Brueckner-Hartree-Fock Calculations of Spherical Nuclei in a Harmonic-Oscillator Basis. II[*]

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An approximation made in previous Brueckner-Hartree-Fock calculations is removed. Both the hole–hole and the particle–hole matrix elements of the single–nucleon potential are now calculated with the correct available energy of the pair. It is shown that, with a given G matrix, the occupied states and energies do not depend on the prescription used for the particle–particle elements. The formalism is easily extended to include Brandow's occupation probabilities.

In Brueckner-Hartree-Fock (BHF) calculations, it is necessary to satisfy both the Hartree-Fock (HF) and the Brueckner self-consistencies. For finite nuclei, the HF self-consistency is easily taken into account by performing the calculations in a harmonic-oscillator representation.[1,2] A recent paper[3] shows how to generalize the matrix method in order to satisfy most of the Brueckner self-consistency also.

Two aspects of this approach might be emphasized. Both are associated with the dependence of the G matrix on ω, the available energy of the correlated pair. First of all, it is not feasible to solve the Bethe-Goldstone equation after each iteration. Instead, one solves this equation beforehand for a few values of ω, and then interpolates during the iteration process. The method of paper I can be used with any reasonable interpolation scheme. The second aspect is that ω refers to the HF representation, *not* to the oscillator representation in which the calculations are actually performed. When one transforms from one basis to the other, the ω dependence introduces some additional one-body matrices which are trivial in ordinary HF. These matrices can be handled, however, and it is found that the computer codes for use in ordinary HF[2] can be simply modified in order to do BHF calculations.

Unfortunately, the present method does not use a self-consistent Pauli operator Q in the calculation of G; it uses a Q appropriate for the oscillator basis, not the actual HF states. Corrections allowing for this additional self-consistency can be reduced by a judicious choice of the oscillator parameter b; the latter should be chosen so that the nuclear size calculated with pure oscillator functions agrees approximately with the size resulting from the BHF calculation. Hopefully, these corrections are small and can be added on by perturbation theory after the main calculation is completed.

The present method also does not try to feed back, into the calculation of the G matrix, the particle spectrum resulting from the BHF calculation — and even less the particle wave functions. Such ultimate self-consistency has now been achieved for nuclear matter,[4] but it would be much harder for finite nuclei.

For computational reasons, an approximation was made in paper I on the particle-hole matrix elements of the single-nucleon potential. The first purpose of this paper is to show how to remove this approximation. The computational complexity is only slightly increased. All calculations done in this paper are with the G matrix of Kuo.[5] Other BHF calculations are presently being done with G matrices developed by Becker, MacKellar, and Morris[6] and by McCarthy.[7] In the following, we also show how to modify the equations in order to include occupation probabilities.[8,9]

We use the notations of paper I. The harmonic-oscillator wave functions are specified by:

$$\alpha, \beta, \gamma, \delta \equiv (nqljm),$$

$$a, b, c, d \equiv (nqlj) = (ns);$$

and the HF wave functions by:

$$\xi, \eta, \zeta \equiv (pqljm),$$

$$x, y, z \equiv (pqlj) = (ps),$$

where n and p are radial quantum numbers and $s \equiv (qlj)$ is the symmetry type.

The matrix elements of the single-nucleon po-

TABLE I. Occupied single-nucleon energies, total energy, and mass and proton rms radii of ^{40}Ca. The calculations are for Kuo's G matrix,[5] with $b = 1.8$ fm, a dimensionality of 3, a maximum relative l of 2 and unit occupation probabilities. All energies are in MeV. Center-of-mass corrections are not included.

	Method of paper I	Method of this paper
Neutron states		
$0s_{1/2}$	−66.3	−66.6
$0p_{3/2}$	−45.0	−45.2
$0p_{1/2}$	−41.2	−41.3
$0d_{5/2}$	−24.0	−24.1
$1s_{1/2}$	−20.6	−20.7
$0d_{3/2}$	−17.9	−17.9
Proton states		
$0s_{1/2}$	−58.3	−58.5
$0p_{3/2}$	−37.3	−37.4
$0p_{1/2}$	−33.6	−33.7
$0d_{5/2}$	−16.5	−16.6
$1s_{1/2}$	−13.1	−13.2
$0d_{3/2}$	−10.6	−10.6
$\mathcal{K}_0$	−153.2	−152.4
r_m (fm)	2.97	2.96
r_p (fm)	2.99	2.98

TABLE II. Unoccupied single-nucleon energies of ^{40}Ca in MeV. The table shows the dependence on $\bar{\epsilon}_{sp}$. All other parameters are the same as for Table I. As $\bar{\epsilon}_{sp}$ increases, the energies decrease, as expected.

$\bar{\epsilon}_{sp}$	$2\epsilon^{av} - \epsilon_{sp}$	ϵ_{sp}	−100.0	+25.0
Neutron states				
$0f_{7/2}$	−0.35	−4.9	2.7	−7.9
$1p_{3/2}$	1.5	−2.9	4.0	−5.5
$1p_{1/2}$	3.5	−0.80	5.6	−3.0
$0f_{5/2}$	6.3	1.9	8.1	0.02
Proton states				
$0f_{7/2}$	7.8	2.4	10.0	0.31
$1p_{3/2}$	9.2	4.2	11.0	2.3
$1p_{1/2}$	10.9	6.1	12.4	4.6
$0f_{5/2}$	13.4	8.8	14.6	7.6

tential are given by[10,11]:

$$\langle \xi | U | \eta \rangle = \tfrac{1}{2} \sum_{\zeta} {}' \langle \xi \zeta | G(\epsilon_x + \epsilon_z) + G(\epsilon_y + \epsilon_z) | \eta \zeta \rangle,$$

$$\xi, \eta \quad \text{both holes}; \quad (1a)$$

$$\langle \xi | U | \eta \rangle = \langle \eta | U | \xi \rangle^* = \sum_{\zeta} {}' \langle \xi \zeta | G(\epsilon_x + \epsilon_z) | \eta \zeta \rangle,$$

$$\xi \text{ a hole}, \ \eta \text{ a particle}; \quad (1b)$$

$$\langle \xi | U | \eta \rangle = \tfrac{1}{2} \sum_{\zeta} {}' \langle \xi \zeta | G(\bar{\epsilon}_x + \epsilon_z) + G(\bar{\epsilon}_y + \epsilon_z) | \eta \zeta \rangle,$$

$$\xi, \eta \quad \text{both particles}; \quad (1c)$$

where the prime means the sum is over occupied states only. The energy $\bar{\epsilon}_x$ differs from ϵ_x be-

cause of the off-shell effect in the particle-particle "bubble diagram," but its correct value is rather uncertain. This uncertainty has been discussed in paper I. Some examples of $\bar{\epsilon}_x$ are:

$$\bar{\epsilon}_x = 2\epsilon^{av} - \epsilon_x, \quad (2a)$$

where ϵ^{av} is the average of all occupied single-nucleon energies;

$$\bar{\epsilon}_x = \epsilon_x \quad \text{(on-shell prescription)}; \quad (2b)$$

$$\bar{\epsilon}_x = \text{a constant}. \quad (2c)$$

For ease of computation, we now write Eqs. (1) in unified form:

$$\langle \xi | U | \eta \rangle = \tfrac{1}{2} \sum_{\zeta} {}' \langle \xi \zeta | G(\epsilon'_{xy} + \epsilon_z) + G(\epsilon'_{yx} + \epsilon_z) | \eta \zeta \rangle, \quad (3)$$

with

$$\epsilon'_{xy} = \epsilon_x \quad \text{if both } \xi \text{ and } \eta \text{ are holes},$$

$$= \epsilon_x \quad \text{if } \xi \text{ is a hole}, \ \eta \text{ a particle},$$

$$= \epsilon_y \quad \text{if } \xi \text{ is a particle}, \ \eta \text{ a hole}, \quad (4)$$

$$= \bar{\epsilon}_x \quad \text{if both } \xi \text{ and } \eta \text{ are particles}.$$

Equation (3) is then transformed to the harmonic-oscillator representation

$$\langle \alpha | U | \beta \rangle = \tfrac{1}{2} \sum_{\alpha' \beta' \gamma \delta} \sum_{\xi \eta} \sum_{\zeta} {}' \langle \alpha | \rho_\xi | \alpha' \rangle \langle \delta | \rho_\zeta | \gamma \rangle \langle \beta' | \rho_\eta | \beta \rangle \langle \alpha' \gamma | G(\epsilon'_{xy} + \epsilon_z) + G(\epsilon'_{yx} + \epsilon_z) | \beta' \delta \rangle, \quad (5)$$

where $\langle \alpha | \rho_\xi | \alpha' \rangle$ is a density matrix for an individual HF orbit

$$\langle \alpha | \rho_\xi | \alpha' \rangle = \langle \alpha | \xi \rangle \langle \xi | \alpha' \rangle. \quad (6)$$

Finally, we perform the geometry[2,3] to obtain

$$(n_1 | U_s | n_2) = \tfrac{1}{2} \sum_{n_1' n_2'} \sum_{P_1 P_2} (n_1 | \rho_{s P_1} | n_1')(n_2' | \rho_{s P_2} | n_2) [(n_1' | \Gamma_s(\epsilon_{s P_1 P_2}') | n_2') + (n_1' | \Gamma_s(\epsilon_{s P_2 P_1}') | n_2')], \quad (7)$$

with

$$(n_1 | \Gamma_s(\epsilon') | n_2) = \sum_{n_3 n_4} \sum_{t P_3} {}' (n_4 | \rho_{t P_3} | n_3)[-(2j_t + 1)^{1/2}(2j_s + 1)^{-1/2} F_0(s n_1, s n_2, t n_4, t n_3; \epsilon' + \epsilon_{t P_3})], \quad (8)$$

and F_0 is a two-body particle-hole matrix element.[2]

TABLE III. Convergence with iteration of some neutron single-nucleon energies of ^{40}Ca. The upper number in each set is for $\bar{\epsilon}_{sp} = 2\epsilon^{av} - \epsilon_{sp}$; the lower number is for $\bar{\epsilon}_{sp} = \epsilon_{sp}$. Energies are in MeV.

| States | Number of iterations | | | | |
	2	4	7	11	19
$0s_{1/2}$	−64.979	−65.961	−66.489	−66.596	−66.607
	−65.305	−66.318	−66.589	−66.606	−66.607
$0p_{3/2}$	−43.824	−44.681	−45.076	−45.150	−45.158
	−44.036	−44.932	−45.147	−45.158	−45.158
$0p_{1/2}$	−40.364	−40.981	−41.257	−41.313	−41.318
	−40.515	−41.168	−41.306	−41.318	−41.318
$0d_{3/2}$	−17.947	−17.920	−17.925	−17.930	−17.930
	−17.959	−17.927	−17.928	−17.930	−17.930
$0f_{7/2}$	−0.9174	−0.4789	−0.3674	−0.3502	−0.3485
	−5.016	−4.918	−4.911	−4.911	−4.911

Equation (7) replaces Eq. (11) of paper I. This method is more exact than the previous method, but it does result in an increase in the iteration time. For example, for ^{40}Ca with a dimensionality of 3, it takes about 1.3 min on the IBM 360/75 to perform 19 iterations, whereas for the method of paper I it takes about 0.65 min. For most cases the iteration time increases by a factor of 2 or 3. This is not expected to be a serious problem since the iteration time is usually small compared to the time required to calculate two-body matrix elements.[2]

In Table I a comparison is made of the ground-state properties of ^{40}Ca using the two methods. It is seen that the approximation made in paper I for the particle-hole matrix element of U was a good one for calcium, although it does get worse for heavy nuclei.[3]

The particle-particle prescription, Eq. (2), is not specified in Table I because *the occupied states are completely independent of* $\bar{\epsilon}_x$. The four very different values of $\bar{\epsilon}_x$ shown in Table II all give exactly the same occupied single-nucleon energies and wave functions. In fact, the occupied states do not depend at all on any assumption made about the particle-particle elements (1c), as long as we work with a given G matrix and do not try to calculate it with a self-consistent particle spectrum. The particle-particle elements could be set equal to zero, for example, and the BHF results (for occupied states) would not change. This behavior is not completely obvious since Eq. (7) involves sums over p_1 and p_2 which include the unoccupied states of symmetry type s. It was not true in paper I, in which prescription (1b) for particle-hole elements was modified. We now give a short proof, based on the fact that both hole-hole and particle-hole matrix elements of U involve only hole energies. The HF equation is

$$(T + U)|\eta\rangle = \epsilon_y |\eta\rangle. \tag{9}$$

Substitute for U its expressions (1a), (1b), *assuming η to be an occupied state*:

$$U|\eta\rangle = \sum_\xi |\xi\rangle\langle\xi|U|\eta\rangle = \sum_\xi \sum_\zeta{}' |\xi\rangle\langle\xi\zeta|G(\epsilon_y + \epsilon_z)|\eta\zeta\rangle + \tfrac{1}{2}\sum_\xi{}' \sum_\zeta{}' |\xi\rangle\langle\xi\zeta|G(\epsilon_x + \epsilon_z) - G(\epsilon_y + \epsilon_z)|\eta\zeta\rangle. \tag{10}$$

The first term is correct by itself when ξ is a particle state; the second term makes the necessary correction when ξ is a hole. Equation (9) can now be written in component form:

$$\sum_\beta (\langle\alpha|T|\beta\rangle + \langle\alpha|U_y|\beta\rangle)\langle\beta|\eta\rangle = \epsilon_y\langle\alpha|\eta\rangle, \tag{11a}$$

with

$$\langle\alpha|U_y|\beta\rangle = \sum_{\gamma\delta} \sum_\zeta{}' \langle\xi|\gamma\rangle\langle\delta|\zeta\rangle[\langle\alpha\gamma|G(\epsilon_y + \epsilon_z)|\beta\delta\rangle + \tfrac{1}{2}\sum_{\alpha'} \sum_\xi{}' \langle\alpha|\xi\rangle\langle\xi|\alpha'\rangle\langle\alpha'\gamma|G(\epsilon_x + \epsilon_z) - G(\epsilon_y + \epsilon_z)|\beta\delta\rangle]. \tag{11b}$$

Note that ξ, η, ζ are all holes, so that Eqs. (11) do not involve either the wave functions of the particle states or their energies. These equations are sufficient to determine the energies and wave functions of the hole states, therefore the latter do not depend at all on the prescription for particle-particle elements,

once a dimensionality has been chosen. The proof is valid only when we have achieved complete self-consistency. This is demonstrated in Table III which compares the convergence with iteration of two prescriptions for $\bar{\epsilon}_x$. It is interesting that the on-shell prescription, which gives complete continuity between particles and holes, converges much better than the off-shell one.

For future use, we now show that our previous equations can be simply modified to take into account two-body correlation corrections for the occupied states, or occupation probabilities.[8,9,12,13] Each term in the sum on the right-hand side of Eq. (3) is multiplied by the occupation probability P_z.

$$\langle \xi | U | \eta \rangle = \tfrac{1}{2} \sum_r {}' \langle \xi \zeta | G(\epsilon'_{xy} + \epsilon_z) + G(\epsilon'_{yx} + \epsilon_z) | \eta \zeta \rangle P_z , \tag{12}$$

and it can be shown that[14]

$$P_x = \left[1 - \sum_\zeta {}' \left\langle \xi\zeta \left| \frac{\partial G(\omega)}{\partial \omega} \right| \xi\zeta \right\rangle P_z \right]^{-1} , \quad \omega = \epsilon_x + \epsilon_z . \tag{13}$$

Equations (6) and (7) are unchanged, and Eq. (8) becomes

$$(n_1 | \Gamma_s(\epsilon') | n_2) = \sum_{n_3 n_4} \sum_{tp_3} {}' (n_4 | \rho_{tp_3} | n_3) P_{tp_3} [- (2j_t + 1)^{1/2} (2j_s + 1)^{-1/2} F_0(sn_1, sn_2, tn_4, tn_3; \epsilon' + \epsilon_{tp_3})] , \tag{14}$$

with

$$P_{sp} = [1 - \sum_{n_1 n_2} (n_2 | \rho_{sp} | n_1)(n_1 | \bar{\Gamma}_s(\epsilon_{sp}) | n_2)]^{-1} , \tag{15}$$

$$(n_1 | \bar{\Gamma}_s(\epsilon_{sp}) | n_2) = \sum_{n_3 n_4} \sum_{tp_3} {}' (n_4 | \rho_{tp_3} | n_3) P_{tp_3} \left[-(2j_t + 1)^{1/2}(2j_s + 1)^{\frac{1}{2}} \frac{\partial F_0}{\partial \omega} (sn, sn_2, tn_4, tn_3; \omega) \right] ,$$

$$\omega = \epsilon_{sp} + \epsilon_{tp_3} . \tag{16}$$

The occupation probabilities can be calculated self-consistently at each iteration, along with the single-particle potential, and it is found that there is only a slight increase in iteration time.

With occupation probabilities included, the total energy $\mathcal{H}_0$ should now include an "overcounting correction"[9]

$$\mathcal{H}_0 = \sum_\xi {}' [\langle \xi | T | \xi \rangle + \tfrac{1}{2}(2 - P_x)\langle \xi | U | \xi \rangle] . \tag{17}$$

In the oscillator representation, this becomes

$$\mathcal{H}_0 = \sum_{n_1 n_2} \sum_{sp} {}' (2j_s + 1)(n_1 | T_{j_s} | n_2)(n_2 | \rho_{sp} | n_1) + \tfrac{1}{2} \sum_{n_1 n_2} \sum_{sp} {}' (2 - P_{sp})(2j_s + 1)(n_1 | U_s | n_2)(n_2 | \rho_{sp} | n_1). \tag{18}$$

Brandow[9] has emphasized that this $\mathcal{H}_0$ admits a variational principle, so that self-consistency implies stationarity.

These correlation corrections were already introduced in Brueckner calculations of light nuclei using pure oscillator wave functions,[12,13] and they are included in a new series of BHF calculations now in progress.[14-16]

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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

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