrix}, \tag{8}$$

where h_{jl} is the single-quasiparticle HF hamiltonian in the jl channel. The solution of this matrix equation can be constructed by using the set of the four linearly independent solutions which satisfy the homogenous system, obtained from (8) by setting the right hand side to zero, and obey the physical boundary conditions [14].

The poles (if any) of the generalized Green's function are determined by zeroes of the generalized Wronskian $W(\epsilon) = 0$, of the four linear-independent solutions, which gives the discrete spectrum of the Bogoliubov quasiparticle states. The spectrum is symmetrical around $\epsilon = 0$. For bound systems $\mu < 0$. If the system is finite one expects $\Delta_\infty = 0$, otherwise the system would be unstable with respect to two particle emission. It follows then that the spectrum is discrete within the energy region $|\epsilon| < |\mu|$ (here $\hat{g}_{jl}$ is a real function at the axis $\mathrm{Im}\,\epsilon = 0$) and continuous if $|\epsilon| > |\mu|$ (there $\hat{g}_{jl}$ is a complex function). These features are reflected in the upper panel of Fig.1 where the branch cuts are shown by the heavy lines extending symmetrically to the left and to the right from the points $\pm\mu$, respectively. The case with only the branch cuts, without poles, corresponds to a drip-line even nucleus. Integrating $\hat{g}_{jl}$ along the upper contour C of Fig.1 one obtains the radial part of the generalized density matrix for a system with even N.

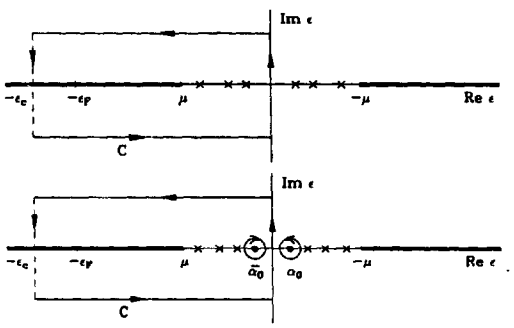

Fig. 1. The contour C in the energy plane to integrate the generalized Green's function for determining the generalized density matrix (top: for even nuclei, bottom: for odd nuclei). The crosses show the positions of the single-particle poles, the heavy lines represent the branch cuts on the $\mathrm{Im}\epsilon = 0$ axis where the energy spectrum is continuous, μ is the chemical potential, ϵ_F is the Fermi energy and ϵ_c is the energy cutoff (see text). The positions α_0 and $\bar{\alpha}_0$ of the poles for the odd quasiparticle are shown by heavy dots. Note that the ways of passing these poles go in the opposite directions

For an odd system the contour for integrating the generalized Green's in the complex energy plane should be modified. Suppose that the addition of an odd particle leads to the appearance of the quasiparticle with the energy E_{α_0} in the ground state of the system and that E_α corresponds to a certain eigenenergy of eq. (8) and belongs to the discrete spectrum, i.e. $|\mu| > E_{\alpha_0} > 0$ ($\alpha_0 = n_0 j_0 l_0 m_0$ is the usual set of the single-particle quantum numbers). As illustrated in Fig.1, E_{α_0} is located in the vicinity of the point $\epsilon = 0$. Generally, E_{α_0} is of the order of $\bar{\Delta}$, the average matrix element of the pairing potential on the the Fermi surface. The case of $E_{\alpha_0} \approx -\mu$ determines the position of the drip line for odd nuclei. The lower contour in Fig.1 clearly illustrates the blocking effect: the presense of the odd particle in the level α_0 prevents it from participating in the pairing correlations because in this case the "conjugate" level $\bar{\alpha}_0$ for an odd system should be empty. The nucleon separation energies S_n are determined by the position of the poles close to $\epsilon = 0$. As easily understood from Fig.1, since these separation energies are measured from the continuum threshold $\epsilon = -\mu$, for an odd system one gets $S_n^{odd} \approx -\mu - E_{\alpha_0}$, and, for an even system, $S_n^{even} \approx -\mu + E_{\bar{\alpha}_0}$. Thus we have $S_n^{even} - S_n^{odd} \approx 2E_{\alpha_0} \approx 2\bar{\Delta}$, i.e. the familiar odd-even effect in nuclear masses.

The calculations were performed with the density functional DF3 [13]. In the anomalous part of the EDF the "gradient" pairing force was used [12] (see eq. (7))

$$\mathcal{F}^{\xi}(x) = C_0 f^{\xi}(x), \quad f^{\xi}(x) = f^{\xi}_{ex} + h^{\xi} x^{q} + f^{\xi}_{grad} r_0^2 \left(\nabla x\right)^2 , \tag{9}$$

where $C_0 = 308$ MeV·fm^{-3}, $q = 2/3$, and $x = (\rho_n + \rho_p)/2\rho_0$ is the isoscalar dimensionless density. The superscript ξ indicates that the interaction corresponds to an energy cutoff ϵ_c (in our case $\epsilon_c = 40$ MeV while the Fermi energy $\epsilon_{0F} = 36.6$ MeV).

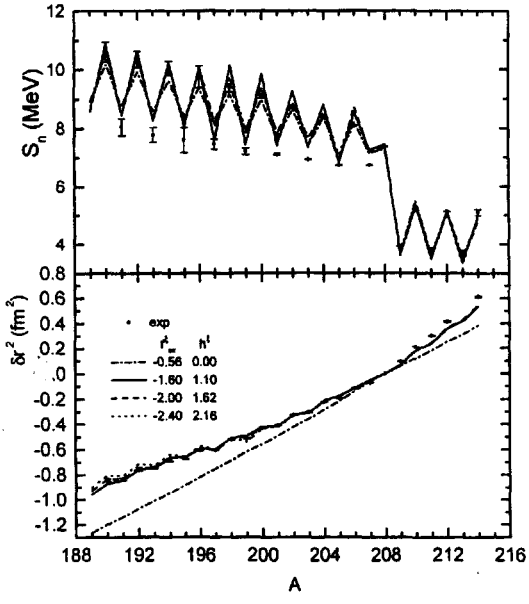

Fig. 2. Calculated neutron separation energies (top) and differences of mean squared charge radii (bottom) for lead isotopes with respect to ^{208}Pb as reference nucleus in comparison with experimental data. All calculations are done self-consistently using the EDF method with different parameter sets of the pairing force of eq. (9). The gradient strength $f^{\xi}_{grad} = 1$ for all sets except the case of "constant" pairing with $f^{\xi}_{ex} = -0.56$

Typical results obtained for the lead isotope chain are shown in Fig. 2. It is seen that the neutron separation energies S_n are described reasonably well with any set of parameters just sufficient to produce an "experimental" average gap at the Fermi surface but the rms charge radii $\langle r^2 \rangle^{1/2}_{ch}$ and their staggering can be explained only if the pairing force (9) contains density dependence and if its parameters are taken in a certain ratio. The physics behind this is discussed in [12]. The success in the simultaneous description of both observables, S_n and $\langle r^2 \rangle^{1/2}_{ch}$, in finite nuclei is due to the gradient term $\propto f^{\xi}_{grad} \approx 1$. This term vanishes in infinite uniform matter. Now the sets of the other two deduced parameters (f^{ξ}_{ex}, h^{ξ}) can be used to predict the pairing gap in nuclear matter. This can be done by solving the gap equation (7). The solution is given by

$$\Delta(x) = 8\epsilon_F(x) \sqrt{\frac{s(x)-1}{s(x)+1}} \exp\left(s(x) - 2 + \frac{2}{f^{\xi}(x) x^{1/3}}\right) , \tag{10}$$

with $s(x) = \sqrt{1 + \epsilon_c/\epsilon_F(x)}$ and $\epsilon_F = \epsilon_{0F} x^{2/3}$. The obtained pairing gap as function of the Fermi momentum (to facilitate the comparison with nuclear matter calculations, e.g. [5]) is shown in Fig. 3. The curve for "constant" pairing $f^{\xi}_{ex} = -0.56$ stands by itself with a positive derivative everywhere. In this case no acceptable description of $\langle r^2 \rangle^{1/2}_{ch}$ is obtained (see Fig. 2). An interesting observation is that all sets of the deduced parameters which give a satisfactory description of S_n and $\langle r^2 \rangle^{1/2}_{ch}$ yield about the same value of

$\Delta \approx 3.3$ MeV at $k_F \approx 1.16\,\mathrm{fm}^{-3}$ (at ≈ 0.66 of the equilbrium density). These sets produce for $\Delta(k_F)$ a characteristic bell form known from the calculations for infinite matter. Our preferred set which gives a slightly better fit compared to others is ($f_{ex}^{\xi} = -1.6$, $h^{\xi} = 1.10$). The corresponding pairing gap, shown in Fig. 3 by solid line, occurs to be in a qualitative agreement with the most recent calculations [5].

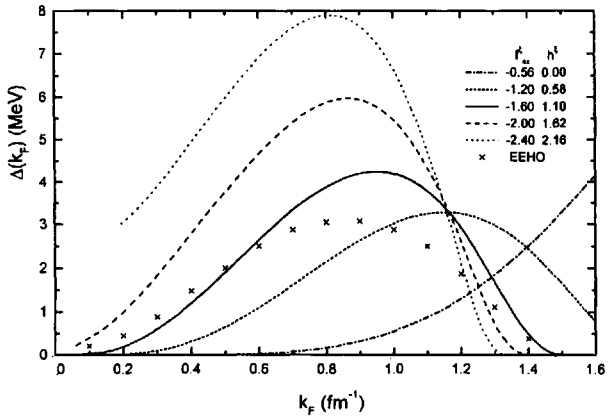

Fig.3. Pairing gap at the Fermi surface in infinite nuclear matter as a function of the Fermi momentum for different parameter sets deduced from the EDF calculations for the lead isotopes. Crosses represent nuclear matter calculation from ref. [5]

The formulated approach based on the local energy density functional method with coordinate-space technique is shown to be quite successful in describing the ground state properties of superfluid finite nuclear systems. The combined analysis of the differential observables such as neutron separation energies and isotopic shifts in charge radii with this approach gives hope to construct an universal density-dependent effective interaction which would allow one to predict pairing properties both for exotic nuclei very far from stability and for nuclear matter.

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