polarization calculations using the Yale-Shakin interaction at a later stage. As has been shown by Bertsch,[11] core polarization mainly effects the pairing matrix elements.

In Table III, we present the Δ values of neutron single-particle levels for some nuclei to compare the gap function Δ obtained for the Yale-Shakin interaction with that for the state-dependent and constant-Δ solutions using the δ-function interaction. It is clearly seen that the δ-function interaction justifies a constant-Δ solution, whereas the Yale-Shakin interaction, though normally giving results similar to the δ-function force, sometimes gives notable differences. These differences in Δ values, it seems, will not cause any substantial change in predicting other properties, e.g., binding energies, spectra, etc.

Thus, the conclusion of this work is that the results of the Yale-Shakin and the δ-function forces agree quite closely, showing that the results are practically independent of the detailed form of the interaction.

[11] G. F. Bertsch, Nucl. Phys. **74**, 234 (1965).

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Number-Conserving Approximation to the Shell Model*

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The broken-pair-approximation (BPA) formalism is presented in this paper in complete form for the description of the nuclear properties of medium and heavy spherical nuclei. Starting from an approximate ground state of even nuclei having BCS-type pair distribution in the valence shells, the model Hilbert space is constructed by replacing one, two, ... pairs in the assumed approximate ground state by arbitrary two, four, ... particle configurations. The BPA states for odd-mass nuclei are obtained by coupling the odd nucleon to zero-, one-, ... broken-pair states. It is shown that the Hilbert spaces spanned in the projected quasiparticle theories and in the BPA are the same in a certain limit, and that in practice these two formalisms are physically equivalent. The BPA is an improvement on the quasiparticle theories and is an approximation to the seniority shell model. All the relevant expressions for calculating energy matrices, transition rates, inelastic electron-scattering form factors, and spectroscopic factors for one- and two-nucleon transfer reactions are presented in a coherent form. The corresponding expressions for the case of first BPA are further elaborated and presented in a form suitable for numerical computation.

I. INTRODUCTION

FOR an accurate description of the nuclear properties in the framework of the shell model one should diagonalize the shell-model Hamiltonian in the Hilbert space containing at least all possible configurations of the nucleons in the partially filled major shell. An orthonormal basis set in this model space is constructed by the well-known shell-model techniques using seniority (w) as quantum number. Defining a pair as two identical nucleons coupled to $J=0$, seniority is then the number of unpaired nucleons or the residue after all pairs have been removed. These configuration-mixing calculations, which are commonly known as exact shell-model (ESM) calculations, are indeed intractable due to the prohibitively large dimensions of energy matrices when the nucleon number exceeds four in valence shells. If one still insists on doing ESM calculations, one is permanently limited to three or four particles in three or four levels. Obviously, a truncation of the basis is obligatory for carrying out such calculations in practice. The simplest one is the

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seniority truncation which has proved quite successful (cf. Ref. 1). In this approximation the Hilbert space is generally limited in such a way that it contains the basis up to seniority four or less for even nuclei and up to seniority three for odd-mass nuclei. Due to the strong pairing part of the interaction, the states with a large number of pairs are energetically favored, so that this is generally a good approximation for low-lying nuclear states. Unfortunately, this approximation is also handicapped by similar problems of large dimensions. For example, let us consider the case of Sn^{116} containing 16 neutrons in five ($2d_{5/2}$, $1g_{7/2}$, $3s_{1/2}$, $2d_{3/2}$, $1h_{11/2}$) valence shells, outside the assumed ($Z=N=50$) core. The number of seniority-zero states in this case is 110 and that of seniority-two ($J^\pi=2^+$) states approaches a thousand. Clearly, such calculations, referred to as lowest-seniority ($w\leq 4$) shell-model (LSSM) calculations, are in practice limited to specific cases.

To preserve the basic concept of the shell model with configuration mixing and to make it more practicable, further approximate methods were developed. The foremost is the quasiparticle or BCS method,[2] which neatly takes into account the pairing interaction between the nucleons by the Bogolubov-Valatin canonical transformation. The quasiparticle vacuum, or BCS state, contains correlated pairs of nucleons. For describing low-lying states it is a reasonably good approximation to diagonalize the Hamiltonian in the Hilbert space containing the zero-, two-, and four-quasiparticle subspaces for even nuclei and the one- and three-quasiparticle subspaces for odd-mass nuclei. This procedure, known by various names such as quasiparticle second Tamm-Dancoff, modified Tamm-Dancoff approximation, etc., has been successfully applied[3–13] to describe many nuclear properties in various nuclear regions.

The most disturbing feature of the quasiparticle theory is the nonconservation of nucleon number. The Hamiltonian in the truncated space containing a limited number of quasiparticles no longer commutes with the particle number, so that its eigenstates are superpositions of states with different numbers of particles. The fact that the quasiparticle theory describes a specific nucleus is reflected only in the imposed condition that the expectation value of the particle number operator in the BCS state coincides with the actual number of valence nucleons. As a result the solutions of the quasiparticle theory describe only average properties of neighboring nuclei and do not pretend to describe the individual nuclear properties, for which one needs a fixed value of the nucleon number. Furthermore, some of the solutions are spurious and do not correspond to any physical state of a single nucleus and must be projected out before energy matrices can be diagonalized.

It has been shown[1,14,15] that the part corresponding to the actual nucleon number n, projected out from the BCS state, when normalized has $\simeq$99% overlap with the ESM ground state of a specific nucleus, which is almost a seniority-zero state. Clearly, this fact supports the use of the projected zero- and two-quasiparticle wave functions in calculating the nuclear properties of low-lying states. This procedure is referred to as projected Tamm-Dancoff approximation (PTDA). The PTDA results[1] of Ni^{62} show that the obtained wave functions for 0^+_1, 2^+_1, 4^+_1, states have about 99% overlaps with the corresponding wave functions of the LSSM ($w\leq 2$) calculations. Ottaviani and Savoia[16] have recently performed PTDA calculations for Sn^{116}. The PTDA results indicate, however, that for an accurate description of the low-lying excited states, the second states of each J^π in particular, the corresponding second approximation is highly desirable. Unfortunately, in practice, these calculations are very involved.

These facts and the success achieved by the quasiparticle theory indicate the necessity of developing a systematic number-conserving formalism utilizing the essential physical contents (inclusion of pairing correlations) of the quasiparticle theory. In this paper, we develop an approximation to the LSSM based on an assumption which takes into account the strong pairing correlation effects. We truncate the LSSM Hilbert space by assuming as a first approximation that the ground state for $2p$ nucleons is built up by the repeated (p times) application on the particle vacuum of the operator S_+ creating a pair distributed among the various levels. This form of the ground state was

[1] M. H. Macfarlane, *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, Colorado 1966), p. 583.
[2] M. Baranger, Phys. Rev. **120**, 957 (1960); this work lists all other earlier publications.
[3] R. Arvieu, Ann. Phys. (Paris) **8**, 407 (1963); R. Arvieu, E. Baranger, M. Baranger, M. Vénéroni, and V. Gillet, Phys. Letters **4**, 119 (1963); R. Arvieu, E. Salusti, and M. Vénéroni, *ibid.* **8**, 334 (1964).
[4] P. L. Ottaviani, M. Savoia, J. Sawicki, and A. Tomasini, Phys. Rev. **153**, 1138 (1967); P. L. Ottaviani, M. Savoia, and J. Sawicki, Phys. Letters **24B**, 353 (1967).
[5] A. Rimini, J. Sawicki, and T. Weber, Phys. Rev. **168**, 1401 (1968).
[6] M. Gmitro, J. Hendeković, and J. Sawicki, Phys. Letters **26B**, 252 (1968); Phys. Rev. **169**, 983 (1968).
[7] M. Gmitro and J. Sawicki, Phys. Letters **26B**, 493 (1968).
[8] A. Rimini, J. Sawicki, and T. Weber, Phys. Rev. Letters **20**, 676 (1968).
[9] B. Gyarmati and J. Sawicki, Nucl. Phys. **A111**, 609 (1968).
[10] T. T. S. Kuo, E. Baranger, and M. Baranger, Nucl. Phys. **79**, 513 (1966).
[11] M. K. Pal, Y. K. Gambhir, and Ram Raj, Phys. Rev. **155**, 1144 (1967); **163**, 1004 (1967).
[12] Y. K. Gambhir, Ram Raj, and M. K. Pal, Phys. Rev. **162**, 1139 (1967); R. Alzetta, A. Rimini, T. Weber, M. Gmitro, and J. Sawicki, *ibid.* **185**, 1233 (1969).
[13] J. B. French and L. S. Hsu, Phys. Letters **19**, 135 (1965); L. S. Hsu, Nucl. Phys. **A96**, 624 (1967).
[14] A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. **124**, 162 (1961); Y. K. Gambhir and Ram Raj, *ibid.* **161**, 1125 (1967).
[15] R. Arvieu, Cargèse Summer School Lectures, 1968 (unpublished); B. Lorazo, thesis, Orsay, 1968 (unpublished).
[16] P. L. Ottaviani and M. Savoia, Phys. Rev. **187**, 1306 (1969).

first proposed by Mottelson.[17] The coefficients of the distribution in S_+ are determined by minimizing the total Hamiltonian with respect to the ground state. Clearly, this approximate ground state is a special seniority-zero state. The state vectors defining the first and second successive approximations are constructed by replacing one and two S_+ operators, respectively, in the ground state by two- and four-particle creation operators. Similarly, the Hilbert space for odd-mass nuclei is obtained by coupling the odd nucleon to the states of zeroth and first approximation for the corresponding even nuclei. The present formalism, which will be referred to as the broken-pair approximation (BPA), is clearly an approximate version of the LSSM. The BPA theory fits directly into the frame of the shell model, avoiding any quasiparticle transformation. It turns out that, in a certain limit, the BPA is equivalent to the projected quasiparticle theory (Sec. II B). The success of the first approximation (PTDA or first BPA) for the first state of a given J^π has already been mentioned. The assumption of the BPA model space is also supported by the study of the breaking of the generalized seniority scheme.[15,18] The coherent presentation of the BPA, given here, is a useful simplification over the projected quasiparticle theories both from the conceptual and practical points of view.

All the relevant expressions for calculating energy matrices, electromagnetic transition rates and static moments, form factors for inelastic electron scattering and spectroscopic factors for one- and two-nucleon transfer reactions are given. The formalism presented in this paper holds both for identical and nonidentical nucleon systems. In the latter case, the pairing correlations between neutrons and protons are neglected in the approximate ground state.

II. HAMILTONIAN

The shell-model Hamiltonian H for spherical nuclei in the second quantized form is given by

$$H=\sum_\alpha \epsilon_a a_\alpha^\dagger a_\alpha+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta\mid V\mid\gamma\delta\rangle_A a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \quad (2.1)$$

The greek subscripts denote all the quantum numbers required to specify the single-particle shell-model states, while the latin subscripts denote all the quantum numbers designated by the corresponding Greek subscripts except the angular momentum projection quantum number. Very frequently we shall also use a, b, ... to denote only the angular momentum quantum numbers and the corresponding Greek letters α, β, ... to denote the respective projection quantum numbers. The occurrence of these symbols in phase factors, weight factors, or in the angular momentum coupling coefficients, will make it obvious wherever such a practice is being followed. $a^\dagger$ and a are the single-particle creation and annihilation operators, respectively, and obey the usual fermion anticommutation rules. ϵ_a is the single-particle energy, V is the two-body effective potential, and the label A denotes matrix elements with respect to normalized antisymmetric states. We introduce the operators

$$A_{JM}^\dagger(ab)=(a_a^\dagger\otimes a_b^\dagger)_{JM}=\sum_{m_\alpha m_\beta}\begin{bmatrix}a & b & J\\ \alpha & \beta & M\end{bmatrix}a_\alpha^\dagger a_\beta^\dagger,$$

$$A_{JM}(ab)=[A_{JM}^\dagger(ab)]^\dagger, \quad (2.2)$$

and

$$H_1(a)=\sum_{m_\alpha} a_\alpha a_\alpha^\dagger,$$

$$H_2(a'b'abI)=\sum_N A_{IN}(a'b')A_{IN}^\dagger(ab), \quad (2.3)$$

where the brackets denote the Clebsch-Gordan coefficient. The Hamiltonian H can then be written in the coupled form

$$H=h_0+\sum_a h_1(a)H_1(a)+\sum_{a\le b,a'\le b',I} h_2(aba'b'I)\times H_2(a'b'abI). \quad (2.4)$$

The quantities h_0, h_1, and h_2 are defined by

$$h_0=\sum_a[\hat{a}^2\epsilon_a+\tfrac{1}{2}\hat{a}\sum_b \hat{b}F(aabb0)],$$

$$h_1(a)=-[\epsilon_a+\hat{a}^{-1}\sum_b \hat{b}F(aabb0)], \quad (2.5)$$

$$h_2(aba'b'I)=(1+\delta_{ab})^{-1}(1+\delta_{a'b'})^{-1}G(aba'b'I),$$

where

$$\langle\alpha\beta\mid V\mid\alpha'\beta'\rangle_A=\sum_{IN}\begin{bmatrix}a & b & I\\ \alpha & \beta & N\end{bmatrix}\begin{bmatrix}a' & b' & I\\ \alpha' & \beta' & N\end{bmatrix}\times G(aba'b'I),$$

$$F(ab'a'bJ)=-\sum_I \hat{I}^2 G(aba'b'I)\begin{Bmatrix}a & b & I\\ a' & b' & J\end{Bmatrix}. \quad (2.6)$$

The symbol $\hat{j}$ stands for $(2j+1)^{1/2}$. It is to be noted that our G and F quantities are -2 times the corresponding ones of Baranger.[2] The form (2.4) of H is valid only if j value, parity and charge are enough to identify the single-particle levels. It is the most convenient form to evaluate the Hamiltonian matrix in the BPA formalism.

III. BPA

A. Basis States

As remarked in the Introduction, the ground state of even nuclei is practically a seniority-zero state. This is due to the strong pairing part $[G(aabb0)]$ of the

[17] B. R. Mottelson, Problème à N Corps, Les Houches, 1958 (unpublished).

[18] O. Bohigas, C. Quesne, and R. Arvieu, Phys. Letters **26B**, 562 (1968).

effective interaction. In order to truncate the prohibitively large dimensions of the lowest seniority ($w \leq 4$) Hilbert space we construct our model space starting from a particular seniority-zero state which approximately takes into account the pairing part of the interaction.

We introduce the operator

$$S_+ = \sum_a \varphi_a \tfrac{1}{2}\hat{a} A_{00}^\dagger(aa), \tag{3.1}$$

in which the coefficients φ give the weight distribution of a pair in the various levels. The approximate ground state for $2p$ nucleons

$$S_+^p \mid 0\rangle \tag{3.2}$$

is then assumed, $\mid 0\rangle$ being the particle vacuum. In practice, it is more convenient to use, instead of the coefficients φ and the operator S_+^p, the quantities u and v defined by

$$\varphi_a = v_a/u_a, \qquad u_a^2 + v_a^2 = 1, \tag{3.3}$$

and the operator

$$\mathfrak{I}_p^\dagger = (p!)^{-1}\Big(\prod_a u_a^{(a+1/2)}\Big) S_+^p. \tag{3.4}$$

The coefficients u and v are to be determined by minimizing H, i.e., by

$$\delta\langle 0 \mid \mathfrak{I}_p H \mathfrak{I}_p^\dagger \mid 0\rangle / \langle 0 \mid \mathfrak{I}_p \mathfrak{I}_p^\dagger \mid 0\rangle = 0. \tag{3.5}$$

We note that $\mathfrak{I}_p^\dagger \mid 0\rangle$ is an exact solution of the pairing part of the interaction in the case when $p=1$. Furthermore, in the general case, $\mathfrak{I}_p^\dagger \mid 0\rangle$ has exactly the same structure as the projected BCS state. In fact, these two states coincide when u_a and v_a are replaced by the corresponding quantities U_a and V_a of the quasiparticle theory defined later through Eqs. (3.19) and (3.20). The results of earlier calculations[1,14,15] show that the projected BCS state has $\simeq 99\%$ overlap with the seniority-zero ground-state wave function. This indicates that our assumed approximate ground state is very near to the true ground state and, moreover, that the replacement of u_a and v_a by U_a and V_a, respectively, is a good approximation.

The remaining state vectors in our model space are constructed by utilizing the idea that the replacement of one operator S_+ by an arbitrary two-particle creation operator requires a large amount of energy, so that the states containing a large number of operators S_+ are energetically favored. This argument is analogous to that which is used to justify the seniority truncations, with the difference that in place of a pair $[A_{00}^\dagger(aa)]$ we have now a pair distributed among the levels in a definite way (S_+). In fact, this difference is responsible for the larger reduction of the dimensions of the shell-model Hilbert space obtained in the BPA. The states defining the first approximation, which are analogous to the seniority two states, are

$$\mathfrak{I}_{p-1}^\dagger A_{JM}^\dagger(rs) \mid 0\rangle. \tag{3.6}$$

These states were first used in Ref. 15 in the $J=0$ case. Clearly, the states (3.6) for $J \neq 0$ are particular seniority two states, in which the distribution of $(p-1)$ zero-coupled pairs is bounded by our assumption of the approximate ground state. For $J=0$, the states (3.6) are $w=0$ states; they are not orthogonal and, furthermore, the approximate ground state $\mathfrak{I}_p^\dagger \mid 0\rangle$ is just a linear combination of these states.

For the successive approximations the states are constructed by replacing more S_+ operators by an equal number of $A^\dagger$ operators. For example, for the two-broken-pair approximation the states are

$$\mathfrak{I}_{p-2}^\dagger [A_{J_1}^\dagger(r_1 s_1) \otimes A_{J_2}^\dagger(r_2 s_2)]_{JM} \mid 0\rangle. \tag{3.7}$$

These states are linear combinations of seniority-zero, -two, and -four states for $2p$ nucleons. For seniorities zero and two, the states (3.6) are linear combinations of the states (3.7). It is to be mentioned that, by breaking all pairs, the ESM Hilbert space is obtained.

The BPA states for $(2p+1)$ particles, corresponding to odd-mass nuclei, are similarly obtained by coupling the odd nucleon to zero- and one-broken-pair states. They are

$$\mathfrak{I}_p^\dagger a_{jm}^\dagger \mid 0\rangle, \tag{3.8}$$

$$\mathfrak{I}_{p-1}^\dagger [a_r^\dagger \otimes A_{J1}^\dagger(r_1 s_1)]_{jm} \mid 0\rangle. \tag{3.9}$$

The states (3.9) are linear combinations of seniority-one and seniority-three states. For seniority-one the states (3.8) are linear combinations of states (3.9).

We shall indicate, in general, the BPA states for $2p$ particles (even nuclei) or $2p+1$ particles (odd-mass nuclei) by

$$\mathfrak{I}_{p-b}^\dagger X_{JM}^\dagger(d, K) \mid 0\rangle, \tag{3.10}$$

where b is the number of broken pairs, $X_{JM}^\dagger(d, K)$ is a vector-coupled product of $2b$ or $2b+1$ creation operators for particles in the levels indicated on the whole by d, K being the set of the intermediate angular momenta. The states

$$X_{JM}^\dagger(d, K) \mid 0\rangle \tag{3.11}$$

will be called few-particle states, in contrast to the BPA states (3.10). The BPA states for different values of d and K are, in general, not orthogonal, even if the corresponding few-particle states are. Therefore an orthonormal basis must be constructed before setting up the Hamiltonian matrix. The orthonormalization procedure requires the knowledge of the scalar products of the BPA states.

An explicit expression for the scalar products can easily be obtained by making use of the seniority representation. We first expand the few-particle states (3.11) in terms of the orthonormal few-particle states

$\mathfrak{X}_{JM}{}^{\dagger}(n_i, w_i, \alpha) \mid 0\rangle$ with definite occupation numbers n_i and seniorities w_i; α is an additional quantum number which may be necessary to specify the state uniquely. The total seniority is

$$w=\sum_i w_i.$$

The expansion coefficients are

$$a_K{}^{w_i\alpha}(d, J)=\langle 0 \mid \mathfrak{X}_{JM}[n_i(d), w_i, \alpha]X_{JM}{}^{\dagger}(d, K) \mid 0\rangle. \tag{3.12}$$

The evaluation of (3.12) requires the operators $\mathfrak{X}^{\dagger}$ in the second quantized form. The operators $\mathfrak{X}^{\dagger}$ for the seniorities zero, one, and two can be written down uniquely in terms of $X^{\dagger}$ operators with specific values of K. The $\mathfrak{X}^{\dagger}$ operators corresponding to the subsequent higher-seniority states can then be obtained by taking only those linear combinations of $X^{\dagger}$ operators which are orthogonal among themselves as well as to the lower-seniority states. This can easily be carried out because only few particles are involved. The procedure is explicitly shown in Refs. 1 and 11. The states $\mathfrak{I}_{p-b}{}^{\dagger}\mathfrak{X}_{JM}{}^{\dagger}(n_i, w_i, \alpha) \mid 0\rangle$ can then be expanded in terms of $2p$- or $(2p+1)$-particle states in the seniority representation and their scalar products can be evaluated. One gets

$$\langle 0 \mid X_{JM}(d', K')\mathfrak{I}_{p-b}\mathfrak{I}_{p-b}{}^{\dagger}X_{JM}{}^{\dagger}(d, K) \mid 0\rangle=\sum_{w_i\alpha} a_K{}^{w_i\alpha}(d, J)a_{K'}{}^{w_i\alpha}(d', J)\mathfrak{D}^{(p-b)}[n_i(d), n_i(d'), w_i], \tag{3.13}$$

where

$$\mathfrak{D}^{(p-b)}(n_i, n_i', w_i)=\sum_{r_1\cdots r_\nu}\prod_{i=1}^{\nu}\frac{u_i{}^{2\Omega_i-r_i+\frac{1}{2}(n_i+n_i')}v_i{}^{r_i-\frac{1}{2}(n_i+n_i')}}{[\frac{1}{2}(r_i-n_i)]![\frac{1}{2}(r_i-n_i')]!}$$
$$\times\frac{[\frac{1}{2}(r_i-w_i)]!}{[\Omega_i-\frac{1}{2}(r_i+w_i)]!}\left[\frac{[\Omega_i-\frac{1}{2}(n_i+w_i)]![\Omega_i-\frac{1}{2}(n_i'+w_i)]!}{[\frac{1}{2}(n_i-w_i)]![\frac{1}{2}(n_i'-w_i)]!}\right]^{1/2}. \tag{3.14}$$

Here ν is the number of valence levels and $\Omega_i=j_i+\frac{1}{2}$. The summation runs over all integer values of $r_1, \cdots, r_\nu$ such that

$$(-)^{r_i}=(-)^{w_i}, \qquad r_i\geq n_i, \qquad r_i\geq n_i', \qquad r_i\leq 2\Omega_i-w_i, \quad \text{and} \quad \sum_i r_i=2(p-b)+\sum_i n_i.$$

The derivation of Eqs. (3.13) and (3.14) is given in Appendix B. Using the facts that the states $\mathfrak{X}_{JM}{}^{\dagger}(n_i, w_i, \alpha) \mid 0\rangle$ form a complete orthonormal set and that the quantities $\mathfrak{D}$ are independent of α, Eq. (3.13) can be put in the form

$$\langle 0 \mid X_{JM}(d', K')\mathfrak{I}_{p-b}\mathfrak{I}_{p-b}{}^{\dagger}X_{JM}{}^{\dagger}(d, K) \mid 0\rangle=\delta_{n_i(d)n_i(d')}\langle 0 \mid X_{JM}(d', K')X_{JM}{}^{\dagger}(d, K) \mid 0\rangle\mathfrak{D}^{(p-b)}[n_i(d), n_i(d), n_i(d)]$$
$$+\sum_{w_i\alpha, \Sigma w_i\leq\mu} a_K{}^{w_i\alpha}(d, J)a_{K'}{}^{w_i\alpha}(d', J)\{\mathfrak{D}^{(p-b)}[n_i(d), n_i(d'), w_i]-\delta_{n_i(d)n_i(d')}\mathfrak{D}^{(p-b)}[n_i(d), n_i(d), n_i(d)]\}, \tag{3.15}$$

where μ is $2b-2$ (even nuclei) or $2b-1$ (odd-mass nuclei). Equation (3.15) is much more convenient than Eq. (3.13) for practical calculations. In fact, it allows one to compute the scalar products between states (3.10), avoiding the expansion on the states of maximum seniority $2b$ or $2b+1$.

B. Relation between BPA and Quasiparticle Tamm-Dancoff Theory

In the quasiparticle theory, the Bogolubov-Valatin canonical transformation is introduced:

$$\alpha_\alpha{}^{\dagger}=U_a a_{am\alpha}{}^{\dagger}-(-)^{a-\alpha}V_a a_{a-m\alpha} \tag{3.16}$$

with

$$U_a{}^2+V_a{}^2=1, \tag{3.17}$$

which is devised to take into account the pairing correlation effects. The quasiparticle vacuum $\mid \mathrm{BCS}\rangle$ is defined, with respect to the new operators which create and destroy quasiparticles, by

$$\alpha_\alpha \mid \mathrm{BCS}\rangle=0, \qquad \text{for all } \alpha. \tag{3.18}$$

In terms of the particle operators, the normalized state $\mid \mathrm{BCS}\rangle$ is given by

$$\mid \mathrm{BCS}\rangle=\prod_{a, m_a>0}[U_a+(-)^{a-\alpha}V_a a_{am\alpha}{}^{\dagger}a_{a-m\alpha}{}^{\dagger}] \mid 0\rangle$$
$$=\sum_p I_p{}^{\dagger} \mid 0\rangle, \tag{3.19}$$

where $I_p{}^{\dagger}$ has the same form as $\mathfrak{I}_p{}^{\dagger}$ [Eq. (3.4)] with the coefficients u_a replaced by U_a. It is apparent from (3.19) that $\mid \mathrm{BCS}\rangle$ contains components corresponding to the different numbers of nucleons which can exist in the valence shells.

The transformation coefficients U (and V) are determined by minimizing H with respect to the state $\mid \mathrm{BCS}\rangle$ with the constraint that the expectation value of the number operator coincides with the actual number n of nucleons present in the valence shells. This is accomplished in practice by replacing H with the Hamiltonian

$$\mathfrak{IC}=H-\lambda\sum_\alpha a_\alpha{}^{\dagger}a_\alpha,$$

λ being a Lagrangian multiplier. Thus, the quantities U and λ are determined through the equations

$$(\partial/\partial U_a)\langle \mathrm{BCS} \mid \mathcal{H} \mid \mathrm{BCS}\rangle = 0, \qquad \text{for all } a \tag{3.20}$$

and

$$\langle \mathrm{BCS} \mid \sum_\alpha a_\alpha^\dagger a_\alpha \mid \mathrm{BCS}\rangle = n. \tag{3.21}$$

These equations are equivalent to the well-known gap and number equations.

The Hamiltonian $\mathcal{H}$ in terms of quasiparticle operators separates into two parts. The first is a diagonal one-quasiparticle operator and the second represents the interaction among the quasiparticles. Their explicit expressions are given in Refs. 4 and 11. The exact solution of the problem would be obtained by diagonalizing $\mathcal{H}$ (i.e., H with the single-particle energies counted from the Fermi level λ) over all the quasiparticle configurations. However, the creation of a quasiparticle requires a fairly large energy which is always greater than the "gap" parameter ($\approx$1 MeV for medium weight nuclei). Therefore, for describing the low-lying nuclear states it is sufficient to consider a space containing a limited number (usually ≤ 4) of quasiparticles. This procedure is known as the quasiparticle Tamm-Dancoff method.

It is apparent that the states with a definite number of quasiparticles contain components corresponding to the different numbers of nucleons which can exist in the valence shells. Therefore these states do not correspond to a specific nucleus. In order to remedy this defect it is desirable to project from these quasiparticle states the part corresponding to the actual nucleon number and use these states in determining the transformation coefficients and in setting up the energy matrices. This procedure is called the projected quasiparticle Tamm-Dancoff method. For simplicity, the minimization after projection is usually not performed and the transformation coefficients obtained through Eqs. (3.20) and (3.21) are used in setting up the energy matrices with projected quasiparticle basis. In fact, the coefficients determined by minimizing before and after projection are, generally, nearly equal.

The quasiparticle states can be written straightforwardly as a sum of components with definite particle number by using the transformation (3.16) and the commutation relations given in Appendix A. For zero- and two-quasiparticle states one gets

$$\mid \mathrm{BCS}\rangle_{2p} = I_p^\dagger \mid 0\rangle, \tag{3.22}$$

$$[(\alpha_r^\dagger \otimes \alpha_s^\dagger)_{JM} \mid \mathrm{BCS}\rangle]_{2p} = (U_r U_s)^{-1} I_{p-1}^\dagger A_{JM}^\dagger(rs) \mid 0\rangle - \delta_{J0}\delta_{rs}\hat{r}(V_r/U_r) I_p^\dagger \mid 0\rangle. \tag{3.23}$$

It is clear from Eqs. (3.22) and (3.23) that the space spanned by the projected zero- and two-quasiparticle states and that spanned by the zero- and one-broken-pair states are the same in the limit in which the coefficients U_a and V_a are equal to u_a and v_a. It can easily be shown that the same is true for higher approximations and for odd-mass nuclei. Therefore, the use of an orthonormal basis constructed either by the projected quasiparticle states or by the broken-pair states would lead, in the said limit, to identical physical results.

C. Hamiltonian Matrix

In this subsection the expressions for the elements of the Hamiltonian matrix are evaluated. Let $\mid \psi_{JM}(k)\rangle$ denote the orthonormal BPA basis states, related to the states (3.10) through

$$\mid \psi_{JM}(k)\rangle = \sum_{d,K} \gamma_k^{d,K}(J) \mid \varphi_{JM}(d, K)\rangle \equiv \sum_{d,K} \gamma_k^{d,K}(J) \mathfrak{I}_{p-b}^\dagger X_{JM}^\dagger(d, K) \mid 0\rangle. \tag{3.24}$$

Using (2.4), the Hamiltonian matrix is given by

$$\langle \psi_{JM}(k') \mid H - h_0 \mid \psi_{JM}(k)\rangle = \sum_{d,K,d',K'} \gamma_{k'}^{d',K'} \gamma_k^{d,K} \times \Big[\sum_a h_1(a) \langle \varphi_{JM}(d', K') \mid H_1(a) \mid \varphi_{JM}(d, K)\rangle + \sum_{a\leq b, a'\leq b', I} h_2(aba'b'I) \times \langle \varphi_{JM}(d', K') \mid H_2(a'b'abI) \mid \varphi_{JM}(d, K)\rangle\Big]. \tag{3.25}$$

The matrix elements in the square bracket in (3.25) are easily reduced in terms of scalar products between BPA states for the nuclei with one or two additional nucleons. The result is

$$\langle \varphi_{JM}(d', K') \mid H_1(a) \mid \varphi_{JM}(d, K)\rangle = \sum_j \hat{j}^2 \hat{J}^{-2} \langle 0 \mid \{[a_a^\dagger \otimes X_J^\dagger(d', K')]_j\}^\dagger \times \mathfrak{I}_{p-b}\mathfrak{I}_{p-b}^\dagger [a_a^\dagger \otimes X_J^\dagger(d, K)]_j \mid 0\rangle, \tag{3.26}$$

$$\langle \varphi_{JM}(d', K') \mid H_2(a'b'abI) \mid \varphi_{JM}(d, K)\rangle = \sum_{J_0} \hat{J}_0^2 \hat{J}^{-2} \langle 0 \mid \{[A_I^\dagger(a'b') \otimes X_J^\dagger(d', K')]_{J_0}\}^\dagger \times \mathfrak{I}_{p-b}\mathfrak{I}_{p-b}^\dagger [A_I^\dagger(ab) \otimes X_J^\dagger(d, K)]_{J_0} \mid 0\rangle. \tag{3.27}$$

The scalar products in the right-hand side of Eqs. (3.26) and (3.27) are given by the general expression (3.15). In a specific BPA the summations over j, I, and J_0 can be carried out explicitly. The resulting expressions for the first BPA are given in Appendix C.

IV. CALCULATION OF ELECTROMAGNETIC PROPERTIES AND SPECTROSCOPIC FACTORS

A. Electromagnetic Transition Rates, Static Moments, and Inelastic-Electron-Scattering Form Factors

The second quantized version of any single-particle tensor operator $\Omega_{\lambda\mu}$ of rank λ is

$$\Omega_{\lambda\mu} = \sum_{\alpha\alpha'} \langle \alpha \mid \Omega_{\lambda\mu} \mid \alpha'\rangle a_\alpha^\dagger a_{\alpha'} = \delta_{\lambda 0}\delta_{\mu 0} \sum_a \hat{a} \langle a \mid\mid \Omega_0 \mid\mid a\rangle - \sum_{aa'} \hat{a}^{-1} \langle a \mid\mid \Omega_\lambda \mid\mid a'\rangle \Omega_1^\lambda(a, a'), \tag{4.1}$$

where

$$\Omega_1^{\lambda}(aa') = \sum_{m_a m_{a'}} \begin{bmatrix} a' & \lambda & a \\ \alpha' & \mu & \alpha \end{bmatrix} a_{a'}\, a_{\alpha}^{\dagger} \qquad (4.2)$$

and the reduced matrix element is defined by

$$\langle \alpha \mid \Omega_{\lambda\mu} \mid \alpha' \rangle = \hat{a}^{-1} \begin{bmatrix} a' & \lambda & a \\ \alpha' & \mu & \alpha \end{bmatrix} \langle a \mid\mid \Omega_{\lambda} \mid\mid a' \rangle. \qquad (4.3)$$

The electromagnetic reduced transition probabilities and static moments are simply related to the quantity

$$\langle J \mid\mid \Omega_{\lambda} \mid\mid J' \rangle \qquad (4.4)$$

in which $\mid JM\rangle$ and $\mid J'M'\rangle$ are the pertinent nuclear states which are linear combinations of states $\mid \varphi_{JM}(d, K)\rangle$ and $\mid \varphi_{J'M'}(d', K')\rangle$, respectively. It is simple to evaluate the expressions for the nuclear reduced matrix elements in terms of scalar products between BPA states. The result (for $\lambda \neq 0$) is

$$\begin{aligned} \langle \varphi_{J'}(d', K') \mid\mid \Omega_{\lambda} \mid\mid \varphi_{J}(d, K) \rangle = & \sum_{aa'} \langle a \mid\mid \Omega_{\lambda} \mid\mid a' \rangle \\ & \times \sum_{j} (-)^{a'-J'-j} \hat{J}^2 \begin{Bmatrix} J & J' & \lambda \\ a' & a & j \end{Bmatrix} \\ & \times \langle 0 \mid \{[a_{a'}^{\dagger} \otimes X_{J'}^{\dagger}(d', K')]_j\}^{\dagger} \\ & \times \mathfrak{I}_{p-b} \mathfrak{I}_{p-b}^{\dagger} [a_a^{\dagger} \otimes X_J^{\dagger}(d, K)]_j \mid 0 \rangle. \end{aligned} \qquad (4.5)$$

In the case of the first BPA, the explicit final expression is given in Appendix C. For $\lambda = 0$ the first term of Eq. (4.1) must be added.

The inelastic-electron-scattering form factor in the first Born approximation is simply related[19] to the nuclear matrix elements of the Coulomb, transverse electric, and transverse magnetic operators. Their expressions are given in Ref. 19. These operators are single-particle tensor operators and can be written in the form (4.1). Therefore, the calculation of the nuclear reduced matrix elements will require exactly the same steps as those followed in the case of the electromagnetic transition rates.

It is possible to incorporate the core contributions in the calculation of electromagnetic transition rates, electromagnetic static moments, form factors of inelastic electron scattering, in an approximate manner by replacing the nucleon charge e by a phenomenological effective charge e_{eff}, or, better, by replacing the quantity $\langle a \mid\mid \Omega_{\lambda} \mid\mid a' \rangle$ in Eq. (4.1) by the corresponding calculated effective quantity $\langle a \mid\mid \Omega_{\lambda}^{\text{eff}} \mid\mid a' \rangle$, as shown in Ref. 20.

[19] T. de Forest, Jr., and J. D. Walecka, Advan. Phys. **15**, 1 (1966).

[20] M. Gmitro, A. Rimini, J. Sawicki, and T. Weber, Phys. Rev. Letters **20**, 1185 (1968); **175**, 1243 (1968).

B. Spectroscopic Factors for One- and Two-Nucleon Transfer Reactions

According to the DWBA theory, the nuclear structure factors s for a one-nucleon transfer reaction can be expressed as the overlap integral between a state of the heavier nucleus $\mid JM\rangle$ and a free state $\mid \chi_{JM}\rangle$ composed of the lighter nucleus with spin J_0 and the transferred neutron with angular momentum j_a, i.e.,

$$s_{j_a}(J_0, J) = \langle JM \mid \chi_{JM}(a, J_0) \rangle \qquad (4.6)$$

with

$$\mid \chi_{JM}(a, J_0) \rangle = \sum_{m_\alpha} \begin{bmatrix} a & J_0 & J \\ \alpha & M_0 & M \end{bmatrix} \mid J_0 M_0 \rangle a_{\alpha}^{\dagger} \mid 0 \rangle. \qquad (4.7)$$

In the framework of the BPA theory $\mid JM\rangle$ is a linear combination of BPA states $\mid \varphi_{JM}(d, K)\rangle$ for the heavier nucleus and $\mid \chi_{JM}\rangle$ is a linear combination of those BPA states which are obtained by coupling the j_a nucleon to the BPA states of angular momentum $J_0 M_0$ of the lighter nucleus. The factor s_{j_a} then reduces to a linear combination of the scalar products of the BPA states evaluated earlier [Eq. (3.15)].

Similarly, the spectroscopic factor B of Yoshida[21] for the stripping reaction $(A \rightarrow A+2)$

$$\begin{aligned} B_{J_1 J_2}(Jab) = & \sum_{M M_2} \begin{bmatrix} J_1 & J & J_2 \\ M_1 & M & M_2 \end{bmatrix} (1+\delta_{ab})^{-1/2} \\ & \times \langle J_2 M_2 (A+2) \mid A_{JM}^{\dagger}(ab) \mid J_1 M_1 (A) \rangle \end{aligned} \qquad (4.8)$$

can easily be evaluated by using (3.15). It is to be noted that in Eq. (3.14) the u's and v's coming from the two states must be kept distinguished.

V. CONCLUDING REMARKS

The BPA theory has been presented as an approximate version of the LSSM for describing the low-lying states of nuclei. It has the advantage over LSSM that it leads to quite reasonable dimensions of the energy matrices. The reduction in dimensions stems from the assumption of an approximate ground state having a particular structure. The BPA theory is an improvement over the quasiparticle theories because its wave functions correspond to a specific nucleus. Physically, the BPA formalism is equivalent to the projected quasiparticle theories.

All the relevant expressions for calculating energy matrices, electromagnetic transition rates and static moments, inelastic-electron-scattering form factors and spectroscopic factors for one- and two-nucleon transfer reactions are presented in a coherent form. The formalism also holds for systems having both neutrons and protons where the pairing effects between the two

[21] S. Yoshida, Nucl. Phys. **33**, 685 (1962); Phys. Rev. **123**, 2122 (1961).

kinds of particles are neglected in the approximate ground state.

The formalism is being applied to the specific cases of Ni and Sn isotopes. The numerical results will be reported in subsequent publications.

A formalism similar to ours has been applied by Lorazo[22] to the 0^+ states of Ni^{62} and Sn^{116}.

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APPENDIX A

We present here the most relevant commutation relations used in this paper. Some of them are given in the form of vacuum expectation values, since their complete expressions are quite lengthy and are not involved in the present work;

$$[A_{J'M'}(a'b'),A_{JM}{}^{\dagger}(ab)]_{-}=\bar{P}(abJ)\Bigg[\delta_{JJ'}\delta_{MM'}\delta_{aa'}\delta_{bb'}-\bar{P}(a'b'J')\delta_{ab'}\sum_{J''}\hat{J}\hat{J}'(-)^{J+J''+M'}\times\begin{Bmatrix}J' & a' & b'\\ b & J & J''\end{Bmatrix}\begin{bmatrix}J & J' & J''\\ M & -M' & M-M'\end{bmatrix}(a_b{}^{\dagger}\otimes\tilde{a}_{a'})_{J'',M-M'}\Bigg], \tag{A1}$$

$$\langle 0\mid[C_{(J')j}(a'b'c'),C_{(J)j}{}^{\dagger}(a,bc)]_{-}\mid 0\rangle=\bar{P}(b'c'J')\left(\delta_{aa'}\delta_{bb'}\delta_{cc'}\delta_{JJ'}+\hat{J}\hat{J}'\bar{P}(bcJ)\delta_{ac'}\delta_{bb'}\delta_{ca'}\begin{Bmatrix}b & c & J\\ j & a & J'\end{Bmatrix}\right), \tag{A2}$$

$$\langle 0\mid[B_{(J_1'J_2')J}(a'b'c'd'),B_{(J_1J_2)J}{}^{\dagger}(abcd)]_{-}\mid 0\rangle=\bar{P}(a'b'J_1')\bar{P}(c'd'J_2')\times\left(\bar{P}[(abJ_1)(cdJ_2)J]\delta_{aa'}\delta_{bb'}\delta_{cc'}\delta_{dd'}\delta_{J_1J_1'}\delta_{J_2J_2'}-\hat{J}_1\hat{J}_2\hat{J}_1'\hat{J}_2'\bar{P}(abJ_1)\bar{P}(cdJ_2)\delta_{aa'}\delta_{bc'}\delta_{cb'}\delta_{dd'}\begin{Bmatrix}a & b & J_1\\ c & d & J_2\\ J_1' & J_2' & J\end{Bmatrix}\right), \tag{A3}$$

$$[a_{\alpha},\mathfrak{I}_p{}^{\dagger}]_{-}=(-)^{a-\alpha}(v_a/u_a)\mathfrak{I}_{p-1}{}^{\dagger}a_{a,-m\alpha}{}^{\dagger}, \tag{A4}$$

$$[A_{JM}(ab),\mathfrak{I}_p{}^{\dagger}]_{-}=(-)^{J-M}\mathfrak{I}_{p-1}{}^{\dagger}[\bar{P}(abJ)(v_a/u_a)(a_a{}^{\dagger}\otimes\tilde{a}_b)_{J-M}+\delta_{ab}\delta_{J0}\delta_{M0}\hat{a}(v_a/u_a)]-(-)^{J-M}(v_av_b/u_au_b)\mathfrak{I}_{p-2}{}^{\dagger}A_{J-M}{}^{\dagger}(ab), \tag{A5}$$

$$[(a_a{}^{\dagger}\otimes\tilde{a}_b)_{JM},\mathfrak{I}_p{}^{\dagger}]_{-}=-(v_b/u_b)\mathfrak{I}_{p-1}{}^{\dagger}A_{JM}{}^{\dagger}(ab), \tag{A6}$$

where

$$\tilde{a}_{am\alpha}=(-)^{a-\alpha}a_{a,-m\alpha}, \tag{A7}$$

$$C_{(J)jm}{}^{\dagger}(a,bc)=[a_a{}^{\dagger}\otimes A_J{}^{\dagger}(bc)]_{jm}, \tag{A8}$$

$$B_{(J_1J_2)JM}{}^{\dagger}(abcd)=[A_{J_1}{}^{\dagger}(ab)\otimes A_{J_2}{}^{\dagger}(cd)]_{JM}, \tag{A9}$$

and

$$\bar{P}(abJ)=1-(-)^{a+b+J}(a\leftrightarrow b), \tag{A10}$$

$$\bar{P}[(abJ_1)(cdJ_2)J]=1+(-)^{J_1+J_2+J}(a\leftrightarrow c,\ b\leftrightarrow d,\ J_1\leftrightarrow J_2). \tag{A11}$$

APPENDIX B

We outline below the derivation of Eqs. (3.13) and (3.14). The main step involved is to express the states

$$\mathfrak{I}_{p-b}{}^{\dagger}\mid n_1w_1,\cdots,n_vw_v\rangle, \tag{B1}$$

which are obtained by applying the operator $\mathfrak{I}_{p-b}{}^{\dagger}$ on the few-particle states in the seniority representation, in terms of $2p$- or $(2p+1)$-particle states in the seniority representation. The operator $\mathfrak{I}_{p-b}{}^{\dagger}$ is first expressed in terms of the operators

$$S_{+}(i)=(\tfrac{1}{2}\Omega_i)^{1/2}A_{00}{}^{\dagger}(ii) \tag{B2}$$

using the definition (3.4) and the algebraic identity

$$(\sum_{i=1}^{\nu}c_i)^m=m!\sum_{p_1\cdots p_\nu,\Sigma_ip_i=m}\prod_{i=1}^{\nu}\frac{1}{p_i!}c_i{}^{p_i}, \tag{B3}$$

where the c_i's are commuting operators. Next, the

[22] B. Lorazo, Phys. Letters **29B**, 150 (1969).

state $|\, n_i w_i\rangle$ is written as

$$|\, n_i w_i\rangle = \mathfrak{N}_{q_i,w_i}^{-1/2} S_+^{q_i}(i)\, |\, w_i w_i\rangle, \tag{B4}$$

where the normalization factor

$$\mathfrak{N}_{q_i,w_i} = \frac{q_i!(\Omega_i - w_i)!}{(\Omega_i - w_i - q_i)!} \quad \text{for} \quad q_i \le \Omega_i - w_i \tag{B5}$$
$$= 0 \qquad \text{otherwise}$$

is derived in Ref. 1. Then the operators $S_+(i)$ coming from $\mathfrak{I}_{p-b}^{\dagger}$ are combined with the $S_+(i)$ introduced through (B4) and, using formula (B4) again, the state (B1) is written as

$$\mathfrak{I}_{p-b}^{\dagger}\, |\, n_1 w_1, \cdots, n_\nu w_\nu\rangle = \sum_{p_1 \cdots p_\nu, \Sigma_i p_i = p-b} \prod_{i=1}^{\nu} u_i^{\Omega_i - p_i} \times v_i^{p_i} (p_i!)^{-1} \mathfrak{N}_{p_i+q_i,w_i}^{1/2} \mathfrak{N}_{q_i,w_i}^{-1/2}\, |\, 2p_i + n_i, w_i\rangle$$
$$= \sum_{r_1 \cdots r_\nu} D(n_1 w_1, \cdots, n_\nu w_\nu; r_1, \cdots, r_\nu)\, |\, r_1 w_1, \cdots, r_\nu w_\nu\rangle. \tag{B6}$$

The coefficient D turns out to be

$$D(n_1 w_1, \cdots, n_\nu w_\nu; r_1, \cdots, r_\nu) = \prod_{i=1}^{\nu} \frac{u_i^{\Omega_i - \frac{1}{2}(r_i - n_i)} v_i^{\frac{1}{2}(r_i - n_i)}}{[\frac{1}{2}(r_i - n_i)]!} \times \left[\frac{[\frac{1}{2}(r_i - w_i)]![\Omega_i - \frac{1}{2}(n_i + w_i)]!}{[\frac{1}{2}(n_i - w_i)]![\Omega_i - \frac{1}{2}(r_i + w_i)]!}\right]^{1/2} \tag{B7}$$

and the summation runs over all integer values of $r_1, \cdots, r_\nu$ such that

$$(-)^{r_i} = (-)^{n_i}, \qquad n_i \le r_i \le 2\Omega_i - w_i$$

and

$$\sum_i r_i = 2(p-b) + \sum_i^{\nu} n_i.$$

It is now straightforward to obtain (3.13) and (3.14).

APPENDIX C

Explicit expressions suitable for numerical computation in the case of first BPA for even nuclei are given in this Appendix. The formulas, as they are presented here, are valid only if the j value is sufficient to identify the single-particle levels.

In the present case, we have

$$|\, \varphi_{JM}(d, K)\rangle \longrightarrow |\, \varphi_{JM}(rs)\rangle = \mathfrak{I}_{p-1}^{\dagger} A_{JM}^{\dagger}(rs)\, |\, 0\rangle. \tag{C1}$$

The indices rs are ordered ($r \le s$). The scalar product between states (C1) is given by

$$\langle \varphi_{JM}(r's')\, |\, \varphi_{JM}(rs)\rangle = (1-\delta_{J0})(1+\delta_{rs})\delta_{rr'}\delta_{ss'} \mathfrak{D}^{(p-1)}[n_i(rs), n_i(rs), n_i(rs)] + 2\delta_{J0}\delta_{rs}\delta_{r's'} \mathfrak{D}^{(p-1)}[n_i(r^2), n_i(r'^2), w=0]. \tag{C2}$$

The matrix element of the second term of the Hamiltonian (2.4) is written as

$$\langle \varphi_{JM}(r's')\, |\, \sum_a h_1(a) H_1(a)\, |\, \varphi_{JM}(rs)\rangle = A_1 + B_1, \tag{C3}$$

$$A_1 = (1+\delta_{rs})\delta_{rr'}\delta_{ss'} \sum_a \hat{a}^2 h_1(a) \mathfrak{D}^{(p-1)}[n_i(ars), n_i(ars), n_i(ars)]$$
$$- \bar{P}(rsJ)\bar{P}(r's'J)\delta_{rr'}\delta_{ss'} h_1(s) \mathfrak{D}^{(p-1)}[n_i(rs^2), n_i(rs^2), n_i(rs^2)], \tag{C4}$$

$$B_1 = 2\sum_a h_1(a)\delta_{mm'}\hat{m}^2(\hat{m}^2 - 2\delta_{lm})^{-1/2}(\hat{m}^2 - 2\delta_{l'm})^{-1/2}\{\mathfrak{D}^{(p-1)}[n_i(l^2m), n_i(l'^2m), w_m = 1]$$
$$- \delta_{ll'}\mathfrak{D}^{(p-1)}[n_i(l^2m), n_i(l^2m), n_i(l^2m)]\}\{\delta_{J0}\delta_{lrs}\delta_{l'r's'}\delta_{am}[\hat{m}^2 - 2P(ll')\delta_{ml'}] + l^{-2}\delta_{all'}\bar{P}(rsJ)\bar{P}(r's'J)\delta_{rr'l}\delta_{ss'm}\}, \tag{C5}$$

where A_1 and B_1 correspond to the first and second terms in Eq. (3.15), respectively. In B_1 only the seniority-one terms can occur, and therefore at least two of the indices $ars(ar's')$ must be equal. The set of indices $llm(l'l'm')$ is then a rearrangement of the set $ars(ar's')$. Similarly, the matrix element of the third term of the Hamiltonian (2.4) is written as

$$\langle \varphi_{JM}(r's')\, |\, \sum_{a\le b, a'\le b', I} h_2(aba'b'I) H_2(a'b'abI)\, |\, \varphi_{JM}(rs)\rangle = A_2 + B_2 + C_2, \tag{C6}$$

$$A_2 = (1+\delta_{rs})(1+\delta_{r's'})\mathfrak{D}^{(p-1)}[n_i(rsr's'), n_i(rsr's'), n_i(rsr's')] h_2(rsr's'J)$$
$$+ \delta_{rr'}\delta_{ss'}(1+\delta_{rs}) \sum_{a\le b} (1+\delta_{ab})\hat{a}\hat{b}\mathfrak{D}^{(p-1)}[n_i(abrs), n_i(abrs), n_i(abrs)] k_2(aabb0)[1 - P(rs)P(ab)\hat{r}^{-2}\delta_{ar}], \tag{C7}$$

$$B_2 = 2 \sum_{a\le b, a'\le b'} \delta_{mm'}\delta_{nn'}[(1+\delta_{mn})\hat{l}^2 - 2(\delta_{lm}+\delta_{ln})^2]^{-1/2}[(1+\delta_{mn})\hat{l}'^2 - 2(\delta_{l'm}+\delta_{l'n})^2]^{-1/2}$$
$$\times \{\mathfrak{D}^{(p-1)}[n_i(l^2mn), n_i(l'^2mn), w(mn)=2] - \delta_{ll'}\mathfrak{D}^{(p-1)}[n_i(l^2mn), n_i(l^2mn), n_i(l^2mn)]\}$$
$$\times \{(1-\delta_{J0})\delta_{abl}\delta_{a'b'l'}\delta_{rr'm}\delta_{ss'n}(1+\delta_{mn})^2\hat{l}\hat{l}' h_2(a'a'aa0)[1 - 2P(mn)P(ll')\hat{l}'^{-2}\delta_{l'm}]$$
$$+ \delta_{J0}\delta_{rsl}\delta_{r's'l'}\delta_{aa'm}\delta_{bb'n}(1+\delta_{mn})^2\hat{l}\hat{l}'[\hat{a}\hat{b}k_2(aabb0) - \delta_{mn}h_2(aaaa0)][1 - 2P(mn)P(ll')l'^{-2}\delta_{l'm}]$$
$$+ P(mn)P(ab)P(a'b')\bar{P}(rsJ)\bar{P}(r's'J)\delta_{arl}\delta_{a'r'l'}\delta_{bm}\delta_{sn}$$
$$\times [\delta_{bs'}\delta_{b's}k_2(a'bab'J) + \delta_{ll'}\delta_{bb'}\delta_{ss'}\hat{l}^{-1}\hat{b}k_2(aabb0) - 2\delta_{mn}\delta_{bb'}\delta_{ss'}\hat{m}^{-2}h_2(a'b'abJ)]\}, \tag{C8}$$

$$C_2=4\sum_{a\leq b,a'\leq b'}\delta_{mn}\delta_{m'n'}h_2(a'b'abJ)[\hat{l}^2+\delta_{lm}(l^2-4)]^{-1/2}[\hat{l}'^2+\delta_{l'm'}(\hat{l}'^2-4)]^{-1/2}$$
$$\times\{\mathfrak{D}^{(p-1)}[n_i(l^2m^2),n_i(l'^2m'^2),w=0]-(1+\delta_{lm})^{-1}(\delta_{ll'}\delta_{mm'}+\delta_{lm'}\delta_{ml'})\mathfrak{D}^{(p-1)}[n_i(l^2m^2),n_i(l^2m^2),n_i(l^2m^2)]\}$$
$$\times\{\delta_{J0}\hat{l}\hat{l}'P(lm)P(l'm')\delta_{abl}\delta_{a'b'l'}\delta_{rsm}\delta_{r's'm'}-4\delta_{J0}\hat{l}\hat{l}'P[(abrslm)(a'b'r's'l'm')]\hat{l}'^{-2}P(lm)\delta_{abl}\delta_{rsm}\delta_{a'b'r's'l'm'}$$
$$+\hat{m}^{-1}\hat{m}'^{-1}\bar{P}(abJ)\bar{P}(a'b'J)\bar{P}(rsJ)\bar{P}(r's'J)\delta_{arl}\delta_{a'r'l'}\delta_{bsm}\delta_{b's'm'}\}. \quad \text{(C9)}$$

Here A_2 corresponds to the first term in Eq. (3.15), while B_2 and C_2 correspond, respectively, to the total seniority-two and the total seniority-zero parts of the second term in Eq. (3.15). Therefore, in B_2 at least two of the indices $abrs(a'b'r's')$ must be equal. The set of indices $llmn(l'l'm'n')$ is a rearrangement of the set $abrs(a'b'r's')$, such that $m\leq n$ and, if $m=n\neq l$, both $l<m$ and $l>m$ are present. In C_2 the indices $abrs(a'b'r's')$ must be pairwise equal. The set of indices $llmm(l'l'm'm')$ is a rearrangement of the set $abrs(a'b'r's')$, such that $l\leq m$. The symbols appearing in the above expressions are defined by

$$k_2(a'bab'J)=-\sum_I \hat{I}^2h_2(aba'b'I)\begin{Bmatrix}a & b & I\\ a' & b' & J\end{Bmatrix}, \quad \text{(C10)}$$

$$\delta_{abc}\cdots=\delta_{ab}\delta_{ac}\cdots, \quad \text{(C11)}$$

$$w(mn)=2\leftrightarrow w_m=w_m=1 \quad \text{if} \quad m\neq n,$$
$$w_m=2 \quad \text{if} \quad m=n, \quad \text{(C12)}$$

$$P(ab)=1+(a\leftrightarrow b), \quad \text{(C13)}$$

$$P[(abc\cdots)(a'b'c'\cdots)]=1+(a\leftrightarrow a',b\leftrightarrow b',c\leftrightarrow c',\cdots). \quad \text{(C14)}$$

The reduced matrix element of any single-particle transition operator between one-broken-pair states is given by

$$\langle\varphi_{J'}(r's')\,||\,\Omega_\lambda\,||\,\varphi_J(rs)\rangle=Z+A_3+B_3, \quad \text{(C15)}$$

$$Z=\delta_{\lambda0}\delta_{JJ'}\hat{J}(\sum_a\hat{a}\langle a\,||\,\Omega_0\,||\,a\rangle)\{(1-\delta_{J0})(1+\delta_{rs})\delta_{rr'}\delta_{ss'}\mathfrak{D}^{(p-1)}[n_i(rs),n_i(rs),n_i(rs)]$$
$$+2\delta_{J0}\delta_{rs}\delta_{r's'}\mathfrak{D}^{(p-1)}[n_i(r^2),n_i(r'^2),w=0]\}, \quad \text{(C16)}$$

$$A_3=-\sum_a\hat{a}\hat{J}'\langle a\,||\,\Omega_\lambda\,||\,a\rangle(1+\delta_{rs})\delta_{rr'}\delta_{JJ'}\delta_{\lambda0}\mathfrak{D}^{(p-1)}[n_i(rsa),n_i(rsa),n_i(rsa)]$$
$$+\hat{J}\hat{J}'\bar{P}(rsJ)\bar{P}(r's'J')\left\{(-)^{r+s+\lambda+J'}\delta_{rr'}\langle s'\,||\,\Omega_\lambda\,||\,s\rangle\begin{Bmatrix}r & s & J\\ \lambda & J' & s'\end{Bmatrix}\mathfrak{D}^{(p-1)}[n_i(rss'),n_i(rss'),n_i(rss')]\right\}, \quad \text{(C17)}$$

$$B_3=2\hat{J}'\sum_{aa'}\delta_{mm'}\hat{a}^{-1}\langle a\,||\,\Omega_\lambda\,||\,a'\rangle\hat{l}\hat{l}'(\hat{l}^2-2\delta_{lm})^{-1/2}(\hat{l}'^2-2\delta_{l'm})^{-1/2}\{\mathfrak{D}^{(p-1)}[n_i(l^2m),n_i(l'^2m),w_m=1]$$
$$-\delta_{ll'}\mathfrak{D}^{(p-1)}[n_i(l^2m),n_i(l^2m),n_i(l^2m)]\}\Big\{-\hat{a}^2\delta_{\lambda0}\delta_{JJ'0}\delta_{lrs}\delta_{l'r's'}\delta_{aa'm}$$
$$+(-)^{a'+J'-m}\hat{a}\hat{J}'^{-1}P[(arslJ)(a'r's'l'J')]\bar{P}(rsJ)\hat{l}^{-1}\delta_{\lambda J}\delta_{J'0}\delta_{a'sm}\delta_{l's'r'}\delta_{lar}$$
$$+\hat{J}\hat{a}'^{-1}(-)^{a+J-m}\begin{Bmatrix}a & m & J\\ J' & \lambda & a'\end{Bmatrix}\bar{P}(rsJ)\bar{P}(r's'J')\delta_{lar}\delta_{l'a'r'}\delta_{ss'm}\Big\}. \quad \text{(C18)}$$

Here Z corresponds to the first term of Eq. (4.1) while A_3 and B_3 correspond, respectively, to the first and second terms in Eq. (3.15). In B_3 only the seniority-one terms occur and the set of indices $llm(l'l'm')$ is a rearrangement of the set $ars(a'r's')$.

In the first approximation for odd-mass nuclei

$$|\,\varphi_{JM}(d,K)\rangle\rightarrow\mathfrak{I}_p{}^\dagger a_\rho{}^\dagger\,|\,0\rangle. \quad \text{(C19)}$$

The corresponding expressions for the expectation values of the Hamiltonian and the nuclear reduced matrix elements can easily be evaluated in a similar way. In the application of Eq. (3.15), at most seniority one will occur in the summation.