Canonical form of transition matrix elements

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The calculation of complicated transition matrix elements between multiquasiparticle states can be essentially simplified by transforming them in a canonical form. This method allows the extension of the basis space of generator coordinate studies aiming to include orthogonal quasiparticle excitations into the commonly considered basis set of collective states. Furthermore, it is shown that the neglect of the exchange contribution of multipole forces may lead to dangerous pole terms in nondiagonal matrix elements. [S0556-2813(98)01508-8]

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I. INTRODUCTION

The self-consistent Hartree-Fock-Bogoliubov (HFB) theory is the appropriate tool to determine the static mean field properties of interacting many-body fermion systems. In order to comprehend the collective dynamics of such systems as well as for the restoration of broken symmetries one needs to superimpose various HFB states. In this respect the generator coordinate method (GCM) [1] provides the appropriate framework to incorporate both collective and single particle dynamics into a unified coherent quantum-mechanical formulation. The GCM is known to be a very powerful and successful method to describe microscopically large amplitude collective motion such as, e.g., pair vibrations, shape coexistence, and shape transitions (see Refs. [2–4]). The rigorous application of the GCM requires that we have stable and efficient algorithms for obtaining the operator brackets, in particular, the Hamiltonian kernel $\langle Z|H|Z'\rangle$ and the overlaps $\langle Z|Z'\rangle$ between arbitrarily chosen HFB states $|Z\rangle$ and $|Z'\rangle$ with any configuration. To have such algorithms at our disposal would allow us to perform the GCM as though it were a shell model diagonalization. The typical basis set of generator states $|Z\rangle$ contains quasicontinuous ''collective'' excitations, i.e., a sequence of nonorthogonal HFB states is formed by shifting a collective variable such as, e.g., the deformation parameter, pair gap, etc., within a chosen interval. When also including excited HFB states into the GCM basis, i.e., discrete (orthogonal) quasiparticle excitations from the ground state configuration, the coupling of collective and single particle degrees of freedom can be taken into account.

The techniques given in the literature [5,6] are not sufficient to evaluate the above brackets between HFB states when also including orthogonal quasiparticle excitations into the GCM basis set since the formulas imply pole terms for zero overlap between the two HFB states involved. Because of these divergencies the nondiagonal matrix elements of a factorized multipole interaction are wrong when neglecting exchange contributions. There are also difficulties in consistently determining the phases of the overlaps and operator matrix elements which are of crucial importance for actual GCM diagonalizations.

With the methods described below it is possible to calculate the necessary operator brackets including their phases in a direct and transparent manner which is otherwise quite complicated [1]. The formulas are formally simple and the numerical effort is considerably lowered by dimensional reduction.

II. CANONICAL FORM OF TRANSITIONAL BRACKETS

For the subsequent consideration it is useful to specify both Bogoliubov (''multiquasiparticle'') states forming the bra and the ket vector of a bracket $\langle Z|Z'\rangle$ in the Thouless representation [7]

$$\langle Z| = \mathcal{N}^*(\mathcal{Z})\langle Z_0| e^{1/2\Sigma_{kk'} Z^*_{kk'} c_{k'} c_k},$$

$$|Z'\rangle = \mathcal{N}(\mathcal{Z}') e^{1/2\Sigma_{kk'} Z'_{kk'} c^+_k c^+_{k'}} |Z_0\rangle. \tag{1}$$

In the above equations c_k and c^+_k denote the n (even) fermion annihilation and creation operators to the c vacuum, i.e., the state $|Z_0\rangle$ satisfying

$$\langle Z_0| c^+_k = 0, \quad c_k |Z_0\rangle = 0. \tag{2}$$

The factors $\mathcal{N}^*(\mathcal{Z})$ and $\mathcal{N}(\mathcal{Z}')$ are for the normalization of the Bogoliubov states (1). The antisymmetric Thouless matrix Z in Eq. (1), and likewise Z' are obtainable from the known Bogoliubov amplitudes U and V using the relation [1,7]

$$Z = (VU^{-1})^*. \tag{3}$$

The UV amplitudes determine the quasiparticle operators

$$a^+_i = \sum_k (U_{ki} c^+_k + V_{ki} c_k) \tag{4}$$

which provide an equivalent definition of the HFB state $|Z\rangle$, Eq. (1), as the quasiparticle a vacuum to the operators $a_i = (a^+_i)^+$, i.e., $|Z\rangle \propto a_1 a_2 \cdots a_n |Z=0\rangle$. The UV matrices are commonly calculated by solving the general HFB equations [1].

The c vacuum (2) can be any HFB state and does not need to be the bare vacuum for real particles. The freedom of this choice enables one to use the representations (1) for systems with both even and odd numbers of particles. An

appropriate vacuum of an odd system is, for instance, one particle excited from the bare vacuum. In order to get the Thouless matrices Z and Z' through the matrix inversion in Eq. (3) both states need to have sufficent overlaps with the chosen vacuum $|Z_0\rangle$ because it holds that [cf. Eq. (6)]

$$|\det U|^{1/2}=|\langle Z_0|Z\rangle|=|\mathcal{N}(\mathcal{Z})|.$$

Hence, the vacuum overlap of the considered states should be numerically well defined (say larger than 10^{-3}) to get stable results. A good choice for the vacuum $|Z_0\rangle$ is a state close enough to both states Z and Z'. Since HFB states are, in general, calculated with the help of parametrized mean field potentials one can simply construct a reasonably overlapping vacuum by appropriately shifting its field parameters relatively to Z and Z', e.g., by changing their potential shape or pairing gaps. This method also normally works for orthogonal states where $\langle Z|Z'\rangle=0$. The latter case happens, in particular, for a symmetry-forbidden bracket implying states of different parity or signature, etc. There one needs to have a vacuum that breaks the symmetry in question to get a finite overlap to both states Z and Z'. For cranking states of good but different signature, for instance, such an appropriate c vacuum is given by a signature-breaking *tilded* cranking state [8]. In practice, it is trivial to find a proper vacuum for two HFB states but the search for a common vacuum for a bundle of states might become more involved.

The Bloch-Messiah theorem [9] enables one to bring the state $|Z\rangle$ in a BCS-like canonical form

$$|Z\rangle=\Pi_i(u_i+v_i d_i^+ d_{\bar{i}}^+)|Z_0\rangle \tag{5}$$

reflecting the pair structure $(i,\bar{i})$ of HFB states and their simple BCS-like occupation amplitudes v_i and $u_i=\sqrt{1-v_i^2}$. With the careful choice of the vacuum state $|Z_0\rangle$ discussed above all u_i become nonzero as implicitly assumed in Eq. (3). Noting that $(d_i^+)^2=0$ we can obviously also write the product state (5) as a simple Thouless state

$$\begin{aligned}|Z\rangle&=(\Pi_i u_i)^{1/2}\Pi_j(1+v_j/u_j d_j^+ d_{\bar{j}}^+)|Z_0\rangle\\&=(\Pi_i u_i)^{1/2}e^{\Sigma z_{i\bar{i}} d_i^+ d_{\bar{i}}^+}|Z_0\rangle,\end{aligned} \tag{6}$$

which has rather convenient cross-diagonal amplitudes $Z_{i\bar{j}}=\delta_{j\bar{i}}v_i/u_i$ compared to the state (1). The great advantage of the canonical states (5), (6) is that they lead to a diagonal density matrix $\rho_{i'i}=\langle Z|d_i^+ d_{i'}|Z\rangle$ and a cross-diagonal pair tensor $\tau_{ii'}=\langle Z|d_i^+ d_{i'}^+|Z\rangle$. Hence, the calculation of expectation values is extremely simple when using the canonical form (6). The above Bloch-Messiah theorem, however, does not facilitate the calculation of the overlaps $\langle Z|Z'\rangle$ and related operator brackets. This is because each state $|Z\rangle$ has, in general, its own set $\{d_i,d_i^+\}$ of canonical operators. Hence, the canonical d operators of the bra vector $\langle Z|$ and those of the ket vector $|Z'\rangle$ cannot be supposed to be the same. The latter problem is solved[1] by constructing a particular set of *transitional* fermion operators $\{d_i,d_i^+\}$ below which indeed brings both states in the brackets $\langle Z|Z'\rangle$ simultaneously to the desired canonical form (6).

Before this general canonical basis transformation is explicitly given we derive some useful relations for complex $n\times n$ matrices A and B. Suppose A and B possess a symmetry with respect to transposition (symmetry or antisymmetry, similar relations exist for hermitean conjugation)

$$\tilde{A}=\alpha A,\quad \tilde{B}=\beta B,\quad \alpha,\beta=\pm 1,\quad \tilde{A}_{ij}\equiv A_{ji}. \tag{7}$$

Then we find for the product $E=AB$ the following identities:

$$EA=ABA=\alpha\beta A\tilde{E},\quad BE=BAB=\alpha\beta\tilde{E}B. \tag{8}$$

On the supposition that the product $E=AB$ can be diagonalized by a nonsingular transformation S, i.e.,

$$ES=Se,\quad e=e_i\delta_{ik}, \tag{9}$$

one obtains from Eq. (8)

$$\begin{aligned}&ea-\alpha\beta ae=0,\quad a\equiv S^{-1}A\tilde{S}^{-1},\\&be-\alpha\beta eb=0,\quad b\equiv\tilde{S}BS.\end{aligned} \tag{10}$$

Since e is diagonal the matrix elements of Eq. (10) read

$$(e_i-\alpha\beta e_k)a_{ik}=(e_i-\alpha\beta e_k)b_{ik}=0, \tag{11}$$

i.e., $a_{ik}=b_{ik}=0$ unless the eigenvalues obey the symmetry relation $e_i=\alpha\beta e_k$.

The above results are used to bring the antisymmetric Z matrices ($\alpha=\beta=-1$) to a canonical form. For this purpose the product matrix

$$E=Z^+Z', \tag{12}$$

well-known to be the key term [1,12] of the brackets $\langle Z|Z'\rangle$, must be diagonalized. Concerning the numerical performance of this basic diagonalization (9) we remark that since this method was proposed by Neergard and Wüst [12] no ill-conditioned cases were found in the numerous practical applications. Otherwise, by optionally changing the reference vacuum state $Z_0\rightarrow Z_1$ the Z matrices of the brackets can be modified as $Z\rightarrow\bar{Z}=(\tilde{U}_1Z+\tilde{V}_1)(\tilde{U}_1+\tilde{V}_1Z)^{-1}$ where (U_1,V_1) are the HFB amplitudes of the new vacuum Z_1. Therefore, with a proper choice of these amplitudes one can always remedy possible diagonalization problems.

The resulting matrix S [cf. Eq. (9)] yields the desired basis transformations of the fermion operators,

$$d_i^+=\sum S_{ik}^{-1}c_k^+,\quad d_i=\sum\tilde{S}_{ik}c_k, \tag{13}$$

$$c_k^+=\sum S_{ki}d_i^+,\quad c_k=\sum\tilde{S}_{ki}^{-1}d_i. \tag{14}$$

These transformations are canonical, i.e., they preserve the fermion commutation relations but they are in general nonunitary ones. In fact, the operators d_i^+ and d_i do form a biorthogonal fermion basis [11] but they can be manipulated as familiar Hermitean conjugated operators since the c

[1]An equivalent but a bit more lengthy derivation to the same subject was independently given by Burzynski and Dobaczewski [10].

vacuum (2) is simultaneously a d vacuum [cf. Eq. (13)]. In particular, the evaluation of contractions can be done in the same manner, i.e., by shifting the fermion operators left or right to the corresponding bra or ket vacuum.[2] Therefore, we do not change the notations in spite of the fact that only for $Z=Z'$ do the above fermion operators get Hermitean conjugated.

When transcribing the Thouless exponents of the bra and ket vector in Eq. (1) into the canonical basis (14) one obtains the following Z matrices:

$$Z^+ \rightarrow z^+ \equiv S^{-1} Z^+ \tilde{S}^{-1}, \quad Z' \rightarrow z' \equiv \tilde{S} Z' S. \tag{15}$$

The transformations conserve the antisymmetry and, in particular, the zero diagonal elements.

Neergard and Wüst [12] proved that the matrix $E = Z^+ Z'$ has twofold degenerate eigenvalues.[3] If we order the eigenvalues as well as eigenvectors in the matrix S into a sequence of degenerate pairs then according to Eq. (11) both matrices (15) get *simultaneously* the canonical 2×2 cross-diagonal block structure where each block implies only two nonzero elements $z_{i\bar{i}} = -z_{\bar{i}i}$ (here $i = \overline{\bar{i}} - 1 = 1,3,\ldots,2n-1$). Thus, one becomes

$$z_{ij} = z_{i\bar{i}}\delta_{j\bar{i}}, \quad z'_{ij} = z'_{i\bar{i}}\delta_{j\bar{i}}, \quad e_i = e_{\bar{i}} = z^*_{i\bar{i}} z'_{\bar{i}i} \tag{16}$$

where for definiteness we introduced the notation i and $\bar{i}$ for the pair of states belonging to degenerate eigenvalues $e_i = e_{\bar{i}}$. Accordingly, we shall refer in what follows to the pair index $i = 1,3,\ldots,2n-1$ for labeling the corresponding pairs (12), (34), ... Hence, in analogy to Eq. (6) the canonical Thouless representation of both the bra and the ket vector, Eq. (1), is

$$\langle Z| = \mathcal{N}^*(\mathcal{Z}) \langle Z_0| e^{\Sigma z^*_{i\bar{i}} d_{\bar{i}} d_i} = \mathcal{N}^*(\mathcal{Z}) \langle Z_0| \Pi_i (1 + z^*_{i\bar{i}} d_{\bar{i}} d_i),$$

$$|Z'\rangle = \mathcal{N}(\mathcal{Z}') e^{\Sigma z'_{i\bar{i}} d^+_i d^+_{\bar{i}}} |Z_0\rangle = \mathcal{N}(\mathcal{Z}') \Pi_i (1 + z'_{i\bar{i}} d^+_i d^+_{\bar{i}}) |Z_0\rangle. \tag{17}$$

Again we emphasize that the bra vector is formally obtained by Hermitean conjugation but, in general, the amplitudes $z^*_{i\bar{i}}$ belong to the inverse transformation (14).

Now, the simple canonical product form (17) can be exploited for any bracket. The basic quantity is the overlap bracket $\langle Z|Z'\rangle$. By using the pair-diagonal structure of z^+ and z', Eq. (16), one obtains

$$\begin{aligned}
\langle Z|Z'\rangle &\equiv D(z^*, z') \\
&= \mathcal{N}^*(\mathcal{Z}) \mathcal{N}(\mathcal{Z}') \langle Z_0| \Pi_{ij} (1 + z^*_{i\bar{i}} d_{\bar{i}} d_i) \\
&\quad \times (1 + z'_{j\bar{j}} d^+_j d^+_{\bar{j}}) |Z_0\rangle \\
&= \mathcal{N}^*(\mathcal{Z}) \mathcal{N}(\mathcal{Z}') \Pi_i (1 + z^*_{i\bar{i}} z'_{\bar{i}i}) \\
&= \mathcal{N}^*(\mathcal{Z}) \mathcal{N}(\mathcal{Z}') \Pi_i (1 + e_i).
\end{aligned} \tag{18}$$

Note that the above expression provides directly[4] the phase of the overlap $\langle Z|Z'\rangle$ which is not given by Onishi's determinantal expression [1,5]. The knowledge of the correct overlap phases is of crucial importance [12] for the performance of GCM calculations when superimposing sets of nonorthogonal quasiparticle states.

III. OPERATOR BRACKETS

The operator brackets can be easily calculated using a similar blocking technique as that applied in Ref. [13]. We define blocked canonical states as

$$|Z', j_1, j_2, \ldots\rangle \equiv \mathcal{N}(\mathcal{Z}') \Pi_{i \neq j_1, j_2, \ldots} (1 + z'_{i\bar{i}} d^+_i d^+_{\bar{i}}) |Z_0\rangle \tag{19}$$

which imply the blocked orbitals $(j_1, \bar{j}_1), (j_2, \bar{j}_2), \ldots$. Notice the useful properties

$$d_j |Z', j\rangle = \langle Z, j| d^+_j = 0. \tag{20}$$

and the identities from Eqs. (17)

$$\begin{aligned}
&\langle Z| d^+_j = \langle Z, j| d_{\bar{j}} z^*_{j\bar{j}}, \quad d_j |Z'\rangle = z'_{j\bar{j}} d^+_{\bar{j}} |Z', j\rangle, \\
&\langle Z| d_j = \langle Z, j| d_j, \quad d^+_j |Z'\rangle = d^+_j |Z', j\rangle.
\end{aligned} \tag{21}$$

By appropriate replacements $d \rightleftharpoons d^+$ and the subsequent shifting of d operators from the bra to the ket vector and vice versa the operators reduce to c numbers and blocked overlaps. This method is demonstrated for the pair operator $\tau = d^+_j d^+_{j'}$:

$$\begin{aligned}
\langle Z| d^+_j d^+_{j'} |Z'\rangle &= \langle Z, j| d_{\bar{j}} z^*_{j\bar{j}} d^+_{j'} |Z'\rangle \\
&= \langle Z, j| z^*_{j\bar{j}} (\delta_{\bar{j}j'} - d^+_{j'} d^+_j z'_{\bar{j}j}) |Z', j\rangle \\
&= z^*_{j\bar{j}} \delta_{\bar{j}j'} \langle Z, j| Z', j\rangle \\
&\equiv \delta_{\bar{j}j'} z^*_{j\bar{j}} D_j(z^*, z')
\end{aligned} \tag{22}$$

where $D_j(z^*, z')$ analogously to Eq. (18) denotes the j-blocked overlap. Treating the density operator $\rho(j', j) = d^+_j d_{j'}$ in the same way gives

$$\langle Z| d^+_j d_{j'} |Z'\rangle = \delta_{jj'} e_j D_j(z^*, z'). \tag{23}$$

One recognizes that the transitional density ρ and the pair density τ get generally diagonal and cross diagonal, respectively, as in the case $Z=Z'$. Hence, the above expressions are much simpler than the ones in the literature [1].

There is another important advantage: Eqs. (22),(23) encounter no problem for zero overlap, i.e., $\langle Z|Z'\rangle = 0$, which to the formulas in the literature do. According to Eq. (18) a zero overlap appears only if one or more factors $(1+e_i)$ in the product vanish or equivalently if at least one of the eigenvalues e_i of the matrix E, Eq. (12), satisfies $e_i = -1$. Let us suppose the term $i = i_0$ belongs to a zero factor. Then, the

[2]The freedom in choosing the normalization of the eigenvectors S, Eq. (7), has no effect to the physical matrix elements.

[3]Accidental higher degeneracies do not change the conclusions.

[4]This phase is the same as that obtained by Neergard and Wüst [12].

brackets (22),(23) of the density and pair matrix produce only for the term $j=i_0$ a nonzero value when the operator takes off the zero factor from the overlap product. The same arguments apply for the two-body matrix elements. For completeness we give the resulting formulas for the two-body operator brackets involving four fermion operators,

$$\begin{aligned}\langle Z|d_i^+ d_{i'}^+ d_j^+ d_{j'}^+|Z'\rangle = & z^*_{i\bar{i}} z'_{j\bar{j}} D_{ij}(z^*,z')\,\delta_{i\bar{i}'}\delta_{j\bar{j}'} \\ & - z^*_{i\bar{i}} z'_{i'\bar{i}'} D_{ii'}(z^*,z')\,\delta_{i\bar{j}}\delta_{i'\bar{j}'} \\ & + z^*_{i\bar{i}} z'_{i'\bar{i}'} D_{i'j'}(z^*,z')\,\delta_{i\bar{j}'}\delta_{i'\bar{j}},\end{aligned} \tag{24}$$

$$\begin{aligned}\langle Z|d_i^+ d_{i'}^+ d_j^+ d_{j'}|Z'\rangle = & z^*_{i\bar{i}} e_j D_{ij}(z^*,z')\,\delta_{i\bar{i}'}\delta_{jj'} \\ & - z^*_{i\bar{i}} e_{i'} D_{ii'}(z^*,z')\,\delta_{i\bar{j}}\delta_{i'j'} \\ & + z^*_{i'\bar{i}'} e_i D_{ii'}(z^*,z')\,\delta_{ij'}\delta_{i'\bar{j}},\end{aligned} \tag{25}$$

$$\begin{aligned}\langle Z|d_i^+ d_{i'}^+ d_j d_{j'}|Z'\rangle = & z^*_{i\bar{i}} z'_{j'\bar{j}'} D_{ij}(z^*,z')\,\delta_{i\bar{i}'}\delta_{j\bar{j}'} \\ & + (\delta_{ij'}\delta_{i'j} - \delta_{ij}\delta_{i'j'}) \\ & \times e_i[D_i(z^*,z') - D_{ii'}(z^*,z')].\end{aligned} \tag{26}$$

Here the analogous notation D_{ij} for a doubly reduced overlap product [cf. Eq. (18)] is used. Note that $D_{ii}=D_{\bar{i}\bar{i}}=0$. The above reduction technique takes fully care of the antisymmetrization of the two body matrix elements.

One realizes that all brackets reduce generally to paired indices and a factorized form which is easy to evaluate. This implies not only a formal simplification but the numerical effort is considerably lowered too. In Eq. (24), for instance, from all the $\binom{n}{4}$ terms on the left-hand side only $\binom{n/2}{2}$ nonzero terms survive to be calculated on the right-hand side. This means that the above-mentioned dimension is reduced by approximately a factor $\frac{1}{10}n^2$ due the pairwise interaction in this representation. Considering, for example, a quartic interaction term one has

$$\begin{aligned}\langle Z|\hat{H}^{40}|Z'\rangle \equiv & \langle Z|\sum_{i,i',j,j'} H^{40}_{ii'jj'} d_i^+ d_{i'}^+ d_j^+ d_{j'}^+|Z'\rangle \\ = & \sum_{i,j} (H^{40}_{i\bar{i}j\bar{j}} - H^{40}_{ij\bar{i}\bar{j}} + H^{40}_{ij\bar{j}\bar{i}}) z^*_{i\bar{i}} z'_{j\bar{j}} D_{ij}(z^*,z').\end{aligned} \tag{27}$$

Due to the transitional canonical basis only the paired part of the interaction matrix element contributes.

IV. POLE TERMS OF WICK CONTRACTIONS

The common method used to evaluate the operator brackets $\langle Z|F|Z'\rangle$ between nonorthogonal HFB states $Z\neq Z'$ is the generalized Wick theorem derived by Balian and Bloch [11]. Defining the generalized contractions as

$$\langle c_i^+ c_k^+\rangle \equiv \frac{\langle Z|c_i^+ c_k^+|Z'\rangle}{\langle Z|Z'\rangle}, \quad \langle c_i c_k\rangle \equiv \frac{\langle Z|c_i c_k|Z'\rangle}{\langle Z|Z'\rangle},$$

$$\langle c_i^+ c_k\rangle \equiv \frac{\langle Z|c_i^+ c_k|Z'\rangle}{\langle Z|Z'\rangle} \tag{28}$$

one can apply the Wick theorem as usual. Using previous methods [1,6] the above division $\langle Z|Z'\rangle$ in Eq. (28) is realized by inverting the corresponding overlap matrix and, therefore, it fails for orthogonal states with zero overlap. This numerically dangerous behavior of the generalized Wick expansion is completely avoided when applying the above canonical representation (22),(23). As discussed before the only difference between brackets of the orthogonal states is the fact that any nonzero contributions remain only if the existing zero factors $(1+e_i)$ in the overlap product (16) are ''bridged'' by the operator which leads to the reduced overlaps in Eqs. (21)–(27). This is because the essential effect of any n-body operator is just to block n overlap factors for those terms $j_1,\ldots,j_n$ on which it is acting. Thus, the canonical form of operator brackets behaves as a well-defined smooth function of the overlap value.

Unfortunately, the zero denominator in the generalized Wick expansion (28) is causing problems so far not noticed in the literature. It is a common practice to calculate the *diagonal* expectation values of the multipole-multipole interaction in the factorization approximation, i.e., by neglecting the exchange contributions. This approximation may lead to severe errors in the GCM calculations when nondiagonal matrix elements of such factorized forces also come into play, such as, e.g., in the self-consistent pairing plus quadrupole model [14]. A typical case in this respect is the monopole pairing force

$$V=P^+P, \quad P^+=\frac{1}{4}\sum_k c_k^+ c_{-k}^+. \tag{29}$$

According to the factorization approximation one takes into account only the direct term in the Wick contraction of the pairing force, i.e.,

$$\langle Z|V|Z'\rangle \approx |\frac{\langle Z|P^+|Z'\rangle}{\langle Z|Z'\rangle}|^2 \langle Z|Z'\rangle. \tag{30}$$

The bracket is in the convenient squared form of the pair operator contraction multiplied by the overlap. Apparently, in the limit $\langle Z|Z'\rangle\to 0$ the total matrix element is diverging because of the second order pole in the square. This is an essential contrast to the case of one-body operators which imply only a simple pole canceled by the overlap.

Considering the same case in the canonical basis (14) one obtains schematically

$$P^+=\sum_{ij} p_{ij}\, d_i^+ d_j^+, \quad P=\sum_{km} \bar{p}_{km} d_m d_k. \tag{31}$$

Substituting the canonical expressions (18), (22), (23) into the Wick contractions (28) the complete pairing matrix element reads

$$\langle Z|V|Z'\rangle=\sum_{ijkm}\bar{p}_{ij}\bar{p}_{km}\left(\frac{z^{*}_{i\bar{i}}\delta_{j\bar{i}}}{1+e_i}\frac{z'_{k\bar{k}}\delta_{m\bar{k}}}{1+e_k}-2\frac{e_i\delta_{im}}{1+e_i}\frac{e_k\delta_{jk}}{1+e_k}\right)\times\langle Z|Z'\rangle, \tag{32}$$

where the direct and the exchange terms appear in the bracket. Obviously, all denominators referring to different pairs $(i,\bar{i})\neq(k,\bar{k})$ cancel out with corresponding factors in the overlap product $\langle Z|Z'\rangle\propto\Pi_i(1+e_i)$, Eq. (18). However, for the contribution $(i,\bar{i})=(k,\bar{k})$ there remains in both the direct and exchange terms a first order singularity at $(1+e_i)\rightarrow 0$, i.e., for zero overlap. Remembering the relation $e_i=z^{*}_{i\bar{i}}z'_{i\bar{i}}$, Eq. (16), those odd terms in the bracket can be summed to

$$\langle Z|V|Z'\rangle_{(1+e_i)\rightarrow 0}\approx 4\bar{p}_{i\bar{i}}\bar{p}_{\bar{i}i}\frac{(z^{*}_{i\bar{i}}z'_{i\bar{i}}+e_i^2)}{(1+e_i)^2}\langle Z|Z'\rangle$$

$$=4\bar{p}_{i\bar{i}}\bar{p}_{\bar{i}i}\frac{e_i}{1+e_i}\langle Z|Z'\rangle. \tag{33}$$

The first order pole drops exactly when multiplied by the overlap. This is the result expected from the above expression (26) containing the pole-free reduced overlaps. Hence, when calculating any interaction matrix elements between nonorthogonal HFB states one cannot neglect the exchange contribution arising due to the Wick contractions.

The same problem arises in the ordinary treatment of the particle number projection. The essential two body matrix element entering the projection integral is

$$\int_0^{2\pi}d\varphi\langle\mathrm{HFB}|Ve^{-iN\varphi}|\mathrm{HFB}\rangle, \tag{34}$$

where N is the particle number operator and φ is the angle of the gauge rotation. When neglecting the exchange contribution the remaining pole is the canonical denominator

$$(u_i^2+v_i^2e^{-2i\varphi}) \tag{35}$$

which becomes zero for $u_i\approx v_i$ at $\varphi=\pi/2$, i.e., for quasiparticle orbitals close to the Fermi level. The existing standard codes for calculating mean field properties should care for the exchange term when calculating particle number projected energies. Without precaution the dangerous pole (35) may originate strange jumps in the calculated potential energy surfaces when changing the input parameters or configurations and approaching by chance the values $u_i\approx v_i$.

Our calculations [15] have shown that the neglect of the exchange contribution leads in other cases to a violation of the rotational symmetry of the interaction. Thus, for instance, the factorized matrix element of the quadrupole interaction between states of opposite signature becomes nonzero in contradiction to the required symmetry.

V. CONCLUSIONS

The above tools permit an effective treatment of the large amplitude collective motion when choosing an appropriate bundle of HFB mean field states as the basis for the GCM diagonalizations. Thereby, the mean field parameters $p=\varepsilon_2,\varepsilon_4,\Delta,\ldots$, for shaping the potential well and pairing properties supply a natural grid of variables for describing the motion on an energy surface:

$$E(p)=H[z^{*}(p),z(p)]=\frac{\langle Z(p)|H|Z(p)\rangle}{\langle Z(p)|Z(p)\rangle}.$$

With the above developed formalism one can construct the GCM Hamiltonian kernel $H[z^{*}(p),z'(p')]$ and overlap function $D[z^{*}(p),z'(p')]$ in a straightforward manner. Following the same spirit of previous GCM studies [4] we expect that the common treatment of the energetically lowest energy surface $E(p)$ might not be sufficient. At parameter points p where an avoided level crossing signals a hidden configuration change, the approaching excited energy surface $E^{\mathrm{ex}}(p)$ needs to be included in order to describe the relevant configuration mixing. In this way an extended subspace can be formed implying both discrete quasiparticle excitations via ''rapid'' configuration changes as well as ''soft'' modes, the latter being related to more smooth variations of mean field parameters outside their self-consistent values. The performance of these more ambitious calculations is considerably facilitated by the techniques presented above.

It was shown that a solid calculation of general matrix elements of the two body interaction must include both direct and the exchange contributions in order to exclude divergencies. Thus, the familiar factorization of multipole forces can only be applied for diagonal terms, or else possible pole contributions may cause severe errors. Similar problems occur in the particle number projection.

The first calculations [15] with the developed technique concerning the signature bifurcation of a rotational band into two signature branches are under way. In this approach one meets the above-mentioned situation where the inclusion of a quasiparticle excitation is necessary in order to describe the signature changing magnetic transitions.

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