Nuclear structure theory in spin- and number-conserving quasiparticle configuration spaces: General formalism

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In the present paper a general survey of the mathematical formalism for microscopic nuclear structure calculations in configuration spaces consisting of arbitrary spin- and number-projected Hartree-Fock-Bogoliubov—type quasiparticle determinants is given. On the basis of this formalism, various levels of approximation are then discussed. These lead to a number of microscopic nuclear structure models in between the standard Hartree-Fock-Bogoliubov theory and the complete diagonalization of a given effective many nucleon Hamiltonian. For all these models variational equations are derived and possibilities for their numerical application are estimated. The second part of the present series of two papers will then present initial results of the applications of the simplest of these models to several nuclei in various mass regions.

I. INTRODUCTION

Microscopic nuclear structure theory usually assumes that the eigenstates of the considered A-nucleon system can be reasonably well approximated within a suitably chosen finite model space spanned by a number of orthonormal single nucleon basis states. Assuming furthermore that the effective many nucleon Hamiltonian appropriate for this model space is known, then obviously the best one can do is to diagonalize this Hamiltonian in the space of all the A-nucleon Slater determinants which can be constructed by distributing the A nucleons over the M orbitals of the single-particle basis system. Such complete shell model configuration mixing (SCM) calculations have been performed for many nuclei during the last two decades and yielded extremely valuable contributions to the microscopic understanding of nuclear structure properties as well as of effective nuclear interactions.[1]

However, because of the very large dimensions of the matrices to be diagonalized the SCM approach is unfortunately restricted to rather small model spaces like the $1s\,0d$ shell or comparable basis systems. Consequently even with the best computers available up to now most of the heavier nuclei as, for example, those of the rare-earth region cannot be studied using this procedure. Equally not accessible to SCM calculations are furthermore, with only a few exceptions, all those problems for which *a priori* the use of several major shells as single-particle basis is required as, for example, the description of negative parity states in doubly even open shell nuclei or the investigation of the structure of the highly excited giant multipole resonances (GMR's). Hence here as well as for many other problems suitable approximations to the numerically inaccessible SCM solutions have to be found.

Faced with the problem of how to truncate the complete set of Slater determinants to a numerically manageable number of configurations, it is obviously desirable to transform the single nucleon basis states in such a way that the residual interaction between the resulting A-nucleon configurations becomes small, i.e., to find such a representation of the model space in which as few configurations as possible account for as many of the correlations as possible in the nuclear states under consideration.

The probably best known approach along these lines is the Hartree-Fock (HF) theory,[2] which provides us with a prescription of how to extract directly from the chosen many nucleon Hamiltonian the optimal average potential each of the nucleons feels due to its interactions with all the others. The ground-state wave function of the considered nucleus in the HF approximation is then given by a single Slater determinant in which the A energetically lowest orbits of this optimal "self-consistent" potential are occupied. A refined description of the nucleus may then be obtained by expanding the ground-state correlations as well as the excited states of the considered system in terms of n-particle—n-hole (np-nh; $n=1,2,\ldots,A$) excitations from the filled into the empty orbits of this reference determinant and by diagonalizing the residual interaction in the resulting configuration space. Defined with respect to the optimal single-particle potential this expansion should converge much faster than the SCM expansion and hence its truncation can be more easily justified than that of the original SCM configuration space.

In doubly closed shell nuclei the HF potential is spherical. Therefore, here the 1p1h excitations as well as the 2p2h ones can be easily coupled to the desired spin quantum numbers. Hence, for example, for the description of the GMR's in spherical nuclei the usual techniques like the Tamm-Dancoff (TDA) or random-phase (RPA) approximations can be easily applied and even refinements like the "spreading" of the GMR's due to the coupling of their 1p1h gross structure to the 2p2h excitations can be taken into account. Indeed such calculations have been performed with great success during the last decade[3]

yielding very essential contributions to our knowledge about the structure of the GMR's in spherical nuclei.

In open shell nuclei, however, the price to be paid for the attempt to account for as many correlations as possible by a single Slater determinant is higher: Here the HF transformation usually breaks the required rotational symmetry. Consequently the resulting configurations cannot be viewed as physical states but only as some "intrinsic" structures from which the physical solutions of the considered problem have still to be obtained by angular momentum projection techniques.[4] Furthermore, since the symmetry breaking configurations are at least partly linearly dependent with respect to rotations it is essential to perform the projection on the desired angular momentum quantum numbers before the diagonalization of the residual interaction. Only in this way can problems with rotational spurious admixtures be avoided and possible spin dependencies of the configuration mixing be taken into account.[5,6]

Using the above description and truncating the intrinsic configuration space after the 1p1h excitations one obtains the angular-momentum-projected deformed particle hole model based on the HF approach (PHM),[6] in which the nuclear wave functions are approximated by linear combinations of the angular-momentum-projected deformed HF reference determinant and the equally spin projected deformed 1p1h configurations with respect to it. Considering doubly even $N=Z$ nuclei in an *sd*-shell model space the PHM approach is an excellent approximation to the exact SCM solutions. However, contrary to the SCM prescription, the PHM method, which contains the usual Tamm-Dancoff approximation as limiting case for doubly closed shell nuclei, can be applied in rather large model spaces and hence could be used with some success for the description of the GMR's as well as of low excited positive and negative parity states of some doubly even $N=Z$ nuclei in the 1s0d-shell mass region.

However, since it is based on an HF reference, the PHM approach is obviously restricted to such nuclei for which the HF description itself can already be considered as a reasonably good approximation. This limits its applicability essentially to light self-conjugate nuclei. As soon as neutron excess nuclei are considered pairing correlations start to play an important role and consequently the PHM method not accounting for such correlations has to fail. Hence, unfortunately, not even light neutron excess nuclei can be described within the PHM limit and for the heavier systems, for example, those of the rare-earth region where pairing becomes one of the essential degrees of freedom, the PHM approximations become even less justified.

In order also to cover these nuclei one has essentially two possibilities: Either one increases the PHM configuration space by including the 2p2h and maybe even higher-order excitations or one skips the HF approximation itself and tries to account for the possible pairing correlations right from the beginning. The first procedure leads to drastically increased dimensions of the matrices involved and therefore, at least in large model spaces, to essentially the same numerical difficulties as the SCM method discussed at the beginning of this section. Therefore, the second possibility, namely to include the pairing correlations directly in the reference potential via the well-known Hartree-Fock-Bogoliubov (HFB) transformation,[7] seems to be much more promising. In contrast to the HF approximation, in which a system of independent particles serves as reference state, the HFB approach yields as reference configuration due to the inclusion of pairing a system of independent "quasiparticles" each of which has, with some probability, particle as well as hole character. Consequently, this reference configuration does not have a sharp Fermi surface and an expansion of the additional correlations in terms of particle-hole states looses its meaning. Instead—considering doubly even nuclei—the 1p1h configurations now have to be replaced by two quasiparticle (2qp) excitations, the 2p2h ones by 4qp states, and so on.

The HF—as well as the HFB—approach in general breaks the required rotational symmetry. Furthermore the HFB transformation violates the particle-number conservation. Hence, here, in addition to the angular momentum projection, projections on the desired proton and neutron numbers are also required, which for similar reasons as discussed above for the spin projection, have to be performed before the diagonalization of the residual interaction.

In the present paper we shall present a quite general survey of different possibilities for approximating the numerically inaccessible solutions of complete SCM calculations in large model spaces using the ideas outlined above. In Sec. II we shall first develop a particular formulation of the HFB theory and the necessary projection techniques, which will turn out to be very suitable to develop models anywhere in between the usual HFB approximation and the exact diagonalization of an effective Hamiltonian in a finite single-particle basis. Using this formalism we shall then discuss in Sec. III various levels of approximation where we can either put the emphasis on how to obtain the optimal mean field (which in general depends on both the chosen configuration space as well as the considered angular momentum) or on the construction and truncation of a suitable set of A-nucleon configurations serving as a basis for a subsequent diagonalization of the residual interaction. Conclusions will then be presented in Sec. IV and some detailed expressions of certain matrix elements will be given in two appendixes.

In paper II of the present series of papers we shall then specialize the ideas developed here with the aim to construct a numerically feasible model. This model—the model for handling large numbers or number- and spin-projected two-quasiparticle excitations with realistic interactions and model spaces (MONSTER) approach—will then be applied to several nuclei in various mass regions and its results be compared with those obtained with other methods and with the experimental data.

II. BASIC FORMALISM FOR CALCULATIONS WITH ARBITRARY HFB-TYPE CONFIGURATIONS

We shall define our model space by a finite, M-dimensional set of orthonormal single nucleon states $\{|i\rangle, |k\rangle, \ldots\}_M$. The corresponding creation and annihilation operators obey the usual Fermion commutation

rules and will be denoted by $\{C_i^\dagger, C_k^\dagger, \ldots\}_M$ and $\{C_i, C_k, \ldots\}_M$, respectively. We shall furthermore assume that the effective many nucleon Hamiltonian appropriate for this model space is known and can be written in the chosen representation as a sum of only one- and two-body terms

$$\hat{H} \equiv \sum_{ir} t(ir) C_i^\dagger C_r + \tfrac{1}{4} \sum_{ikrs} v(ikrs) C_i^\dagger C_k^\dagger C_s C_r \ , \tag{1}$$

where $t(ir) \equiv \langle i \mid \hat{t} \mid r \rangle$ and $v(ikrs) \equiv \langle ik \mid \hat{V} \mid rs - sr \rangle$ are shorthand notations for the one-body matrix elements and the antisymmetrized two-body matrix elements of the effective interaction, respectively.

The exact solutions of the A-nucleon problem in the chosen finite model space can then be obtained by diagonalizing the given Hamiltonian in the space of all the A-nucleon Slater determinants which can be constructed out of the M single nucleon basis states.

Obviously these solutions are invariant with respect to a unitary transformation of the single-particle basis

$$d_\alpha^\dagger \equiv \sum_i D_{i\alpha}^* C_i^\dagger \tag{2}$$

or, in matrix notation

$$d^\dagger = D^\dagger C^\dagger \ , \tag{3}$$

where the unitarity

$$D^\dagger D = D D^\dagger = U_M \tag{4}$$

with U_M being the $(M \times M)$ unit matrix, guarantees the Fermion properties of the new particle creation and annihilation operators $d_\alpha^\dagger$ and d_β. In other words, when diagonalizing H in the complete space of A-nucleon Slater determinants it does not matter whether these are constructed using as building blocks the eigenstates of the originally chosen basis creating potential or the orbits $d_\alpha^\dagger$ of some other average potential in the model space.

If, on the other hand, only a subspace of the total configuration space is taken into account—and this is usually the case since at least on present day computers complete "shell model configuration mixing" (SCM) calculations[1] are unfortunately restricted to rather small model space—then the choice of the average potential becomes essential. In fact, for each particular incomplete set of m A-nucleon Slater determinants there exists an optimal average potential, which can be obtained minimizing the total energy by treating not only the mixing coefficients of these Slater determinants but also their building blocks, i.e., the elements of the transformation matrix D, as variational parameters. The resulting wave functions are then the optimal approximation to the exact solutions, which can be reached in the truncated space of only m A-nucleon Slater determinants provided that these are all defined with respect to one and the same average potential. For $m=1$ this "multiconfiguration-Hartree-Fock" (MCHF) procedure[8] obviously reduces to the well-known Hartree-Fock (HF) method,[2] which approximates the nuclear ground state by a single Slater determinant, in which the A energetically lowest orbits of the optimal average potential each of the nucleons feels due to its interaction with all the others are occupied and the remaining $(M-A)$ ones are empty.

The number of correlations accounted for by a given number of configurations can even be further increased, if instead of the HF-type single-particle states (2) the quasiparticle states of the well-known Hartree-Fock-Bogoliubov (HFB) theory[7,9,10] are used as building blocks for the many nucleon configurations, because then the important pair correlations between the nucleons induced by the short-range attraction of the effective interaction can be included in the average field itself and hence do not have to be taken into account explicitly via configuration mixing. Such a theory, which tries to optimize its truncated configuration space using HFB-type quasiparticle determinants as basis states will be described in detail in the following sections.

A. HFB-configuration space

Elementary building blocks of the theory presented here are the HFB quasiparticles

$$a_\alpha^\dagger \equiv \sum_i [A_{i\alpha}(q) C_i^\dagger + B_{i\alpha}(q) C_i] \tag{5}$$

or, in matrix notation

$$\begin{bmatrix} a^\dagger(q) \\ a(q) \end{bmatrix} = F(q) \begin{bmatrix} C^\dagger \\ C \end{bmatrix} = \begin{bmatrix} A^T(q) B^T(q) \\ B^\dagger(q) A^\dagger(q) \end{bmatrix} \begin{bmatrix} C^\dagger \\ C \end{bmatrix} , \tag{6}$$

where the unitarity of the transformation $F(q)$

$$F(q) F^\dagger(q) = F^\dagger(q) F(q) = U_{2M} \tag{7}$$

with U_{2M} being the $(2M \times 2M)$ unit matrix, is required to ensure that the quasiparticle operators (6) fulfil the Fermion commutation rules. The parameter q has been introduced in order to distinguish between different transformations of the type (6) and can hence be interpreted as a sort of "quasiparticle representation label."

Each of the quasiparticle operators (6) is a linear combination of both particle creation and annihilation operators and therefore has with some probability "particle" as well as "hole" character. So the "smearing" of the sharp HF-Fermion surface due to the virtual scattering of correlated nucleon pairs into the unoccupied orbits is taken into account.

Using (7) one obtains from (6) immediately the inverse transformation

$$\begin{bmatrix} C^\dagger \\ C \end{bmatrix} = F^\dagger(q) \begin{bmatrix} a^\dagger(q) \\ a(q) \end{bmatrix} = \begin{bmatrix} A^*(q) B(q) \\ B^*(q) A(q) \end{bmatrix} \begin{bmatrix} a^\dagger(q) \\ a(q) \end{bmatrix} \tag{8}$$

which expresses the creators and annihilators of the single nucleon basis states in terms of the quasiparticle operators (6) and can hence be used to transform any arbitrary operator whose basis representation is known into the quasiparticle representation q. As an example the quasiparticle representations of the total Hamiltonian (1) and the nucleon number operators are given in Appendix A.

The condition (7) ensures that $a_\alpha^2(q) = 0$ for all $\alpha = 1, \ldots, M$. Therefore the configuration

$$| \{q\}_0 \rangle \equiv \prod_{\alpha=1}^{M} a_\alpha(q) \mid 0 \rangle \ , \tag{9}$$

where $|0\rangle$ denotes the particle vacuum, is obviously the vacuum state of the quasiparticle operators (6) and hence the equivalent of the HF ground-state Slater determinant, which has been mentioned above.

It is obvious from the transformation (6) that the state (9) does not conserve the total number of nucleons. Instead, if M is even as is usually the case, the configuration (9) is a linear superposition of different components corresponding to all the even nucleon numbers A $(0 \leq A \leq M)$ which are possible in the chosen model space. This is the price for taking into account the pair correlations implicitly via the transformation (6) rather than explicitly via configuration mixing.

On the other hand, the "one-quasiparticle" (1qp) states

$$|\{q\}_1\rangle \equiv a^\dagger_{q_1}(q)\,|\{q\}_0\rangle, \quad q_1 = 1, \ldots, M \tag{10}$$

contain only the odd A components $(1 \leq A \leq M-1)$. These states are also known as "blocked" HFB states since in them the quasiparticle orbit q_1 is not participating in the virtual pair scattering.

Generally, each arbitrary "n-quasiparticle" ($n$qp) state

$$|\{q\}_n\rangle \equiv \begin{cases} |\{q\}_0\rangle \quad \text{for } n=0 \\ \prod_{i=1}^{n} a^\dagger_{q_i}(q)\,|\{q\}_0\rangle, \quad q_1 > q_2 > \cdots > q_n = 1, \ldots, M; \text{ for } n = 1, \ldots, M \end{cases} \tag{11}$$

consists for even n only out of even A, for odd n only out of odd A components. Following Mang[10] we shall refer to this property of the HFB states (11) as "number parity."

It is interesting to note that each of the states (11) can be considered as a vacuum of a particular set of quasiparticle operators defined by a transformation matrix $F(q')$ which is obtained from the original transformation $F(q)$ by interchanging the n rows corresponding to the operators $a^\dagger_{q_i}(q)(i=1,\ldots,n)$ with those corresponding to the operators a_{q_i} $(i=1,\ldots,M)$.

Because of the unitarity (7) of $F(q)$ the states (11) for $n=0,\ldots,M$ form a complete set of orthogonal configurations for all the possible model space nuclei with $0 \leq A \leq M$. Its dimension

$$\dim(|\{q\}\rangle) \equiv \sum_{n=0}^{M} \dim(|\{q\}_n\rangle) = \sum_{n=0}^{M} \binom{M}{N} = 2^M \tag{12}$$

equals the sum of the total SCM dimensions for all these nuclei. Therefore, the diagonalization of the Hamiltonian (1) in the complete space (11) yielding the exact solutions for all the model space nuclei simultaneously is obviously numerically even more involved than a complete SCM calculation for a given particle number A. However, each of the configurations (11) is already a rather complicated linear combination of very many Slater determinants and hence contains many more correlations than any of the latter. Consequently, with a suitable choice of $F(q)$ in any incomplete subset of m configurations out of the complete space (11) one can obviously reach a better approximation of the exact solutions than would be possible by using the same number of Slater determinants as basis states.

Again for any incomplete set of m quasiparticle determinants of the type (11) there exists an optimal basis transformation $F(q)$ of the form (6) corresponding to an optimal average field which, at least in principle, can be obtained by treating the mixing coefficients of these determinants and the matrix elements of $F(q)$ simultaneously as parameters in a variational principle for the total energy. For $m=1$ this procedure now reduces to the standard HFB theory.[7,9,10]

Unfortunately, as already mentioned in the Introduction, in general the configurations (11) are eigenstates neither to the square of the total angular momentum operator nor to its projection along the z axis of the chosen frame of reference. Consequently the determinants (11) cannot be considered as physical states but only as some "intrinsic" structures from which the physical states in the laboratory system have still to be obtained by restoring the broken rotational symmetry. The easiest way to achieve this would be to diagonalize the Hamiltonian first in the chosen truncated subspace of (11) and then projecting the required spin quantum numbers out of the resulting wave function. However, this procedure would lead to severe difficulties. First, obviously spin dependencies of the configuration mixing are not accounted for and second, and even more serious, the results would depend on the orientation of the chosen intrinsic frame of reference since truncated subspaces of (11) are in general not invariant under rotations. Hence diagonalizing $\hat{H}$ in the intrinsic system we would give the system the possibility to gain energy by simply changing its orientation. In order to avoid these spurious effects and to take into account possible spin dependencies of the configuration mixing it is therefore essential to restore the broken rotational symmetry before the diagonalization of the residual interaction.[5,6]

It has furthermore already been mentioned above that the configurations (11) do mix rather different nucleon numbers. Also here a diagonalization in a truncated subspace of (11) would yield spurious effects due to the mixing with components corresponding to other nuclei than the considered one. Consequently, the desired nucleon numbers also have to be restored before the diagonalization of the residual interaction.

Last but not least, in general also $F(q)$ will depend on spin and nucleon number. Hence in principle also the variation of the transformation $F(q)$ should be performed after restoring the broken symmetries. We shall come back to this problem in Sec. III of the present paper.

For the moment we shall assume that $F(q)$ is given and a particular subset of (11) has been chosen. The tech-

niques to restore the broken symmetries in such a set of HFB configurations are well known.[4,11,12] However, since they are very essential for our theory we shall describe them in detail in the following two sections.

B. Particle number and angular momentum projection

Let $\{|NZIK\chi\rangle\}$ be a complete basis of orthonormal shell model configurations for the chosen model space. Here N denotes the neutron, Z denotes the proton number, I is the total angular momentum, K is its projection on the z axis of the chosen intrinsic frame of reference, and χ represents all the necessary additional quantum numbers. The total number of those configurations is 2^M (12). Each of the configurations $|\{q\}\rangle$ out of the last section can then be expanded as

$$|\{q\}\rangle = \sum_{NZIK\chi} |NZIK\chi\rangle\langle NZIK\chi|\{q\}\rangle \equiv \sum_{NZIK\chi} |NZIK\chi\rangle y^{(NZI)}_{\chi;\{q\}K} . \tag{13}$$

Obviously the operators

$$\hat{Q}(N_0) \equiv \sum_{ZIK\chi} |N_0ZIK\chi\rangle\langle N_0ZIK\chi| \tag{14}$$

and

$$\hat{Q}(Z_0) \equiv \sum_{NIK\chi} |NZ_0IK\chi\rangle\langle NZ_0IK\chi| \tag{15}$$

project from the expansion (13) onto the components with fixed neutron number N_0 and proton number Z_0, respectively. Both operators are Hermitian and idempotent and hence true mathematical projectors.

Conceptionally more difficult is the projection onto good angular momentum states. Here one usually introduces the operator

$$\hat{P}(IM;K) \equiv \sum_{NZ\chi} |NZIM\chi\rangle\langle NZIK\chi| \tag{16}$$

which produces a state with spin I and projection M in the laboratory frame of reference from the (I,K) component of (13) in the intrinsic system. Obviously this operator is a mathematical projector only for $M=K$. However, as we shall see below, the use of the nondiagonal form (16) is essential, since only then the resulting total wave functions will become independent of the particular orientation of the intrinsic reference frame.

The three operators defined above do commute with each other and can hence be applied in arbitrary order. Application of

$$\hat{P}(N_0Z_0IM;K) \equiv \hat{P}(IM;K)\hat{Q}(Z_0)\hat{Q}(N_0) = \sum_{\chi} |N_0Z_0IM\chi\rangle\langle N_0Z_0IK\chi| \tag{17}$$

on the expansion (13) yields a set of configurations

$$|\{q\}N_0Z_0IM;K\rangle \equiv \hat{P}(N_0Z_0IM;K)|\{q\}\rangle = \sum_{\chi} |N_0Z_0IM\chi\rangle y^{(N_0Z_0I)}_{\chi;\{q\}K} \tag{18}$$

which already have the required number and spin quantum numbers, but which still depend on the orientation of the intrinsic system via their K dependence. Furthermore they are obviously neither normalized nor orthogonal.

Let us now assume that we have a number of intrinsic configurations $|\{q\}\rangle$ of the type (11), which do not necessarily have to belong to only one quasiparticle representation q. The most general wave function constructable in the defined truncated subspace of the total shell model configuration space has then the form

$$|i;N_0Z_0IM\rangle = \sum_{\{q\}K} |\{q\}N_0Z_0IM;K\rangle f^{(N_0Z_0I)}_{\{q\}K;i} = \sum_{\chi} |N_0Z_0IM\chi\rangle (yf)_{\chi i} \tag{19}$$

where the first sum runs over all the HFB configurations $|\{q\}\rangle$ to be included as well as over all the $2I+1$ K values and the f's are variational parameters being restricted only by the constraint

$$f^{\dagger}Nf \equiv (yf)^{\dagger}(yf) = U \tag{20}$$

which guarantees the orthonormality of the states (19). Here U is the unit matrix and the overlap matrix N is defined by

$$N^{(N_0Z_0I)}_{\{q\}K;\{q'\}K'} \equiv \langle\{q\}N_0Z_0IM;K|\{q'\}N_0Z_0IM;K'\rangle = (y^{\dagger}y)_{\{q\}K;\{q'\}K'} . \tag{21}$$

N is Hermitian by construction and furthermore, since for any arbitrary column vector z with the proper dimension

$$z^{\dagger}Nz = z^{\dagger}(y^{\dagger}y)z = (yz)^{\dagger}(yz) \geq 0 \tag{22}$$

also positive definite.

The configuration mixing coefficients f can then be obtained by requiring a minimum of the expectation value of the Hamiltonian (1) in the state (19) with respect to variations of the parameters f constrained by the orthonormality condition (20). One gets

$$(H-EN)f = 0 \tag{23}$$

with N out of Eq. (21) and H being defined as

$$H^{(N_0Z_0I)}_{\{q\}K;\{q'\}K'} \equiv \langle\{q\}N_0Z_0IM;K|\hat{H}|\{q'\}N_0Z_0IM;K'\rangle = (y^{\dagger}h^s y)_{\{q\}K;\{q'\}K'} , \tag{24}$$

where

$$h^s_{\chi\chi'}(N_0Z_0I) \equiv \langle N_0Z_0IM\chi|\hat{H}|N_0Z_0IM\chi'\rangle \tag{25}$$

is the representation of $\hat{H}$ in the shell model basis.

The solution of (23) under the constraint (20) is equivalent to the diagonalization of $\hat{H}$ in the subspace of all the shell model configurations for given N_0, Z_0, and I, which are contained in the chosen truncated intrinsic configuration space. This can be seen by rewriting (23) with the help of Eqs. (21) and (24). One obtains

$$y^{\dagger}(h^s-EU)(yf) = 0 \tag{26}$$

which has to be compared to the equation

$$(h^s - EU)g = 0 \tag{27}$$

giving the exact model space solutions for given N_0, Z_0, and I.

Furthermore, it can easily be shown that the wave functions (19) indeed do not depend on the intrinsic orientation. For this purpose we apply the usual rotation operator[13]

$$\begin{aligned}\hat{R}(\Omega) &\equiv \hat{R}(\alpha,\beta,\gamma) \\ &\equiv \exp(-i\alpha\hat{I}_z)\exp(-i\beta\hat{I}_y)\exp(-i\gamma\hat{I}_z)\end{aligned} \tag{28}$$

where $\Omega \equiv (\alpha,\beta,\gamma)$ are the three Euler angles, on the intrinsic configurations (13). This yields a new set of rotated configurations

$$\begin{aligned}|\{\tilde{q}\}\rangle &\equiv \hat{R}(\Omega)|\{q\}\rangle \\ &= \sum_{NZIK\chi} |NZIK\chi\rangle \left[\sum_{K'} y^{(NZI)}_{\chi;\{q\}K'} D^I_{KK'}(\Omega)\right] \\ &\equiv \sum_{NZIK\chi} |NZIK\chi\rangle \tilde{y}^{(NZI)}_{\chi;\{q\}K}\end{aligned} \tag{29}$$

where the D function

$$D^I_{KK'}(\Omega) \equiv \langle IK|\hat{R}(\Omega)|IK'\rangle \tag{30}$$

is the familiar representation of the rotation operator in good angular momentum states.[13] Diagonalizing $\hat{H}$ in the resulting set of projected configurations (18), now with $\tilde{f}$'s as variational parameters, it becomes obvious that (29) induces only a unitary transformation on the original f's. By writing

$$\tilde{f}^{(N_0Z_0I)}_{\{q\}K;i} = \sum_{K'} D^*_{KK'}(\Omega) f^{(N_0Z_0I)}_{\{q\}K';i} \tag{31}$$

it follows immediately that

$$\tilde{y}\tilde{f} = yf \tag{32}$$

and hence the resulting wave functions (19) remain unchanged.

Note that the use of the nondiagonal form (16) of the angular momentum projector requires the diagonalization of $\hat{H}$ according to Eqs. (23) and (20) even if only a single HFB state is included in the intrinsic configuration space. The projection procedure discussed in the present section therefore leads us already some steps beyond the mean-field concept underlying the standard HFB theory.

Unfortunately, in most cases the decompositions (13) of the intrinsic configurations in terms of shell model states are very hard to obtain. Therefore, in general the forms (14)—(16) of the projectors cannot be used in practical calculations but other representations have to be chosen. Using the identity operator

$$\hat{U} \equiv \sum_{NZIK\chi} |NZIK\chi\rangle\langle NZIK\chi| \tag{33}$$

and the definition

$$\hat{S}_n(\phi_n) \equiv \exp(-i\phi_n\hat{N}) \tag{34}$$

where $\hat{N}$ is the neutron number operator, we may for example write

$$\begin{aligned}\hat{S}_n(\phi_n) &= \hat{U}\hat{S}_n(\phi_n)\hat{U} \\ &= \sum_{NZIK\chi} |NZIK\chi\rangle\exp(-i\phi_n N)\langle NZIK\chi| \ .\end{aligned} \tag{35}$$

Multiplying this identity from the left with $(1/2\pi)\exp(i\phi_n N_0)$ and integrating over ϕ_n from 0 to 2π yields then immediately

$$\begin{aligned}\hat{Q}(N_0) &\equiv \sum_{2IK\chi} |N_0ZIK\chi\rangle\langle N_0ZIK\chi| \\ &= (1/2\pi)\int_0^{2\pi} d\phi_n \exp(i\phi_n N_0)\hat{S}_n(\phi_n)\end{aligned} \tag{36}$$

which is the more familiar integral representation[11] of the neutron number projector (14). In the same way one obtains

$$\begin{aligned}\hat{Q}(Z_0) &\equiv \sum_{NIK\chi} |NZ_0IK\chi\rangle\langle NZ_0IK\chi| \\ &= (1/2\pi)\int_0^{2\pi} d\phi_p \exp(i\phi_p Z_0)\hat{S}_p(\phi_p) \ ,\end{aligned} \tag{37}$$

where

$$\hat{S}_p(\phi_p) \equiv \exp(-i\phi_p\hat{Z}) \tag{38}$$

with $\hat{Z}$ being the proton number operator.

To derive an integral expression for the operator (16) we can use exactly the same method. Here we write the rotation operator (28) as

$$\begin{aligned}\hat{R}(\Omega) &= \hat{U}\hat{R}(\Omega)\hat{U} \\ &= \sum_{NZIK\chi K'} |NZIK\chi\rangle D^I_{KK'}(\Omega)\langle NZIK'\chi|\end{aligned} \tag{39}$$

and multiply from the left with $(2I+1)/8\pi^2 D^{I*}_{MK}(\Omega)$. Integration over Ω ($d\Omega = d\alpha\, d\gamma \sin\beta\, d\beta$, α and γ from 0 to 2π, β from 0 to π) gives then the result

$$\begin{aligned}\hat{P}(IM;K) &\equiv \sum_{NZ\chi} |NZIM\chi\rangle\langle NZIK\chi| \\ &= \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I*}_{MK}(\Omega)\hat{R}(\Omega)\end{aligned} \tag{40}$$

which is the well-known integral form[4] of the spin projector (16).

Introducing the shorthand notations

$$\hat{\tilde{R}}(\tilde{\Omega}) \equiv \hat{\tilde{R}}(\Omega,\phi_p,\phi_n) = \hat{R}(\Omega)\hat{S}_n(\phi_n)\hat{S}_p(\phi_p) \ , \tag{41}$$

$$d\tilde{\Omega} \equiv d\Omega\, d\phi_p d\phi_n \ , \tag{42}$$

and

$$\omega^{N_0Z_0I*}_{MK}(\tilde{\Omega}) \equiv \frac{2I+1}{8\pi^2}\frac{1}{(2\pi)^2} D^{I*}_{MK}(\Omega) e^{i\phi_p Z_0} e^{i\phi_n N_0} \ , \tag{43}$$

we may then write the combined projector (17) as

$$\hat{P}(N_0Z_0IM;K)\equiv\sum_{\chi}|N_0Z_0IM\chi\rangle\langle N_0Z_0IK\chi| = \int d\tilde{\Omega}\,\omega_{MK}^{N_0Z_0I^*}(\tilde{\Omega})\hat{\tilde{R}}(\tilde{\Omega})\,. \tag{44}$$

Using this operator now the reduced matrix elements of any arbitrary tensor operator $\hat{T}^L_\mu(\Delta N_0,\Delta Z_0)$, which may even change the neutron and proton number by ΔN_0 and ΔZ_0, respectively, in between arbitrary configurations of the type (11), which may not even belong to the same quasiparticle representation, can be calculated without knowing the decompositions (13) explicitly. With the help of the well-known transformation properties of tensor operators under rotations[13] one obtains straightforwardly

$$\langle\{q\}N_0+\Delta N_0,Z_0+\Delta Z_0,I_f;K_f||\hat{T}^L(\Delta N_0,\Delta Z_0)||\{q'\}N_0Z_0I_i;K_i\rangle = (2I_f+1)^{1/2}\sum_{\mu=-L}^{+L}(I_iLI_f\,|\,K_f-\mu\mu K_f)\int d\tilde{\Omega}\,\omega_{K_f-\mu K_i}^{N_0Z_0I_i^*}(\tilde{\Omega})\langle\{q\}\,|\,\hat{T}^L_\mu(\Delta N_0,\Delta Z_0)\hat{\tilde{R}}(\tilde{\Omega})\,|\,\{q'\}\rangle\,, \tag{45}$$

where the reduced matrix element is defined using Edmond's convention.[13]

Obviously the evaluation of the rotated matrix element under the integral is in general rather complicated but nevertheless straightforward. The special techniques which are necessary to perform this evaluation are the subject of the following section.

C. Evaluation of general rotated matrix elements

Let $|\{q\}\rangle$ be an arbitrary $n$qp state out of the set (11) and $|\{q'\}\rangle$ an arbitrary $m$qp state out of a similar set generally being based on a different quasiparticle representation q'. In order to evaluate the general rotated matrix element under the integral in Eq. (45) we shall then first introduce a set of rotated quasiparticle operators

$$\begin{bmatrix}b^\dagger(q',\tilde{\Omega})\\ b(q',\tilde{\Omega})\end{bmatrix}\equiv\hat{\tilde{R}}(\tilde{\Omega})\begin{bmatrix}a^\dagger(q')\\ a(q')\end{bmatrix}\hat{\tilde{R}}^\dagger(\tilde{\Omega}) \tag{46}$$

in terms of which the rotated vacuum configuration of the representation q' can be written as

$$|\{q'(\tilde{\Omega})\}_0\rangle\equiv\hat{\tilde{R}}(\tilde{\Omega})\,|\,\{q'\}_0\rangle=\prod_{\alpha=1}^{M}b_\alpha(q',\tilde{\Omega})\,|\,0\rangle\,. \tag{47}$$

Using the basis representation of the generalized rotation operator (41)

$$\tilde{R}_{ik}(\tilde{\Omega})\equiv\langle i\,|\,\hat{\tilde{R}}(\tilde{\Omega})\,|\,k\rangle\equiv\langle 0\,|\,C_i\hat{\tilde{R}}(\tilde{\Omega})C_k^\dagger\,|\,0\rangle \tag{48}$$

and the well-known transformation properties of the basis creators and annihilators $C^\dagger$ and C under this operator one obtains from (46) immediately

$$\begin{bmatrix}b^\dagger(q',\tilde{\Omega})\\ b(q',\tilde{\Omega})\end{bmatrix}=\tilde{F}(q',\tilde{\Omega})\begin{bmatrix}C^\dagger\\ C\end{bmatrix} = \begin{bmatrix}A^T(q')\tilde{R}^T(\tilde{\Omega}),B^T(q')\tilde{R}^\dagger(\tilde{\Omega})\\ B^\dagger(q')\tilde{R}^T(\tilde{\Omega}),A^\dagger(q')\tilde{R}^\dagger(\tilde{\Omega})\end{bmatrix}\begin{bmatrix}C^\dagger\\ C\end{bmatrix}. \tag{49}$$

Because of the unitarity of $\tilde{R}(\tilde{\Omega})$ and of $F(q')$ also, $\tilde{F}(q',\tilde{\Omega})$ is a unitary transformation. With the help of the inverse transformation $F^\dagger(q)$ out of Eq. (8) we are then able to express the rotated quasiparticle operators (46) through the unrotated ones belonging to the representation q. We get straightforwardly

$$\begin{bmatrix}b^\dagger(q',\tilde{\Omega})\\ b(q',\tilde{\Omega})\end{bmatrix}=\tilde{F}(q',\tilde{\Omega})F^\dagger(q)\begin{bmatrix}a^\dagger(q)\\ a(q)\end{bmatrix} =\tilde{F}(q',q,\tilde{\Omega})\begin{bmatrix}a^\dagger(q)\\ a(q)\end{bmatrix}, \tag{50}$$

where

$$\tilde{F}(q',q,\tilde{\Omega})\equiv\tilde{F}(q',\tilde{\Omega})F^\dagger(q) = \begin{bmatrix}\tilde{A}^T(q',q,\tilde{\Omega}) & \tilde{B}^T(q',q,\tilde{\Omega})\\ \tilde{B}^\dagger(q',q,\tilde{\Omega}) & \tilde{A}^\dagger(q',q,\tilde{\Omega})\end{bmatrix} \tag{51}$$

is again a unitary transformation with its components being defined as

$$\tilde{A}(q',q,\tilde{\Omega})\equiv A^\dagger(q)\tilde{R}(\tilde{\Omega})A(q')+B^\dagger(q)\tilde{R}^*(\tilde{\Omega})B(q') \tag{52}$$

and

$$\tilde{B}(q',q,\tilde{\Omega})\equiv B^T(q)\tilde{R}(\tilde{\Omega})A(q')+A^T(q)\tilde{R}^*(\tilde{\Omega})B(q')\,. \tag{53}$$

By using Thouless's theorem[14] the rotated vacuum (47) can now be expressed through the unrotated quasiparticle operators of the representation q as

$$|\{q'(\tilde{\Omega})\}_0\rangle=n_0(q',q,\tilde{\Omega})\exp\{\hat{Q}^\dagger(q',q,\tilde{\Omega})\}\,|\,\{q\}_0\rangle\,, \tag{54}$$

where

$$\hat{Q}^\dagger(q',q,\tilde{\Omega})\equiv\tfrac{1}{2}\sum_{\alpha\beta}g_{\alpha\beta}(q',q,\tilde{\Omega})a_\alpha^\dagger(q)a_\beta^\dagger(q) \tag{55}$$

with

$$g(q',q,\tilde{\Omega})\equiv\tilde{B}^*(q',q,\tilde{\Omega})X^T(q',q,\tilde{\Omega})=-g^T(q',q,\tilde{\Omega}) \tag{56}$$

being an antisymmetric matrix and $X(q',q,\tilde{\Omega})$ defined as

$$X(q',q,\tilde{\Omega})\equiv[\tilde{A}^\dagger(q',q,\tilde{\Omega})]^{-1}\,. \tag{57}$$

The rotated overlap $n_0(q',q,\tilde{\Omega})$ can be calculated following Onishi and Yoshida.[12] One obtains

$$n_0(q',q,\tilde{\Omega}) \equiv \langle \{q\}_0 | \{q'(\tilde{\Omega})\}_0 \rangle = [\det \tilde{A}^{\dagger}(q',q,\tilde{\Omega})]^{1/2} \times \exp\{-(i/2)(\phi_n M_n + \phi_p M_p)\} , \quad (58)$$

where use has been made of the assumption that the single nucleon basis $\{|i\rangle, |k\rangle, \ldots\}_M$ has the isospin projection as a good quantum number and consists of M_n neutron and M_p proton states ($M_n + M_p = M$).

With the commutators

$$[a_\alpha^\dagger(q), \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\}] = 0 \quad (59)$$

and

$$[a_\alpha(q), \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\}] = \sum_\beta g_{\alpha\beta}(q',q,\tilde{\Omega}) a_\beta^\dagger(q) \quad (60)$$

which can be easily derived, and Eq. (50) one can easily check that (54) is indeed the vacuum for the operators $b_\alpha(q',\tilde{\Omega})$, and such, because of the uniqueness of the vacuum, prove Thouless's theorem. Furthermore, it follows immediately that

$$b_{q_1'}^\dagger(q',\tilde{\Omega}) \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\} = \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\} \sum_\alpha [\{\tilde{A}(q',q,\tilde{\Omega}) - g(q',q,\tilde{\Omega})\tilde{B}(q',q,\tilde{\Omega})\}_{\alpha q_1'} a_\alpha^\dagger(q) + \tilde{B}_{\alpha q_1'}(q',q,\tilde{\Omega}) a_\alpha(q)]$$
$$= \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\} \sum_\alpha [X_{\alpha q_1'}(q',q,\tilde{\Omega}) a_\alpha^\dagger(q) + \tilde{B}_{\alpha q_1'}(q',q,\tilde{\Omega}) a_\alpha(q)] , \quad (61)$$

where use has been made of the relation

$$\tilde{A}(q',q,\tilde{\Omega}) - g(q',q,\tilde{\Omega})\tilde{B}(q',q,\tilde{\Omega}) = X(q',q,\tilde{\Omega}) \quad (62)$$

which results directly from the definition (56) and the unitarity of $\tilde{F}(q',q,\tilde{\Omega})$.

Expression (61) now enables us to write also the rotated $m$qp states of the representation q' in terms of the unrotated operators $a_\alpha^\dagger(q)$. So one obtains, for example, for the rotated 1qp states

$$b_{q_1'}^\dagger(q',\tilde{\Omega}) | \{q'(\tilde{\Omega})\}_0 \rangle \equiv \hat{\tilde{R}}(\tilde{\Omega}) a_{q_1'}^\dagger(q') | \{q'\}_0 \rangle = n_0(q',q,\tilde{\Omega}) \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\} \sum_\alpha X_{\alpha q_1'}(q',q,\tilde{\Omega}) a_\alpha^\dagger(q) | \{q\}_0 \rangle . \quad (63)$$

Similarly one gets for the rotated 2qp states

$$b_{q_1'}^\dagger(q',\tilde{\Omega}) b_{q_2'}^\dagger(q',\tilde{\Omega}) | \{q'(\tilde{\Omega})\}_0 \rangle \equiv \hat{\tilde{R}}(\tilde{\Omega}) a_{q_1'}^\dagger(q') a_{q_2'}^\dagger(q') | \{q'\}_0 \rangle$$
$$= n_0(q',q,\tilde{\Omega}) \exp\{\hat{Q}^{\dagger}(q',q,\tilde{\Omega})\}$$
$$\times \left[\tilde{g}_{q_1' q_2'}(q',q,\tilde{\Omega}) + \sum_{\alpha\beta} X_{\alpha q_1'}(q',q,\tilde{\Omega}) X_{\beta q_2'}(q',q,\tilde{\Omega}) a_\alpha^\dagger(q) a_\beta^\dagger(q) \right] | \{q\}_0 \rangle , \quad (64)$$

where

$$\tilde{g}(q',q,\tilde{\Omega}) \equiv \tilde{B}^T(q',q,\tilde{\Omega}) X(q',q,\tilde{\Omega}) = -\tilde{g}^T(q',q,\tilde{\Omega}) \quad (65)$$

and so on.

With the use of the above form of the rotated $m$qp states, which has been first proposed in Ref. 15 and was also used in Ref. 16, the rotated matrix element in Eq. (45) can now be calculated using a sort of generalized Wick's theorem. For this purpose first the operator $\hat{T}_\mu^L(\Delta N_0, \Delta Z_0)$ is transformed into the quasiparticle representation q with the help of the inverse transformation (8). The rotated matrix element can then always be written as a linear combination of terms of the following type

$$M_{\{q\}_n;\{q'\}_m}^{pp'} \equiv \langle \{q\}_0 | a_{q_n}(q) \cdots a_{q_1}(q) a_{\alpha_1}^\dagger(q) \cdots a_{\alpha_p}^\dagger(q) a_{\beta_1}(q) \cdots a_{\beta_{p'}}(q) b_{q_1'}^\dagger(q',\tilde{\Omega}) \cdots b_{q_m'}^\dagger(q',\tilde{\Omega}) | \{q'(\tilde{\Omega})\}_0 \rangle \quad (66)$$

which in turn can be written as the product of the overlap $n_0(q',q,\tilde{\Omega})$ with the sum of all the possible terms, in which all the operators in (66) are pairwise contracted, while the sign of each term is given by the number of permutations as in the usual Wick's theorem. The only difference with respect to the ordinary theorem, which considers only one and the same vacuum state on both sides, is that here not only one but four nonvanishing elementary contraction possibilities have to be taken into account. These can be easily derived considering the matrix elements

$$\langle \{q\}_0 | a_{q_2}(q) a_{q_1}(q) | \{q'(\tilde{\Omega})\}_0 \rangle \equiv n_0(q',q,\tilde{\Omega}) \langle \{q\}_0 | [a_{q_2}(q) a_{q_1}(q)]_c | \{q'(\tilde{\Omega})\}_0 \rangle , \quad (67)$$

$$\langle \{q\}_0 | b_{q_1'}^\dagger(q',\tilde{\Omega}) b_{q_2'}^\dagger(q',\tilde{\Omega}) | \{q'(\tilde{\Omega})\}_0 \rangle \equiv n_0(q',q,\tilde{\Omega}) \langle \{q\}_0 | [b_{q_1'}^\dagger(q',\tilde{\Omega}) b_{q_2'}^\dagger(q',\tilde{\Omega})]_c | \{q'(\tilde{\Omega})\}_0 \rangle , \quad (68)$$

$$\langle \{q\}_0 | a_{q_1}(q) b_{q_1'}^\dagger(q',\tilde{\Omega}) | \{q'(\tilde{\Omega})\}_0 \rangle \equiv n_0(q',q,\tilde{\Omega}) \langle \{q\}_0 | [a_{q_1}(q) b_{q_1'}^\dagger(q',\tilde{\Omega})]_c | \{q'(\tilde{\Omega})\}_0 \rangle , \quad (69)$$

and

$$\langle\{q\}_0\,|\,a_{q_1}(q)a^\dagger_\alpha(q)\,|\,\{q'(\widetilde{\Omega})\}_0\rangle\equiv n_0(q',q,\widetilde{\Omega})\langle\{q\}_0\,|\,[a_{q_1}(q)a^\dagger_\alpha(q)]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle\ . \tag{70}$$

With the above Eqs. (54), (63), and (64) and the commutators (59) and (60) follows immediately

$$\langle\{q\}_0\,|\,[a_{q_1}(q)a^\dagger_\alpha(q)]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle=\delta(\alpha q_1) \tag{71}$$

and

$$\langle\{q\}_0\,|\,[a_{q_2}(q)a_{q_1}(q)]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle=\langle\{q\}_0\,|\left[a_{q_2}(q)+\sum_\beta g_{q_2\beta}(q',q,\widetilde{\Omega})a^\dagger_\beta(q)\right]$$
$$\times\left[a_{q_1}(q)+\sum_\alpha g_{q_1\alpha}(q',q,\widetilde{\Omega})a^\dagger_\alpha(q)\right]|\,\{q\}_0\rangle=g_{q_1q_2}(q',q,\widetilde{\Omega})\ . \tag{72}$$

Furthermore

$$\langle\{q\}_0\,|\,[b^\dagger_{q'_1}(q',\widetilde{\Omega})b^\dagger_{q'_2}(q',\widetilde{\Omega})]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle=\tilde{g}_{q'_1q'_2}(q',q,\widetilde{\Omega}) \tag{73}$$

and finally

$$\langle\{q\}_0\,|\,[a_{q_1}(q)b^\dagger_{q'_1}(q',\widetilde{\Omega})]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle=\langle\{q\}_0\,|\left[a_{q_1}(q)+\sum_\beta g_{q_1\beta}(q',q,\widetilde{\Omega})a^\dagger_\beta(q)\right]$$
$$\times\sum_\alpha X_{\alpha q'_1}(q',q,\widetilde{\Omega})a^\dagger_\alpha(q)\,|\,\{q\}_0\rangle=X_{q_1q'_1}(q',q,\widetilde{\Omega})\ . \tag{74}$$

As an example for the application of this generalized Wick's theorem we consider now the overlap between two arbitrary two quasiparticle states. We obtain

$$\langle\{q\}_0\,|\,a_{q_2}(q)a_{q_1}(q)b^\dagger_{q'_1}(q',\widetilde{\Omega})b^\dagger_{q'_2}(q',\widetilde{\Omega})\,|\,\{q'(\widetilde{\Omega})\}_0\rangle$$
$$=n_0(q',q,\widetilde{\Omega})\{\langle\{q\}_0\,|\,[a_{q_2}(q)a_{q_1}(q)]_c[b^\dagger_{q'_1}(q',\widetilde{\Omega})b^\dagger_{q'_2}(q',\widetilde{\Omega})]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle$$
$$+\langle\{q\}_0\,|\,[a_{q_2}(q)b^\dagger_{q'_2}(q',\widetilde{\Omega})]_c[a_{q_1}(q)b^\dagger_{q'_1}(q',\widetilde{\Omega})]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle$$
$$-\langle\{q\}_0\,|\,[a_{q_2}(a)b^\dagger_{q'_1}(q',\widetilde{\Omega})]_c[a_{q_1}(q)b^\dagger_{q'_2}(q',\widetilde{\Omega})]_c\,|\,\{q'(\widetilde{\Omega})\}_0\rangle$$
$$=n_0(q',q,\widetilde{\Omega})\{g_{q_1q_2}(q',q,\widetilde{\Omega})\tilde{g}_{q'_1q'_2}(q',q,\widetilde{\Omega})+X_{q_1q'_1}(q',q,\widetilde{\Omega})X_{q_2q'_2}(q',q,\widetilde{\Omega})$$
$$-X_{q_1q'_2}(q',q,\widetilde{\Omega})X_{q_2q'_1}(q',q,\widetilde{\Omega})\}\ . \tag{75}$$

Expressions for the rotated overlap and energy matrices needed in a space of 0qp and 2qp states are given in Appendix B of the present paper.

III. TRUNCATION SCHEMES FOR GENERAL HFB-BASED CONFIGURATION SPACES

After having developed a formalism to calculate the matrix elements of an arbitrary operator within general angular momentum and particle number projected HFB-type configurations we shall now come back to the problem of how to determine the transformation $F(q)$ of Eq. (6) for various truncated model spaces. Obviously there are different ways to obtain this transformation corresponding to different levels of approximation. Some of these will be discussed in the present section.

A. HFB theory with number and spin projection before the variation

We shall first consider the case that the chosen intrinsic configuration space consists only of the quasiparticle vacuum $|\,\{q\}_0\rangle$. According to Sec. II B the most general number and spin conserving wave function constructable from this single determinant has then the form

$$|\,\{q_i\}_0N_0Z_0IM;i\,\rangle=\sum_K|\,\{q_i\}_0N_0Z_0IM;K\,\rangle f_{K;i}(N_0Z_0I;q_i) \tag{76}$$

with the mixing coefficients $f(N_0Z_0I;q_i)$ to be obtained as solutions of the matrix equation

$$\sum_{K'} \{H^{(N_0Z_0I)}_{\{q_i\}_0K;\{q_i\}_0K'} - E_i(N_0Z_0I;q_i)N^{(N_0Z_0I)}_{\{q_i\}_0K;\{q_i\}_0K'}\} f_{K';i}(N_0Z_0I;q_i) = 0 \tag{77}$$

being subject to the constraint

$$f^{\dagger}(N_0Z_0I;q_i)N(N_0Z_0I)f(N_0Z_0I;q_i) = U \ , \tag{78}$$

where U is the unit matrix and N and H are defined by Eqs. (21) and (24), respectively.

Left to be determined then is the optimal quasiparticle transformation $F(q_i)$ for the energetically lowest solution i of Eqs. (77) and (78). This can be done in a very elegant way with the help of Thouless's theorem[14] as has been demonstrated, for example, by Mang.[10] This theorem allows us to write any variation of the vacuum $|\{q_i\}_0\rangle$ in the form

$$|\{q_i+\delta q\}_0\rangle = c_0 \exp\left[\tfrac{1}{2}\sum_{\alpha\beta} d_{\alpha\beta}a^{\dagger}_{\alpha}(q_i)a^{\dagger}_{\beta}(q_i)\right]|\{q_i\}_0\rangle \tag{79}$$

with c_0 being a normalization constant and d an antisymmetric $(M\times M)$ matrix. Consequently the total energy can be written as a function of the matrix elements of d and the variational problem for the average HFB field be formulated as

$$\frac{\partial}{\partial d^*_{\gamma\delta}}\{E_i[\{d\}]\}_{d=0} = \frac{\partial}{\partial d^*_{\gamma\delta}}\left[\frac{\langle\{q_i+\delta q\}_0N_0Z_0IM;i\,|\,\hat{H}\,|\,\{q_i+\delta q\}_0N_0Z_0IM;i\rangle}{\langle\{q_i+\delta q\}_0N_0Z_0IM;i\,|\,\{q_i+\delta q\}_0N_0Z_0IM;i\rangle}\right]_{d=0} = 0 \ . \tag{80}$$

This yields straightforwardly the set of equations

$$\mathscr{H}^{q_iN_0Z_0I^*}_{20}(\gamma\delta) \equiv \int d\tilde{\Omega} \sum_{KK'} f^*_{K;i}(N_0Z_0I;q_i)\omega^{N_0Z_0I^*}_{KK'}(\tilde{\Omega})$$

$$\times f_{K';i}(N_0Z_0I;q_i)\langle\{q_i\}_0\,|\,a_{\delta}(q_i)a_{\gamma}(q_i)[\hat{H}-E_i(N_0Z_0I;q_i)]\hat{\tilde{R}}(\tilde{\Omega})\,|\,\{q_i\}_0\rangle = 0 \ , \tag{81}$$

which expresses the stability of the state i (76) with respect to arbitrary spin- and number-projected 2qp admixtures within the same representation q_i. The explicit expression for the rotated matrix element in Eq. (81) is given in Appendix B. Furthermore, in addition to the above equations the unitarity of the transformation matrix $F(q_i)$

$$F(q_i)F^{\dagger}(q_i) = F^{\dagger}(q_i)F(q_i) = U \tag{82}$$

has to be ensured.

However, the above set of equations is not yet sufficient to determine $F(q_i)$ in a unique way. This is due to the fact that any unitary transformation t of the form

$$a_{\alpha}(q'_i) = \sum_{\beta} t_{\alpha\beta}a_{\beta}(q_i) \tag{83}$$

leaves the vacuum $|\{q_i\}_0\rangle$ invariant. The resulting ambiguity in $F(q_i)$ is usually resolved by using (83), the so-called "third Bloch-Messiah transformation,"[17] to diagonalize the $\hat{H}^{q_i}_{11}$ part of the Hamiltonian requiring that

$$H^{q_i}_{11}(\alpha\beta) \equiv \langle\{q_i\}_0\,|\,a_{\alpha}(q_i)\hat{H}a^{\dagger}_{\beta}(q_i)\,|\,\{q_i\}_0\rangle - \langle\{q_i\}_0\,|\,\hat{H}\,|\,\{q_i\}_0\rangle\delta(\alpha,\beta)$$

$$= E_{\alpha}\delta(\alpha,\beta) \ . \tag{84}$$

Here E_{α} are the usual "quasiparticle energies." The explicit expression for $H^{q_i}_{11}(\alpha\beta)$ is given in Appendix A.

Together with (84) now the system of equations (77), (78), (81), and (82) determines the stationary points of the state (76) in the variational space spanned by the matrices $f(N_0Z_0I;q_i)$ and $F(q_i)$ in a unique way. Similar equations have already been proposed by several authors a long time ago.[18,19] At least in principle, they can be solved numerically using a straightforward extension of the iteration scheme for the variational equations of the HF problem with spin projection before the variation which has been recently discussed.[5]

B. The "optimal" truncation scheme

As for the spin conserving HF approach described in Ref. 5 the above procedure can also be easily extended to construct an optimal truncated configuration space for each spin value of the considered nucleus. For this purpose the equations of the last section are repeatedly solved requiring in addition that each new solution i (76) should be orthogonal to all the already obtained solutions $j=1,\ldots,i-1$. This can be formulated mathematically by additional constraints

$$n_{ij}(N_0Z_0I) \equiv \sum_{KK'} f^*_{K;i}(N_0Z_0I;q_i)N^{(N_0Z_0I)}_{\{q_i\}_0K;\{q_j\}_0K'} \times f_{K';j}(N_0Z_0I;q_j) + \text{H.c.} = 0 \tag{85}$$

which have to be added with Lagrangian multipliers μ_j to the total energy functional before performing the variation. Equation (77) is then generalized to

$$\sum_{K'}\{[H^{(N_0Z_0I)}_{\{q_i\}_0K;\{q_i\}_0K'}-E_i(N_0Z_0I;q_i)N^{(N_0Z_0I)}_{\{q_i\}_0K;\{q_i\}_0K'}]f_{K';i}(N_0Z_0I;q_i)-\sum_{j=1}^{i-1}N^{(N_0Z_0I)}_{\{q_i\}_0K;\{q_j\}_0K'}f_{K';j}(N_0K_0I;q_j)\mu_j\}=0 \tag{86}$$

and instead of Eqs. (81) now the set

$$\mathscr{H}^{q_i^*}_{20}(\gamma\delta)-\sum_{j=1}^{i-1}\mu_j\int d\tilde{\Omega}\sum_{KK'}f^*_{K;i}(N_0Z_0I;q_i)\omega^{N_0Z_0I^*}_{KK'}(\tilde{\Omega})f_{K';j}(N_0Z_0I;q_j)\langle\{q_i\}_0\,|\,a_\delta(q_i)a_\gamma(q_i)\hat{\tilde{R}}(\tilde{\Omega})\,|\,\{q_j\}_0\rangle=0 \tag{87}$$

has to be used.

Solving Eqs. (86) and (87) together with (85), (84), (82), and (78) successively the optimal one determinant approximation for each nuclear state of a given spin value can be obtained. Truncating after m configurations and diagonalizing the residual interaction in the resulting space according to Sec. II B yields then the optimal approximation to the m lowest exact solutions which can be reached using only m HFB states as basis configurations.

Obviously the procedure described above using a different $F(q_i)$ for each number of the truncated configuration space becomes more and more difficult with increasing number of configurations. For problems requiring the use of very many configurations as, for example, the investigation of the giant multipole resonances, the above method is therefore not very suitable. Here it is obviously preferable to start with a certain number of intrinsic configurations right from the beginning and to require that these are all built on the same quasiparticle transformation $F(q)$. While the configuration mixing has then always to be obtained according to Sec. II B, there are different ways to determine $F(q)$. These will be discussed in the following three sections.

C. The "second best" approach: Spin and configuration space-dependent $F(q)$

The optimal quasiparticle transformation $F(q)$ for a given incomplete set of configurations $|\{q\}\rangle$, $|\{q'\}\rangle, \ldots,$ of the type (11) is obviously the simultaneous variation of the configuration mixing and the matrix elements of $F(q)$ in order to minimize the total energy. The resulting variational equations look very much like those derived in Sec. III A except that now all the sums run not only over the $(2I+1)$ K values but also over all the configurations $|\{q\}\rangle, |\{q'\}\rangle, \ldots,$ included in the configuration space. Equation (77) therefore has to be replaced by

$$\sum_{\{q'\},K}\{H^{(N_0Z_0I)}_{\{q\}K;\{q'\}K'}-E_i(N_0Z_0I)N^{(N_0Z_0I)}_{\{q\}K;\{q'\}K'}\}\times f_{\{q'\}K;i}(N_0Z_0I)=0 \tag{88}$$

and instead of Eqs. (81) now the system of equations

$$\sum_{\{q\},K,\{q'\},K'}\int d\tilde{\Omega}\,f^*_{\{q\}K;i}(N_0Z_0I)\times\omega^{N_0Z_0I^*}_{KK'}(\tilde{\Omega})f_{\{q'\}K';i}(N_0Z_0I)\times\langle\{q\}\,|\,a_\delta(q)a_\gamma(q)[\hat{H}-E_i(N_0Z_0I)]\hat{\tilde{R}}(\tilde{\Omega})\,|\,\{q'\}\rangle=0 \tag{89}$$

has to be used.

The solution of the coupled system of Eqs. (88), (89), (82), and (84) together with the orthonormality condition (20) yields then the optimal approximation to the exact solutions which can be reached within a given subset of HFB configurations being all based on the same quasiparticle transformation $F(q)$. This $F(q)$ obviously depends on both the actual spin I (and particle numbers N_0 and Z_0) as well as on the chosen set of intrinsic configurations.

Unfortunately even the approach described above which is the natural extension of the MCHF approximation (see Schmid *et al.*, Ref. 8), which is based on particle Slater determinants, can hardly be used in realistic calculations because of the extremely time consuming iterative procedure necessary for the solution of the corresponding coupled systems of equations. Therefore, additional approximations have to be made.

D. The "third best" approach: Configuration space-independent $F(q)$

A drastic simplification can be reached, if the set of Eqs. (89) is completely discarded and instead the fixed transformation $F(q)$, which results from the solution of the spin and number conserving HFB equations in Sec. III B, is used to build up the configuration space in which the Hamiltonian is then diagonalized according to Eqs. (88) and (20). Since the coupling of the configuration mixing to the quasiparticle degrees of freedom is neglected, however, both $f(N_0Z_0I)$ and $F(q)$ do still depend on the given spin value.

Note that in this case because of Eqs. (81) the vacuum state (76) does not mix with the spin- and number-projected 2qp excitations belonging to the same quasiparticle representation. Restricting the truncated configuration space to the vacuum and the 2qp excitations with respect to it, the yrast states of the nucleus would therefore have the form (76) while the excited states would be linear superpositions of projected 2qp states. Thus the extension of the well-known TDA or RPA to open shell quasiparticle systems could be easily constructed using the spin-dependent but configuration-space-independent transformation $F(q)$ resulting from the above prescription.

However, even for this drastic simplification of the more general approach described in Sec. III C the solutions of the variational equations of Sec. III A would be needed, which at least for realistic model spaces have never been obtained numerically up to now. Hence for practical calculations in general even more drastic approximations are necessary.

E. The "fourth best" approach: Spin and configuration space-independent $F(q)$

With the use of a configuration space based on HF-type Slater determinants it could be shown that often the use of a fixed HF transformation for all the spin values still yields a very good approximation to the exact solutions provided that at least the configuration mixing is done after restoring the rotational symmetry.[6] We shall therefore make the same approximation in the following for configuration spaces consisting of HFB determinants of the type (11). This procedure has the advantage that $F(q)$ has only to be determined once via the standard HFB prescription in the intrinsic system and can then be kept fixed for all further steps of the calculation.

In standard HFB theory a minimum for the vacuum expectation value of the Hamiltonian $\hat{H}'$

$$\langle\{q\}_0|\hat{H}'|\{q\}_0\rangle\equiv\langle\{q\}_0|\hat{H}-\lambda_n\hat{N}-\lambda_p\hat{Z}|\{q\}_0\rangle = \text{minimum!} \tag{90}$$

with respect to variations of $F(q)$ is required, where the additional constraints

$$\langle\{q\}_0|\hat{N}|\{q\}_0\rangle=N_0(q)=N_0 \tag{91}$$

and

$$\langle\{q\}_0|\hat{Z}|\{q\}_0\rangle=Z_0(q)=Z_0\,, \tag{92}$$

which ensure that at least the average nucleon numbers have the desired values, have been coupled with Lagrangian multipliers λ_p and λ_n (the "chemical potentials" or "Fermi energies") to the original Hamiltonian. Using exactly the same methods as in Sec. III A one then obtains a set of equations

$$H^{q*}_{20}(\gamma\delta)-\lambda_n N^{q*}_{20}(\gamma\delta)-\lambda_p Z^{q*}_{20}(\gamma\delta)\equiv\langle\{q\}_0|a_\delta(q)a_\gamma(q)(\hat{H}-\lambda_n\hat{N}-\lambda_p\hat{Z})|\{q\}_0\rangle=0 \tag{93}$$

which are the equivalent of the Eqs. (81) in the intrinsic system and express the stability of the intrinsic vacuum versus intrinsic 2qp admixtures. These equations have been first derived by Belyaev.[20] Explicit expressions for $H_0(q)$, $N_0(q)$, $Z_0(q)$ and the matrices H^q_{20}, N^q_{20}, and Z^q_{20} are given in Appendix A. Furthermore, because of the additional constraints (91) and (92), Eqs. (84) are modified, too. Here one obtains

$$H^q_{11}(\alpha\beta)-\lambda_n N^q_{11}(\alpha\beta)-\lambda_p Z^q_{11}(\alpha\beta)=E_\alpha\delta(\alpha,\beta) \tag{94}$$

with all the matrix elements again given in Appendix A.

Together with the unitarity constraint (7) Eqs. (91)—(94) are the usual HFB variational equations. For their numerical solution elegant methods are available.[21]

With the solutions $F(q)$ of the above equations the intrinsic configuration space can now be built up and the Hamiltonian can be diagonalized according to Sec. II B. Note that in this approach now the number- and spin-projected 2qp excitations do mix with their projected vacuum since Eqs. (93) guarantee stability of the vacuum with respect to 2qp excitations only for the unprojected intrinsic configurations.

Naturally, using a fixed $F(q)$ for all spin values the possible spin dependencies in the total wave functions (19) can only be accounted for via the configuration mixing coefficients and not by the quasiparticle transformation itself. Therefore, to reach an approximation to the exact solutions as good as with the approaches using spin-dependent transformations $F(q)$ described in Secs. III B—III D here obviously more configurations have to be taken into account. However, from the computational point of view working with a spin- and space-independent quasiparticle transformation seems at least at the moment the only possibility for the realization of practical calculations using realistic interactions in large model spaces.

The numerical realization of the procedure described in the present section for the case that the truncated intrinsic configuration space consists only of the quasiparticle vacuum and the 2qp excitations with respect to it was the goal of the computer code MONSTER, which has been developed during the last three years and whose main details will be presented in paper II of the present series of papers. Paper II will also contain the results of first applications of this approach to nuclei in various mass regions.

IV. CONCLUSIONS

Many nuclear structure problems, as, for example, the microscopic description of the giant multipole resonances or the theoretical analysis of the various high spin phenomena in heavy nuclei require the use of single-particle basis systems, which are far too large to allow for the diagonalization of a given effective many nucleon Hamiltonian in the complete shell model configuration space at least on present day computers. One is therefore forced to approximate the inaccessible complete shell model expansion of the nuclear wave function within a truncated space consisting only of a numerically manageable number of A-nucleon configurations. Thus it is desirable to account for as much of the correlations as possible between the nucleons by as few A-nucleon basis states as possible.

In the present paper we have described and discussed a variety of such truncation schemes which are all based on the HFB theory. The essential idea behind this is to incorporate the most important collective correlations in the nucleus as, for example, pairing and deformation via a mean-field approach already in the reference configuration and thus to increase the changes to account for the essential residual correlations within a relatively small configuration space.

Unfortunately such an approach in general conserves neither the particle numbers Z_0 and N_0 nor the total angular momentum I of the considered nucleus. A physical basis can therefore only be obtained by restoring these broken symmetries with the help of projection techniques which lead to rather drastic complications both in the

mathematical formulation as well as in the numerical realization of such a theory. We have therefore tried to give in Sec. II a rather general review and survey about the methods which are necessary in order to handle general spin- and number-projected HFB-type quasiparticle determinants. Special emphasis has been put here on the properties of the projection operators and on how to evaluate the matrix elements of general operators in between arbitrary HFB-type configurations which may even be based on completely different quasiparticle transformations.

Left to be answered then is the question of how these quasiparticle transformations themselves are to be determined. This was the main subject of Sec. III. The obviously most sophisticated answer to this question is to require an optimized HFB transformation for each configuration of the chosen truncated space separately. This can be achieved by successively constructing these configurations using the HFB procedure with spin and number projection before the variation out of Sec. III A requiring in addition orthogonality of the different solutions obtained for a given spin value. For each state of a given spin the optimal one determinant approximation can be calculated. Truncating the resulting configuration space after m solutions and then diagonalizing the residual interaction yields obviously the best approximation to the lowest m states of a given spin value which can be reached using only m general quasiparticle determinants.

Unfortunately this procedure, which has been discussed in Sec. III B and which is the natural extension of the HF-based truncation scheme proposed in Ref. 5, is numerically extremely involved especially if highly excited states as, for example, the giant multipole resonances are to be described. Here it is preferable to fix the number of configurations to be included for a given spin value right from the beginning and to construct them all out of one and the same HFB transformation. In general this transformation will then still depend on both the spin as well as the chosen configuration space and can be determined via the solution of the variational equations for the multiconfiguration HFB procedure with spin and number projection before the variation which have been derived and discussed in Sec. III C of the present paper.

However, for large single-particle basis systems these variational equations can hardly be solved numerically at least with present day computer facilities. Therefore, in general additional approximations are unavoidable. A great simplification of the variational equations is reached if, for example, the configuration space dependence of the HFB transformation is neglected. In this case the still spin-dependent reference configurations for the considered nucleus are again given by the solutions of the variational equations discussed in Sec. III A, which are stable against arbitrary spin- and number-projected 2qp admixtures being based on the same HFB transformation. Hence this procedure, which has been discussed in Sec. III D, is the natural starting point for the extension of quasiparticle TDA- or RPA-like theories to deformed nuclei. Still the numerical realization of even this method is rather involved. Nevertheless, we think there is a fair chance for its application within the next few years.

For the moment, however, we probably have to be content with an even less general approximation, which has been discussed as "fourth-best" solution in Sec. III E. In this approach the transformation is forced to be not only configuration space but also spin independent and determined by a standard HFB calculation in the intrinsic (i.e., symmetry breaking) frame of reference. All the spin-dependent structure changes in the nuclear wave functions therefore have to be described entirely by changes in the configuration mixing. Hence in order to obtain as good a description of the nucleus as with the more sophisticated methods discussed above, here obviously a larger configuration space is necessary out of numerical reasons; however, this is at present still much more practical than the complicated iteration schemes which are necessary to obtain solutions for the other methods.

Restricting the configuration space to the reference determinant and the 2qp excitations with respect to it the method of Sec. III E reduces to the MONSTER approach (model for handling large numbers of number- and spin-projected two quasiparticle excitations with realistic interactions and model spaces) being the basis of the equal-named computer code, which has been developed during the last three years. This approach and the essential additional approximations which were made for its numerical realization are the subject of paper II of the present series of papers. This part will also present the results of first applications of the MONSTER to nuclei in various mass regions.

APPENDIX A: QUASIPARTICLE REPRESENTATION OF THE HAMILTONIAN AND THE NUMBER OPERATORS

With the use of the transformation (8) any arbitrary operator whose basis representation is known can be transformed into its "quasiparticle representation" q. In this appendix we shall do this for the Hamiltonian (1) and for the neutron- and proton-number operators.

For the Hamiltonian one obtains[10]

$$\hat{H} \equiv H_0(q) + \hat{H}^{q}_{11} + \hat{H}^{q}_{20} + \hat{H}^{q}_{22} + \hat{H}^{q}_{31} + \hat{H}^{q}_{40} , \tag{A1}$$

where

$$H_0(q) \equiv \sum_{ik} \{ [t(ik) + \tfrac{1}{2}\Gamma^{q}_{ik}]\rho^{q}_{ki} + \tfrac{1}{2}\Delta^{q}_{ik}\kappa^{q*}_{ki} \} \tag{A2}$$

and

$$\rho^{q}_{ki} \equiv [B^*(q)B^T(q)]_{ki} , \tag{A3}$$

$$\kappa^{q}_{ki} \equiv [B^*(q)A^T(q)]_{ki} , \tag{A4}$$

$$\Gamma^{q}_{ik} \equiv \sum_{rs} v(irks)\rho^{q}_{sr} , \tag{A5}$$

$$\Delta^{q}_{ik} \equiv \tfrac{1}{2} \sum_{rs} v(ikrs)\kappa^{q}_{sr} . \tag{A6}$$

Furthermore,

$$\hat{H}^{q}_{11} \equiv \sum_{\alpha\beta} H^{q}_{11}(\alpha\beta) a^{\dagger}_{\alpha}(q) a_{\beta}(q) \tag{A7}$$

with

$$H^q_{11}(\alpha\beta)\equiv[A^\dagger(q)h(q)A(q)+B^\dagger(q)h^T(q)B(q) +B^\dagger(q)\Delta^{q*}A(q)-A^\dagger(q)\Delta^qB(q)]_{\alpha\beta} \tag{A8}$$

and

$$h_{ik}(q)\equiv t(ik)+\Gamma^q_{ik}\ . \tag{A9}$$

Similarly

$$\hat{H}^q_{20}\equiv\sum_{\alpha\beta}[H^q_{20}(\alpha\beta)a^\dagger_\alpha(q)a^\dagger_\beta(q) +H^{q*}_{20}(\alpha\beta)a_\beta(q)a_\alpha(q)]\ , \tag{A10}$$

where

$$H^q_{20}(\alpha\beta)\equiv\tfrac{1}{2}[A^\dagger(q)h(q)B^*(q)-B^\dagger(q)h^T(q)A^*(q) +B^\dagger(q)\Delta^{q*}B^*(q)-A^\dagger(q)\Delta^qA^*(q)]_{\alpha\beta}\ . \tag{A11}$$

Finally

$$\hat{H}^q_{22}\equiv\sum_{\alpha\beta\gamma\delta}H^q_{22}(\alpha\beta\gamma\delta)a^\dagger_\alpha(q)a^\dagger_\beta(q)a_\delta(q)a_\gamma(q)\ , \tag{A12}$$

$$\hat{H}^q_{31}\equiv\sum_{\alpha\beta\gamma\delta}[H^q_{31}(\alpha\beta\gamma\delta)a^\dagger_\delta(q)a^\dagger_\gamma(q)a^\dagger_\beta(q)a_\alpha(q) +H^{q*}_{31}(\alpha\beta\gamma\delta)a^\dagger_\alpha(q)a_\beta(q)a_\gamma(q)a_\delta(q)]\ , \tag{A13}$$

and

$$\hat{H}^q_{40}\equiv\sum_{\alpha\beta\gamma\delta}[H^q_{40}(\alpha\beta\gamma\delta)a^\dagger_\alpha(q)a^\dagger_\beta(q)a^\dagger_\gamma(q)a^\dagger_\delta(q) +H^{q*}_{40}(\alpha\beta\gamma\delta)a_\delta(q)a_\gamma(q)a_\beta(q)a_\alpha(q)]\ , \tag{A14}$$

where

$$H^q_{22}(\alpha\beta\gamma\delta)\equiv\tfrac{1}{4}\sum_{ikrs}v(ikrs)\{A^*_{i\alpha}(q)A^*_{k\beta}(q)A_{r\gamma}(q)A_{s\delta}(q)+B^*_{i\alpha}(q)B^*_{k\beta}(q)B_{r\gamma}(q)B_{s\delta}(q) -A^*_{i\alpha}(q)B_{k\delta}(q)A_{r\gamma}(q)B^*_{s\beta}(q)-B^*_{i\alpha}(q)A_{k\delta}(q)B_{r\gamma}(q)A^*_{s\beta}(q) +A^*_{i\alpha}(q)B_{k\delta}(q)A_{s\gamma}(q)B^*_{r\beta}(q)+B^*_{i\alpha}(q)A_{k\delta}(q)B_{s\gamma}(q)A^*_{r\beta}(q)\} \tag{A15}$$

while

$$H^q_{31}(\alpha\beta\gamma\delta)\equiv\tfrac{1}{6}\sum_{ikrs}v(ikrs)\{A_{i\alpha}(q)B^*_{k\beta}(q)A^*_{r\delta}(q)A^*_{s\gamma}(q)+B_{i\alpha}(q)A^*_{k\beta}(q)B^*_{r\delta}(q)B^*_{s\gamma}(q) -A_{i\alpha}(q)B^*_{k\gamma}(q)A^*_{r\delta}(q)A^*_{s\beta}(q)-B_{i\alpha}(q)A^*_{k\gamma}(q)B^*_{r\delta}(q)B^*_{s\beta}(q) +A_{i\alpha}(q)B^*_{k\delta}(q)A^*_{r\gamma}(q)A^*_{s\beta}(q)+B_{i\alpha}(q)A^*_{k\delta}(q)B_{r\gamma}(q)B^*_{s\beta}(q)\} \tag{A16}$$

and

$$H^q_{40}(\alpha\beta\gamma\delta)\equiv\tfrac{1}{24}\sum_{ikrs}v(ikrs)\{A^*_{i\alpha}(q)A^*_{k\gamma}(q)B^*_{r\delta}(q)B^*_{s\beta}(q)+B^*_{i\alpha}(q)B^*_{k\gamma}(q)A^*_{r\delta}(q)A^*_{s\beta}(q) -A^*_{i\alpha}(q)A^*_{k\delta}(q)B^*_{r\gamma}(q)B^*_{s\beta}(q)-B^*_{i\alpha}(q)B^*_{k\delta}(q)A^*_{r\gamma}(q)A^*_{s\beta}(q) -A^*_{i\alpha}(q)A^*_{k\beta}(q)B^*_{r\delta}(q)B^*_{s\gamma}(q)-B^*_{i\alpha}(q)B^*_{k\beta}(q)A^*_{r\delta}(q)A^*_{s\gamma}(q)\}\ . \tag{A17}$$

Much simpler are the quasiparticle representations of the neutron- and proton-number operators. We obtain for

$$_{1/2}\hat{N}\equiv\hat{N} \tag{A18}$$

and

$$_{-1/2}\hat{N}\equiv\hat{Z}\ , \tag{A19}$$

$$_\tau\hat{N}\equiv{}_\tau N_0(q)+{}_\tau\hat{N}^q_{11}+{}_\tau\hat{N}^q_{20}\ , \tag{A20}$$

where

$$_\tau N_0(q)\equiv\sum_i\delta(\tau_i,\tau)\rho^q_{ii} \tag{A21}$$

and

$$_\tau\hat{N}^q_{11}\equiv\sum_{\alpha\beta}{}_\tau N^q_{11}(\alpha\beta)a^\dagger_\alpha(q)a_\beta(q) \tag{A22}$$

with

$$_\tau N^q_{11}(\alpha\beta)\equiv[A^\dagger(q)\xi_\tau A(q)-B^\dagger(q)\xi_\tau B(q)]_{\alpha\beta} \tag{A23}$$

and

$$(\xi_\tau)_{ik}\equiv\delta(i,k)\delta(\tau_i,\tau) \tag{A24}$$

while

$$_\tau\hat{N}^q_{20}\equiv\sum_{\alpha\beta}[{}_\tau N^q_{20}(\alpha\beta)a^\dagger_\alpha(q)a^\dagger_\beta(q) +{}_\tau N^{q*}_{20}(\alpha\beta)a_\beta(q)a_\alpha(q)] \tag{A25}$$

with

$$ {}_{\tau}N^{q}_{20}(\alpha\beta)\equiv\tfrac{1}{2}[A^{\dagger}(q)\xi_{\tau}B^{*}(q)-B^{\dagger}(q)\xi_{\tau}A^{*}(q)]_{\alpha\beta}\ . \tag{A26} $$

Note that in Eqs. (A18)—(A26) it has been assumed that τ_i is a good quantum number of the basis orbits $\{|i\rangle,\ldots\}_M$. The transformation $F(q)$ of Eq. (6), on the other hand, may still mix proton and neutron orbits as it is necessary to account for proton-neutron pairing.

APPENDIX B: ROTATED OVERLAP AND ENERGY MATRICES

Here we shall give explicit expressions for the spin- and number-rotated matrix elements needed for the evaluation of the overlap and energy matrices of Eqs. (21) and (24), respectively. For simplicity we shall restrict ourselves to only 0qp and 2qp configurations which nevertheless may be based on various different quasiparticle representations $q,q',\ldots$. Higher-order configurations ($n$qp) may be treated using exactly the same methods.

With the help of the generalized Wick's theorem of Sec. II C one obtains straightforwardly

$$ \langle\{q\}_0|\hat{\tilde{R}}(\tilde{\Omega})|\{q'\}_0\rangle=n_0(q',q,\tilde{\Omega}) \tag{B1} $$

with $n_0(q',q,\tilde{\Omega})$ given by Eq. (58). Furthermore

$$ \langle\{q\}_0|\hat{\tilde{R}}(\tilde{\Omega})a^{\dagger}_{q'_1}(q')a^{\dagger}_{q'_2}(q')|\{q'\}_0\rangle =n_0(q',q,\tilde{\Omega})\tilde{g}_{q'_1q'_2}(q',q,\tilde{\Omega}) \tag{B2} $$

with $\tilde{g}_{q'_1q'_2}(q',q,\tilde{\Omega})$ given by the definition (65). Similarly one gets

$$ \langle\{q\}_0|a_{q_2}(q)a_{q_1}(q)\hat{\tilde{R}}(\tilde{\Omega})|\{q'\}_0\rangle=n_0(q',q,\tilde{\Omega})g_{q_1q_2}(q',q,\tilde{\Omega}) \tag{B3} $$

with $g_{q_1q_2}(q',q,\tilde{\Omega})$ of Eq. (56) and finally

$$ \begin{aligned}\langle\{q\}_0|a_{q_2}(q)a_{q_1}(q)\hat{\tilde{R}}(\tilde{\Omega})a^{\dagger}_{q'_1}(q')a^{\dagger}_{q'_2}(q')|\{q'\}_0\rangle=n_0(q',q,\tilde{\Omega})\{&g_{q_1q_2}(q',q,\tilde{\Omega})\tilde{g}_{q'_1q'_2}(q',q,\tilde{\Omega})\\ &+X_{q_1q'_1}(q',q,\tilde{\Omega})X_{q_2q'_2}(q',q,\tilde{\Omega})\\ &-X_{q_1q'_2}(q',q,\tilde{\Omega})X_{q_2q'_1}(q',q,\tilde{\Omega})\}\ .\end{aligned} \tag{B4} $$

With $X_{q_1q'_1}(q',q,\tilde{\Omega})$ defined by Eq. (57). Equation (B4) has been considered as an example already at the end of Sec. II C [see Eq. (75)].

For the rotated energy matrix one obtains

$$ \langle\{q\}_0|\hat{H}\hat{\tilde{R}}(\tilde{\Omega})|\{q'\}_0\rangle=n_0(q',q,\tilde{\Omega})h_0(q',q,\tilde{\Omega})\ , \tag{B5} $$

where

$$ h_0(q',q,\tilde{\Omega})\equiv H_0(q)+\tfrac{1}{4}\sum_{\alpha\beta}[2H^{q*}_{20}+12\tilde{H}^{q'q*}_{40}(\tilde{\Omega})]_{\alpha\beta}g_{\alpha\beta}(q',q,\tilde{\Omega}) \tag{B6} $$

with

$$ [\tilde{H}^{q'q*}_{40}(\tilde{\Omega})]_{\alpha\beta}\equiv\sum_{\gamma\delta}H^{q*}_{40}(\alpha\beta\gamma\delta)g_{\gamma\delta}(q',q,\tilde{\Omega}) \tag{B7} $$

and $H_0(q)$, $H^{q*}_{20}(\alpha\beta)$, and $H^{q*}_{40}(\alpha\beta\gamma\delta)$ as given in Appendix A. Similarly one gets

$$ \langle\{q\}_0|\hat{H}\hat{\tilde{R}}(\tilde{\Omega})a^{\dagger}_{q'_1}(q)q^{\dagger}_{q'_2}(q')|\{q'\}_0\rangle=n_0(q',q,\tilde{\Omega})\{h^{02}_{q'_1q'_2}(q',q,\tilde{\Omega})+h_0(q',q,\tilde{\Omega})\tilde{g}_{q'_1q'_2}(q',q,\tilde{\Omega})\}\ , \tag{B8} $$

where

$$ h^{02}_{q'_1q'_2}(q',q,\tilde{\Omega})\equiv X^{T}(q',q,\tilde{\Omega})[2H^{q*}_{20}+12\tilde{H}^{q'q*}_{40}(\tilde{\Omega})]X(q',q,\tilde{\Omega})_{q'_1q'_2} \tag{B9} $$

and

$$ \langle\{q\}_0|a_{q_2}(q)a_{q_1}(q)\hat{H}\hat{\tilde{R}}(\tilde{\Omega})|\{q'\}_0\rangle=n_0(q',q,\tilde{\Omega})\{h^{20}_{q_1q_2}(q',q,\tilde{\Omega})+h_0(q',q,\tilde{\Omega})g_{q_1q_2}(q',q,\tilde{\Omega})\} \tag{B10} $$

with

$$ \begin{aligned}h^{20}_{q_1q_2}(q',q,\tilde{\Omega})\equiv&(2H^{q}_{20}+2\tilde{H}^{q'q}_{22}(\tilde{\Omega})+g(q',q,\tilde{\Omega})[2H^{q*}_{20}+12\tilde{H}^{q'q*}_{40}(\tilde{\Omega})]g(q',q,\tilde{\Omega})\\ &+\{[H^{q}_{11}-3\tilde{H}^{q'q*}_{31}(\tilde{\Omega})]g(q',q,\tilde{\Omega})\}-\{[H^{q}_{11}-3\tilde{H}^{q'q*}_{31}(\tilde{\Omega})]g(q',q,\tilde{\Omega})\}^{T})q_1q_2\ ,\end{aligned} \tag{B11} $$

where

$$[\tilde{H}^{q'q}_{22}(\tilde{\Omega})]_{\alpha\beta}\equiv\sum_{\gamma\delta}H^{q}_{22}(\alpha\beta\gamma\delta)g_{\gamma\delta}(q',q,\tilde{\Omega}) \tag{B12}$$

and

$$[\tilde{H}^{q'q^*}_{31}(\tilde{\Omega})]_{\alpha\beta}\equiv\sum_{\gamma\delta}H^{q^*}_{31}(\alpha\beta\gamma\delta)g_{\gamma\delta}(q',q,\tilde{\Omega}) \tag{B13}$$

with $H^{q}_{11},H^{q}_{22},H^{q^*}_{31}$ again given by Appendix A. Finally we obtain

$$\begin{aligned}
&\langle\{q\}_0\,|\,a_{q_2}(q)a_{q_1}(q)\hat{H}\hat{\tilde{R}}(\tilde{\Omega})a^{\dagger}_{q'_1}(q')a^{\dagger}_{q'_2}(q')\,|\,\{q'\}_0\rangle\\
&=n_0(q',q,\tilde{\Omega})\{h_0(q',q,\tilde{\Omega})[g_{q_1q_2}(q',q,\tilde{\Omega})\tilde{g}_{q'_1q'_2}(q',q,\tilde{\Omega})+X_{q_1q'_1}(q',q,\tilde{\Omega})X_{q_2q'_2}(q',q,\tilde{\Omega})-X_{q_1q'_2}(q',q,\tilde{\Omega})X_{q_2q'_1}(q',q,\tilde{\Omega})]\\
&\quad+h^{20}_{q_1q_2}(q',q,\tilde{\Omega})\tilde{g}_{q'_1q'_2}(q',q,\tilde{\Omega})+h^{02}_{q'_1q'_2}(q',q,\tilde{\Omega})g_{q_1q_2}(q',q,\tilde{\Omega})\\
&\quad+h^{11}_{q_1q'_1}(q',q,\tilde{\Omega})X_{q_2q'_2}(q',q,\tilde{\Omega})+h^{11}_{q_2q'_2}(q',q,\tilde{\Omega})X_{q_1q'_1}(q',q,\tilde{\Omega})\\
&\quad-h^{11}_{q_1q'_2}(q',q,\tilde{\Omega})X_{q_2q'_1}(q',q,\tilde{\Omega})-h^{11}_{q_2q'_1}(q',q,\tilde{\Omega})X_{q_1q'_2}(q',q,\tilde{\Omega})+v^{q'q\tilde{\Omega}}_{22}(q_1q_2;q'_1q'_2)\}\,,
\end{aligned} \tag{B14}$$

where

$$h^{11}_{\alpha\beta}(q',q,\tilde{\Omega})\equiv\{[H^{q}_{11}-3\tilde{H}^{q'q^*}_{31}(\tilde{\Omega})]+g(q',q,\tilde{\Omega})[2H^{q^*}_{20}+12\tilde{H}^{q'q^*}_{40}(\tilde{\Omega})]\}X(q',q,\tilde{\Omega})_{\alpha\beta} \tag{B15}$$

and

$$\begin{aligned}
v^{q'q\tilde{\Omega}}_{22}(q_1q_2;q'_1q'_2)\equiv\sum_{\gamma\delta}\Big\{&[4H^{q}_{22}(q_1q_2\gamma\delta)]+6\sum_{\beta}[g_{q_2\beta}(q',q,\tilde{\Omega})H^{q^*}_{31}(q_1\beta\gamma\delta)-g_{q_1\beta}(q',q,\tilde{\Omega})H^{*}_{31}(q_2\beta\gamma\delta)]\\
&-24\sum_{\alpha\beta}[g_{q_1\alpha}(q',q,\tilde{\Omega})g_{q_2\beta}(q',q,\tilde{\Omega})H^{q^*}_{40}(\alpha\beta\gamma\delta)]\Big\}X_{\gamma q'_1}(q',q,\tilde{\Omega})X_{\delta q'_2}(q',q,\tilde{\Omega})\,.
\end{aligned} \tag{B16}$$

Similar expressions can be easily obtained for the rotated matrix elements of general tensor operators. These will not be given explicitly in the present paper.

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