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Self-Consistent Occupation Probabilities in Brueckner-Hartree-Fock Calculations *

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A method is developed for evaluating self-consistent occupation probabilities in Brueckner-Hartree-Fock calculations of finite nuclei. The method does not involve explicitly the overlaps of defect wave functions but is based instead on the energy dependence of the G matrix elements. Results are presented for ^{16}O using a G matrix which shifts only the low-lying intermediate-particle spectrum.

It is well known that first-order Hartree-Fock (HF) or Brueckner-Hartree-Fock (BHF) calculations with realistic forces consistently fail to yield the correct saturation properties of finite nuclei.[1-9] Typical results yield too little binding energy and/or too small an rms radius. Moreover, simple estimates of the average kinetic energy per nucleon (based on known nuclear radii) combined with experimental information[10] on the single-particle (SP) energies of occupied states indicate that the simple HF definition of SP energies cannot be correct.[11] In heavy nuclei this problem is expected to be especially serious. It is, perhaps, not so well known that a relatively simple correction term can be incorporated into existing BHF codes to mitigate the above-mentioned deficiencies.

For some time now, several authors[7,8,12-20] have advocated the inclusion of occupation-probability diagrams (also called saturation-potential diagrams, rearrangement diagrams, or correlation corrections) in the definition of SP potentials. The lowest-order correction term is shown in Fig. 1(b). Figure 1(a) defines the usual HF potential, while 1(c) illustrates the correct prescription in which Figs. 1(a) and 1(b) are the leading terms.

Brandow, in a series of recent publications,[14-16] has suggested the following prescription for use in BHF calculations. The total energy is given by

$$\mathcal{H}_0 = \sum_A T_A + \tfrac{1}{2} \sum_{A,B} \langle AB| G(\omega) |AB\rangle P_A P_B + \sum_A (1 - P_A) U_A , \quad (1)$$

where:

$$\omega = E_A + E_B , \tag{2}$$

$$E_A = T_A + U_A , \tag{3}$$

$$U_A = \sum_B \langle AB | G(\omega) | AB \rangle P_B , \tag{4}$$

$$P_A = [1 + \tfrac{1}{2} \sum_B \langle \chi_{AB} | \chi_{AB} \rangle P_B]^{-1} . \tag{5}$$

In the above equations, A and B represent occupied states whose wave functions are the eigenstates of the BHF equations; each G matrix element is antisymmetrized and evaluated on the energy shell with self-consistent starting energy ω; and χ_{AB} is an antisymmetrized two-body defect wave function. Equations (1)–(4) reduce to the usual BHF formalism when the occupation probabilities P_A and P_B, are set equal to unity. The last term in Eq. (1) is an "over-counting correction" which must be included when SP energies are renormalized with occupation probabilities.

We will not be concerned here with the solution of the BHF equations or the evaluation of the reaction matrix G. Details can be found in Refs. 4, 18, and 19. In this paper we simply wish to illustrate the ease with which self-consistent occupation probabilities can be included in the calculations and the extent to which the results are improved.

One frequently used method of renormalizing with occupation probabilities is to expand Eq. (5) and retain only the first two terms, so that

$$P_A \approx 1 - \tfrac{1}{2} \sum_B \langle \chi_{AB} | \chi_{AB} \rangle . \tag{6}$$

Equations (5) and (6) are both difficult to solve because of the necessity of evaluating overlaps of two-body defect wave functions. We propose a method which does not involve explicitly the defect wave functions and is much simpler and more natural to use in BHF calculations. Moreover, it is exact to all orders and can be used to calculate self-consistently both the SP potential and the occupation probabilities.[19]

We begin by re-expressing Eq. (5) as

$$P_A = \left[1 + \sum_B \left\langle AB \left| G(\omega) \left(\frac{Q}{\omega - H_0} \right)^2 G(\omega) \right| AB \right\rangle P_B \right]^{-1} , \tag{7}$$

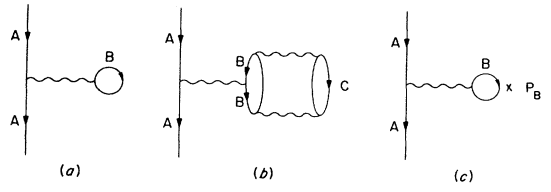

FIG. 1. Diagrammatic definitions of SP potential (see text for discussion).

where Q is a projection operator restricting the intermediate states to lie above the Fermi surface. Then consider two slightly different G matrices:

$$G(\omega) = V + V \frac{Q}{\omega - H_0} G(\omega) , \tag{8}$$

$$G(\omega') = V + V \frac{Q}{\omega' - H_0} G(\omega') , \tag{9}$$

which are related by the equation

$$G(\omega') = G(\omega) + G(\omega) \left[\frac{Q}{\omega' - H_0} - \frac{Q}{\omega - H_0} \right] G(\omega') . \tag{10}$$

Expanding Eq. (10), we obtain

$$G(\omega') - G(\omega) = -(\omega' - \omega) G(\omega) \left(\frac{Q}{\omega - H_0} \right)^2 G(\omega) + \eta , \tag{11}$$

where η contains terms in $(\omega' - \omega)^2$ and higher powers. The derivative of the G matrix is given by

$$\frac{\partial G(\omega)}{\partial \omega} = \lim_{\omega' \to \omega} \frac{G(\omega') - G(\omega)}{\omega' - \omega} = -G(\omega) \left(\frac{Q}{\omega - H_0} \right)^2 G(\omega) , \tag{12}$$

and from Eqs. (7) and (12) we find that[14–16]

$$P_A = \left[1 - \sum_B \left\langle AB \left| \frac{\partial G(\omega)}{\partial \omega} \right| AB \right\rangle P_B \right]^{-1} , \tag{13}$$

where the derivative is evaluated at $\omega = E_A + E_B$.

The main point here is that the denominator of Eq. (13) can be calculated simultaneously with the SP potential at each iteration. To evaluate the SP potential from Eq. (4), we must interpolate on $G(\omega)$, e.g.,

$$G(\omega) = G_0 + \omega G_1 + \omega^2 G_2 + \omega^3 G_3 , \tag{14}$$

where the coefficients G_0, G_1, G_2, and G_3 are stored in the memory of the computer. These same coefficients can be used to obtain

$$\partial G / \partial \omega = G_1 + 2\omega G_2 + 3\omega^2 G_3 , \tag{15}$$

which is then substituted into Eq. (13) to calculate the occupation probabilities. The method is applicable to any interpolation scheme.

In Table I we give the results of calculations of ^{16}O, both with and without occupation probability renormalization. The G matrix is calculated according to the prescription of Ref. 18, with harmonic-oscillator energies for the high-lying intermediate states and shifted harmonic-oscillator energies for all intermediate states with $2n_1 + l_1 + 2n_2 + l_2 \leq 14$. ($n_1$ and n_2 are the number of radial nodes for the SP wave functions.) All states below this level are shifted downward by the amount B_0 indicated in the table.

The nucleus is still underbound, but this is not surprising since nuclear-matter calculations[20]

TABLE I. Occupied SP energies, occupation probabilities, binding energy/nucleon, and charge radius for ^{16}O. The numbers in parentheses are for unrenormalized BHF calculations, with unit occupation probabilities, and B_0 is the shift of the low-lying particle spectrum. The calculations are done with the Hamada-Johnson potential, for $\hbar\Omega = 12.5$, a maximum relative l of 3, and a dimensionality of 4. All energies are in MeV. The binding energy/nucleon and r_c are corrected for center-of-mass motion.

B_0	0	30
Neutron states:		
$E_{0s_{1/2}}$	−27.8 (−33.6)	−29.6 (−38.1)
$E_{0p_{3/2}}$	−11.0 (−14.6)	−13.0 (−18.4)
$E_{0p_{1/2}}$	−8.7 (−11.4)	−10.7 (−15.0)
$P_{0s_{1/2}}$	0.874 (1.0)	0.834 (1.0)
$P_{0p_{3/2}}$	0.903 (1.0)	0.826 (1.0)
$P_{0p_{1/2}}$	0.905 (1.0)	0.823 (1.0)
Proton states:		
$E_{0s_{1/2}}$	−25.0 (−30.4)	−27.0 (−34.8)
$E_{0p_{3/2}}$	−8.3 (−11.5)	−10.5 (−15.3)
$E_{0p_{1/2}}$	−6.1 (− 8.4)	−8.3 (−11.9)
$P_{0s_{1/2}}$	0.873 (1.0)	0.832 (1.0)
$P_{0p_{3/2}}$	0.904 (1.0)	0.825 (1.0)
$P_{0p_{1/2}}$	0.906 (1.0)	0.822 (1.0)
$\mathcal{K}_0/A$	1.93 (1.73)	3.64 (3.06)
r_c(fm)	2.90 (2.76)	2.80 (2.65)

using the Hamada-Johnston potential also yield too little binding. Of more interest is that the renormalized calculation gives more total binding energy and a larger rms radius than the unrenormalized results. Then, comparing the effects of shifting the intermediate-state spectrum, we see that increasing B_0 tends to bring the binding energy/nucleon and r_c closer to the experimental values[21,22] of 7.98 MeV and 2.75 fm, respectively. Also, notice that the occupied SP levels become more repulsive when we renormalize; thus, it is expected that introducing occupation probabilities will bring the SP levels of heavy nuclei into better agreement with experiment. This latter point is also consistent with the proposal of Baranger[23] that the SP potential be defined in terms of all self-energy insertions that are attached to a hole line at a single point.

The choice of intermediate-state spectrum for use in BHF calculations remains open. Many authors use plane-wave intermediate states while others prefer harmonic-oscillator states with various kinds of energy shifts. The final choice will depend greatly on more accurate evaluations of the three-body cluster energy for both nuclear matter and finite nuclei. We also note that occupation probabilities for low-lying excited states might be important,[24] as might the lowest-order diagrams with potential insertions in particle lines.[18]

We point out that our method gives results very close to those obtained by Becker *et al.*,[17] who calculate occupation probabilities from the overlaps of the defect wave functions. The method described here is presently being used in other BHF calculations.[25,26]

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Inclusion of Nuclear-Structure Calculations in Nucleon-Nucleus Scattering

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It is shown how one can use the results of a nuclear-structure calculation in the theory of nucleon-nucleus scattering. We restrict ourselves to the simple case of nucleon scattering on a hole nucleus. The correlations of the ground state have been included.

INTRODUCTION

In a previous work[1] we have developed the general theory of nucleon-nucleus scattering on a hole nucleus in the framework of linear-response theory extending Migdal's approach[2] to the scattering problem. With a similar goal, the unrenormalized random-phase approximation (RPA) has been applied to the scattering problem, using a schematic model.[3] The details and restrictions of these methods can be found in Refs. 1 and 3, as well as in further references. It turns out that a calculation of the scattering process using an effective particle-hole interaction would be rather complicated, since one has to solve a complicated Fredholm problem.[1] Therefore, one has so far studied the problem only in the framework of a schematic model,[1,3] where the corresponding Fredholm determinant degenerates. But it is well known that the schematic model is only a poor approximation to the real situation (see for instance, Mikeska.[4]) For this reason we think one can obtain an improvement of the present status of the theory by including the results of the nuclear-structure calculation obtained with a normal effective particle-hole interaction. The deviations from the nuclear-structure calculation – caused by the matrix elements of the interaction between continuum-bound and continuum-continuum single-particle states – will be treated in this work by a schematic approach. This implies that these special matrix elements can be approximately represented by a separable particle-hole force with the help of a fitting procedure to the real particle-hole force. One may get further improvement using perturbation theory for the difference of the particle-hole force and the separable force as a final step. In the first section, we give a short summary of the nucleon-nucleus scattering theory on a hole nucleus in terms of Migdal's renormalized quantities. The explicit treatment of the model will then be given in the second section.

I. GENERAL FORMALISM

It has been shown in Ref. 1, that the scattering