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Microscopic Approach to the Generator Coordinate Method*

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Abstract

In this paper, we solve different theoretical problems associated with the calculation of the kernel occurring in the Hill-Wheeler integral equations within the framework of generator coordinate method. In particular, we extend the Wick's theorem to non-orthogonal Bogoliubov states. Expressions for the overlap between Bogoliubov states and for the generalised density matrix are also derived. These expressions are valid even when using an incomplete basis, as in the case of actual calculations. Finally, the Hill-Wheeler formalism is developed for a finite range interaction and the Skyrme force, and evaluated for the latter.

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1 Introduction

About fifteen years ago, the ability of the density-dependent Hartree-Fock aprroximation[1,2] to describe reasonably the mean field in nuclei was demonstrated by the accuracy of its predictions in several nuclear structure calculations. This success provided the incentive to go beyond the static description and attack on theoretical grounds the problem of finding coherent microscopic descriptions for some specific collective phenomenon in nuclei. By "specific" we mean those phenomenon whose dynamics is expected to depend essentially on the time evolution of the mean field. As an example, let us recall here that various giant resonances are satisfactorily described by assuming that they are associated with small oscillations of the mean field. As is well known, the linearization of the time-dependent Hartree-Fock theory with respect to these small oscillations provide the microscopic description for their time evolution (*e.g.* the RPA approximation).

In this paper, we are interested in large amplitude motions such as those encountered in fission or in the description of low-lying excited states of soft nuclei. The derivation of a microscopic theory adapted to this case is not as straightforward as in the case of giant resonances. The time-dependent Hartree-Fock approximation with the adiabatic hypothesis (ATDHF) can again be the foundation for the theoretical formulation of large amplitude motions. In this approximation, Baranger and Veneroni[3] derived a set of coupled equations whose resolution would, in principle, provide the collective paths and the mass parameters. With this information, it is possible to construct the semi-classical collective Hamiltonian and to quantize it.

In Villars'[4] approach to large amplitude motions, the collective Hamiltonian is extracted from the kernel of the Hill-Wheeler theory[5] by a simple expansion around the locality in the collective variables. As a result, the collective potential is corrected by some zero-point energies. In contrast to the ATDHF theory which is semi-classical, Villars' procedure is quantized to start with and gives a collective Hamiltonian which is automatically and uniquely quantized.

These theoretical works have certainly contributed towards a coherent foundation to a previous phenomenological collective model, as proposed by the Copenhagen group[6]. However, a couple of remarks regarding these theories are in order. First, it is clear that the resolution of the set of coupled equations would require a considerable amount of effort.

Second, there is no general proof of the existence of their solutions. That is why in actual applications, the collective paths are generally not determined from these equations. In order to bypass these difficulties, one has recourse to the mean-field approximation with additional external fields. By varying their strength, one can deform the mean field and generate a set of Hartree-Fock solutions which can be labelled by the mean values of the operators associated with these external fields. Somehow these mean values will define a set of collective variables. The choice of the fields will depend on the type of processes we want to describe. For instance in fission[7], it seems sufficient to consider the following collective variables:

1. q_{20}: quadrupole deformation (stretching),
2. q_{30}: octupole deformation (left-right asymmetry),
3. q_{40}: hexadecapole deformation (necking).

Evidently, pairing correlations can be included in the description by using the Hartree-Fock-Bogoliubov[1,8] approximation instead of only Hartree-Fock. The dynamics of fission in this collective space is then described with the microscopic collective Hamiltonian.

Our motivation in this paper is to go, among other things, beyond the collective model and solve the full Hill-Wheeler[5] equations. We have in mind further applications to the predictions of possible shape isomeric states, if they exist, and on their characteristics. The paper is organized as follows. In Sec.2, we derive, for completeness, the Hill-Wheeler equations. Sections 3, 4 and 5 are devoted to the presentation of all the technical aspects which are necessary to calculate the kernel occurring in the Hill-Wheeler integral equations. In Secs.6 and 7, we apply the formalism to non-zero finite range interaction and to the Skyrme interaction, respectively. The paper is concluded in Sec.8.

2 Derivation of the Hill-Wheeler equations

In the generator coordinate method (GCM)[9], the stationary wave function describing a system is chosen in the factorized form

$$| \Psi >= \int d\{q\} \chi(\{q\}) \, | \Phi_{\{q\}} >, \tag{1}$$

where $\{q\}$ denotes a set of "collective variables" — the so-called generator coordinates, and the function $\mid \Phi_{\{q\}} >$ are supposed to take into account the internal degrees of freedom. In the Hill-Wheeler theory[5], it is assumed that the $\mid \Phi_{\{q\}} >$ are predetermined and only the $\chi(\{q\})$ are the unknowns. As long as we are interested in the low-lying excited states, this approximation can be justified by arguing that the collective oscillations are much slower than the internal motion. Thus applying the variational principle to $\mid \Psi >$ which states that the total energy $< \Psi \mid \mathcal{H} \mid \Psi > / < \Psi \mid \Psi >$ be stationary with respect to variations in the functional space spanned by the function χ, we obtain the following system of equations:

$$\int \mathcal{H}(q,q')\chi(q')dq' = E \int I(q,q')\chi(q')dq', \tag{2}$$

where $I(q,q')$ is the overlap between the states Φ_q and $\Phi_{q'}$, *i.e.* $I(q,q') =< \Phi_q \mid \Phi_{q'} >$. (For the sake of simplicity, we shall henceforth use the notation q instead of $\{q\}$. The notations and conventions used in this paper are outlined in Appendix A.) By defining a set of new functions as

$$\bar{\chi}(q) = \int I^{1/2}(q,q')\chi(q')dq', \tag{3}$$

we can rewrite Eq.(2) as

$$\int K(q,q')\bar{\chi}(q')dq' = E\bar{\chi}(q), \tag{4}$$

which is in the form of the familiar Hill-Wheeler[5] type integral equations. The kernel $K(q,q')$ is given by the expression

$$K(q,q') = \int I^{-1/2}(q,q')\mathcal{H}(q',q''')I^{-1/2}(q''',q'')dq''dq''', \tag{5}$$

where $\mathcal{H}(q,q')$ are the matrix elements of a given effective Hamiltonian, *i.e.* $\mathcal{H}(q,q') = < \Phi_q \mid \mathcal{H} \mid \Phi_{q'} >$. The kernel K being Hermitian, the resolution of Eq.(4) is a simple eigenvalue problem

$$\int K(q,q')\bar{\chi}_n(q')dq' = E_n\bar{\chi}_n(q), \tag{6}$$

with the eigenfunctions normalized according to

$$\int \bar{\chi}_n(q)\bar{\chi}_{n'}(q)dq = \delta_{nn'}. \tag{7}$$

This guarantees the normalization of $\mid \Psi >$, defined in Eq.(1), to be unity. The eigenvalues of Eq.(6) can be interpreted as those of the ground state (lowest E_n), the first (collective) excited state (next higher E_n), and so on. The wave functions of these states, according to Eq.(1), are

$$| \Psi_n >= \int \chi_n(q) \mid \Phi_q > dq, \tag{8}$$

where

$$\chi_n(q) = \int I^{-1/2}(q,q') \tilde{\chi}_n(q') dq'. \tag{9}$$

It remains to be specified how we choose the function $| \Phi_q >$ and define the collective variables. In our approach, the set of functions $| \Phi_q >$ are the independent quasi-particle (q.p.) states obtained by means of the Hartree-Fock + BCS theory[10-12], or more generally, by the Hartree-Fock-Bogoliubov (HFB) method[1,8] with several external constraining fields. For instance, the external fields can be some low order multipolar one-body operator $\hat{Q}_{lm}$. Then the set of collective variables $\{q_{lm}\}$ are the mean values

$$q_{lm} =< \Phi_q \mid \hat{Q}_{lm} \mid \Phi_q > . \tag{10}$$

It is worth pointing out that our approach is fully consistent and microscopic in the sense that the mean-field, the pairing field and the kernel of the Hill-Wheeler equations are calculated with the same Hamiltonian, the only input being the effective interaction between nucleons and the choice of the constraining fields. In the next section, we develop the formalism for the calculation of the kernel when using independent q.p. states.

3 Calculation of the kernel $K(q,q')$

For the sake of completeness, we present here an extension of Wick's theorem[13] to the case of non-orthogonal independent q.p. states. This theorem will allow us to express in terms of simple contractions the expectation values of the one- and two-body operators occurring in the definition of the kernel $K(q,q')$ in Eq.(5). We mention that the Wick's theorem for non-orthogonal Slater determinants has been worked out by Blaizot and Ripka[14].

3.1 Wick's theorem

The extension of Wick's theorem is readily established by using the Bloch-Messiah theorem[15] concerning the decomposition of the most general Bogoliubov transformation[16]. Let us recall briefly that a general Bogoliubov transformation maps a given set of creation and annihilation operators $(a^\dagger, a)$ onto a new set $(\eta^\dagger, \eta)$ associated with the creation and annihilation operators of the so-called "quasi-particles". We write the transformation in the form

$$\begin{pmatrix} \eta^\dagger \\ \eta \end{pmatrix} = \begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix} \begin{pmatrix} a^\dagger \\ a \end{pmatrix} = B \begin{pmatrix} a^\dagger \\ a \end{pmatrix}. \tag{11}$$

The transformation B has to be unitary ($BB^\dagger = B^\dagger B$) in order to preserve the anticommutation relations between the fermion operators $(a^\dagger, a)$. Also, to avoid writing explicitly the quantum labels, we use compact notations where U and V represent block matrices. Thus,

$$\eta^\dagger_\alpha = \sum_\beta (u_{\alpha\beta} a^\dagger_\beta + v_{\alpha\beta} a_\beta), \tag{12}$$

$$\eta_\alpha = \sum_\beta (u^*_{\alpha\beta} a_\beta + v^*_{\alpha\beta} a^\dagger_\beta) \tag{13}$$

The Bloch-Messiah theorem stipulates that the transformation given by Eq.(11) can be factorized into product of three transformations. More specifically, the first transformation just rotates $a^\dagger$ and a separately and defines new operators $b^\dagger$ and b: $b^\dagger = Da^\dagger$ and $b = Da$. D is real and it diagonalizes the matrix $\tilde{V}V$. The second transformation is of the BCS type and defines the q.p. operators $\xi^\dagger$ and ξ as

$$\begin{pmatrix} \xi^\dagger_i \\ \xi_{\bar{i}} \end{pmatrix} = \begin{pmatrix} u_i & -v_i \\ v_i & u_i \end{pmatrix} \begin{pmatrix} b^\dagger_i \\ b_{\bar{i}} \end{pmatrix}. \tag{14}$$

In the above equation, the transformation matrix is of the order 2×2 and $\mid i >$ and $\mid \bar{i} >$ denote states which allow the pairing tensors to be cast in the canonical form. However, in all the applications we present in this paper, $\mid \bar{i} >$ represents the time-reversed state of $\mid i >$. Furthermore, the ratio v_i/u_i is simply related to the eigenvalues of $\tilde{V}V$. Finally, the third transformation rotates $\xi^\dagger$ and ξ and defines the q.p. operators $\eta^\dagger$ and η according to the relations $\eta^\dagger = C\xi^\dagger$ and $\eta = C\xi$.

This decomposition of the most general Bogoliubov transformation allows us to express the vacuum $\mid \tilde{0} >$ of the q.p. operator η ($\eta \mid \tilde{0} >= 0$) in terms of the vacuum $\mid 0 >$ of the operator a ($a \mid 0 >= 0$). The relationship is given by

$$\mid \tilde{0} >=< 0 \mid \tilde{0} > e^X \mid 0 >, \tag{15}$$

where

$$X = \sum_{i>} \frac{v_i}{u_i} b^\dagger_i b^\dagger_{\bar{i}}. \tag{16}$$

(The notation $i_>$ implies that the time-reversed states $|\,\bar{i}\,>$ are not included in the summation.)

It is now quite straightforward to establish the connection between two independent q.p. states $|\,\Phi_q\,>$ and $|\,\Phi_{q'}\,>$, as defined in the previous section, since they are both by definition the vacuum of two q.p. sets η^q and $\eta^{q'}$ which are related according to the Bogoliubov transformation

$$\begin{pmatrix} \eta^{q'\dagger} \\ \eta^{q'} \end{pmatrix} = B^{q q'} \begin{pmatrix} \eta^{q\dagger} \\ \eta^{q} \end{pmatrix} = B^{q'} B^{q} \begin{pmatrix} \eta^{q\dagger} \\ \eta^{q} \end{pmatrix}. \tag{17}$$

In fact, by using the same arguments that led to Eq.(15), we find that

$$|\,\Phi_{q'}\,> = <\,\Phi_q\,|\,\Phi_{q'}\,>\, e^{X_{q'q}}\,|\,\Phi_q\,>, \tag{18}$$

where

$$X_{q'q} = \sum_{i_>} \frac{v_i^{q'q}}{u_i^{q'q}} b_i^{q\dagger} \bar{b}_i^{q\dagger}, \tag{19}$$

and $b_i^q\,|\,\Phi_q\,> = 0\;\forall\, i$.

Equation (18) makes it much easier to calculate any general contraction of the form

$$<\,\Phi_q\,|\,b_{i_1}^{q\dagger}\cdots b_{i_m}^{q\dagger} b_{j_1}^{q}\cdots b_{j_m}^{q}\,|\,\Phi_{q'}\,>\,. \tag{20}$$

Using Eq.(18) and inserting $e^{X_{q'q}} e^{-X_{q'q}}$ as many times as necessary, this contraction becomes

$$<\,\Phi_q\,|\,\Phi_{q'}\,><\,\Phi_q\,|\,\bar{b}_{i_1}^{q\dagger}\cdots\bar{b}_{i_m}^{q\dagger}\bar{b}_{j_1}^{q}\cdots\bar{b}_{j_m}^{q}\,|\,\Phi_q\,>, \tag{21}$$

where we have used the fact that $<\,\Phi_q\,|\,e^{X_{q'q}} = <\,\Phi_q\,|$. The new operators $\bar{b}^{q\dagger}$ and $\bar{b}^q$ are defined as

$$\bar{b}^{q\dagger} = e^{-X_{q'q}} b^{q\dagger} e^{X_{q'q}}, \tag{22}$$

$$\bar{b}^{q} = e^{-X_{q'q}} b^{q} e^{X_{q'q}}, \tag{23}$$

and obey the same commutation relations as b^q and $b^{q\dagger}$. Consequently, we can use Wick's theorem and express contraction (20) in terms of the simple contractions

$$<\,\Phi_q\,|\,\Phi_{q'}\,>^{-1} <\,\Phi_q\,|\,b^{q\dagger} b^{q}\,|\,\Phi_{q'}\,>, \tag{24}$$

$$<\,\Phi_q\,|\,\Phi_{q'}\,>^{-1} <\,\Phi_q\,|\,b^{q\dagger} b^{q\dagger}\,|\,\Phi_{q'}\,>, \tag{25}$$

$$< \Phi_q \mid \Phi_{q'} >^{-1} < \Phi_q \mid \delta^q b^q \mid \Phi_{q'} > . \tag{26}$$

The usual Wick's theorem still applies under the condition that we use the contractions defined in (24)-(26) and multiply by the overlap $< \Phi_q \mid \Phi_{q'} >$ the final result. As an example, we show how to use this new theorem for the contraction occurring in a two-body operator:

$$\begin{aligned} < \Phi_q \mid b^{q\dagger}_\alpha b^{q\dagger}_\beta b^q_\delta b^q_\gamma \mid \Phi_{q'} > = & < \Phi_q \mid \Phi_{q'} > \\ & [\frac{< \Phi_q \mid b^{q\dagger}_\alpha b^q_\iota \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >} \frac{< \Phi_q \mid b^{q\dagger}_\beta b^q_\delta \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >} \\ & - \frac{< \Phi_q \mid b^{q\dagger}_\alpha b^q_\delta \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >} \frac{< \Phi_q \mid b^{q\dagger}_\beta b^q_\gamma \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >} \\ & + \frac{< \Phi_q \mid b^{q\dagger}_\iota b^{q\dagger}_\beta \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >} \frac{< \Phi_q \mid b^q_\delta b^q_\gamma \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >}]. \end{aligned} \tag{27}$$

In the next subsection, we calculate by a direct method the overlap $< \Phi_q \mid \Phi_{q'} >$ and the elements of the generalized density matrix that appear in the contractions given by (24)-(26). They are needed for the calculation of the kernel.

3.2 Evaluation of the overlap and the elements of the generalized density matrices

In order to calculate the overlap, we define the quantity

$$R(x) = < 0 \mid e^{xX^\dagger_q} e^{X_{q'}} \mid 0 > \equiv \frac{< \Phi_q ; x \mid \Phi_{q'} >}{< 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >}, \tag{28}$$

where x is some parameter. According to Eq.(15), we can express the independent q.p. state $\mid \Phi_q >$ in the form

$$\mid \Phi_q > = < 0 \mid \Phi_q > e^{X_q} \mid 0 > . \tag{29}$$

Consequently, the overlap is simply related to $R(x)$ by

$$< \Phi_q \mid \Phi_{q'} > = < 0 \mid \Phi_{q'} >< \Phi_q \mid 0 > R(1). \tag{30}$$

For convenience, we set

$$\tan \theta^q_i = \frac{v^q_i}{u^q_i}, \tag{31}$$

so that X_q becomes

$$X_q = \sum_{i>} \tan\theta_i^q b_i^{q\dagger} b_i^q. \tag{32}$$

We now show that $R(x)$ satisfies a simple differential equation by calculating the first derivative $R'(x)$ with respect to x. Starting from Eq.(28), we immediately find

$$R'(x) = tr[\tan\theta^q A(x)], \tag{33}$$

where the elements of the matrix $A(x)$ are

$$A_{ij}(x) = \frac{< \Phi_q, x \mid b_j^q b_i^q \mid \Phi_{q'} >}{< 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >}. \tag{34}$$

As shown in Appendix B, the evaluation of $A(x)$ necessitates the introduction of another matrix $B(x)$ with elements

$$B_{ij}(x) = \frac{< \Phi_q, x \mid b_j^{q'\dagger} b_i^{q'\dagger} \mid \Phi_{q'} >}{< 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >}, \tag{35}$$

and to solve the set of coupled equations

$$A(x) = \tau^{qq'} \tan\theta^{q'} \tau^{qq'\dagger} R(x) - \tau^{qq'} \tan\theta^{q'} B(x) \tan\theta^{q'} \tau^{qq'\dagger}, \tag{36}$$

$$B(x) = x\tau^{qq'\dagger} \tan\theta^q \tau^{qq'} R(x) - x^2 \tau^{qq'\dagger} \tan\theta^q A(x) \tan\theta^q \tau^{qq'}, \tag{37}$$

where $\tau^{qq'} = \{b^{q'\dagger}, b^q\}$. (See Appendix A.)

We note that the matrices $A(x)$ and $B(x)$ enter also in the calculation of the elements of the generalized density matrix since, as shown in Appendix C, we have the relations

$$< \Phi_q \mid b_i^{q'\dagger} b_j^{q'} \mid \Phi_{q'} >= \tan\theta_j^{q'} B_{ji} < 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >, \tag{38}$$

$$< \Phi_q \mid b_i^{q'} b_j^{q'} \mid \Phi_{q'} >= - < \Phi_q \mid \Phi_{q'} > \tan\theta_i^{q'} \delta_{ij}$$

$$+ \tan\theta_j^{q'} \tan\theta_i^{q'} B_{ij} < 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >, \tag{39}$$

$$< \Phi_q \mid b_i^{q'\dagger} b_j^{q'\dagger} \mid \Phi_{q'} >= B_{ji} < 0 \mid \Phi_{q'} >< \Phi_q \mid 0 > . \tag{40}$$

Due to the structure of $\mid \Phi_q >$ and $\mid \Phi_{q'} >$, the matrix elements $< \Phi_q \mid b_i^{q'\dagger} b_j^{q'} \mid \Phi_{q'} >$, $< \Phi_q \mid b_i^{q'} b_j^{q'} \mid \Phi_{q'} >$ and $< \Phi_q \mid b_i^{q'\dagger} b_j^{q'\dagger} \mid \Phi_{q'} >$ are all zero.

3.2.1 Overlap

To calculate the overlap matrix [Eq.(30)], we need to evaluate $R'(x)$ as given by Eq.(33). Introducing the notations

$$C_1(x) = \tan\theta^q A(x), \tag{41}$$

$$C_2(x) = (r^{qq'\dagger})^{-1} B(x) \tan\theta^{q'} r^{qq'\dagger}, \tag{42}$$

$$M^q = \tan\theta^q r^{qq'} \tan\theta^{q'} r^{qq'\dagger}, \tag{43}$$

we find with the help of Eqs.(38) and (37) the following equations for $C_1(x)$ and $C_2(x)$:

$$C_1(x) = M^q R(x) - M^q C_2(x), \tag{44}$$

$$C_2(x) = xM^q R(x) - x^2 C_1(x) M^q. \tag{45}$$

The second equation allows us to eliminate $C_2(x)$ in the first and, consequently, $C_1(x)$ must be the solution of

$$C_1(x) = M^q R(x) - x(M^q)^2 R(x) + x^2 M^q C_1(x) M^q. \tag{46}$$

A solution of Eq.(46) in the form of a series can be found by iteration and it is

$$\begin{aligned} C_1(x) &= [1 - xM^q + x^2(M^q)^2 - x^3(M^q)^3 + \cdots] M^q R(x) \\ &= (1 + xM^q)^{-1} M^q R(x). \end{aligned} \tag{47}$$

While the above is quite general, in actual calculation, the Bogoliubov transformation is performed in a restricted basis. Consequently, we calculate a restricted set of q.p. operators $\eta_i^{q\dagger}$ (or $\eta_i^{q'\dagger}$) characterized by the Bogoliubov angles θ_i^q (or $\theta_i^{q'}$) such that $\tan\theta_i^q \neq 0$ (or $\tan\theta_i^{q'} \neq 0$). In that case, M^q can be written as $P^q M^q$ where P^q is the projector in the space spanned by the q.p. set $\eta_i^{q\dagger}$. Then with the present notation, Eq.(47) becomes

$$C_1(x) = [P^q M^q - xP^q M^q P^q + x^2 (P^q M^q P^q)^2 + \cdots] P^q M^q R(x), \tag{48}$$

which has the important consequence that, indeed, we do invert $(1 + xM^q)$ in the restricted space.

Combining Eqs.(33), (41) and (47), we obtain

$$R'(x) = R(x) tr[(1 + xM^q)^{-1} M^q]. \tag{49}$$

Equation (49) can be readily integrated (between 0 and 1) to give

$$R(1) = \exp[tr\{\log(1 + M^q)\}] = \det[1 + M^q]. \tag{50}$$

Thus we find for the overlap [Eq.(30)]

$$< \Phi_q \mid \Phi_{q'} >=< 0 \mid \Phi_{q'} >< \Phi_q \mid 0 > \det[1 + M^q], \tag{51}$$

where

$$< \Phi_q \mid 0 >= \prod_{i>} u_i^q, \tag{52}$$

with a similar definition for $< 0 \mid \Phi_{q'} >$. We emphasize once again that when working in a restricted space, $[1 + M^q]$ has to be defined only in this space ($[1 + P^q M^q] P^q$).

3.2.2 Generalized density matrix

To calculate the overlap matrix, we had to only evaluate $\tan\theta^q A(x)$. However, to completely determine the elements of the generalized density matrix as given by Eqs.(38)-(40), we need to calculate $B(x)$ as well as $\tan\theta^{q'} B(x)$. (Details are given in Appendix C.)

The calculation of $\tan\theta^{q'} B(x)$ is very similar to that of $\tan\theta^q A(x)$ and we shall content ourselves to quote the result only:

$$\tan\theta^{q'} B(x) = xR(x)(1 + M^{q'})^{-1} M^{q'}, \tag{53}$$

where

$$M^{q'} = \tan\theta^{q'} \tau^{qq'\dagger} \tan\theta^q \tau^{qq'}. \tag{54}$$

Again, in actual calculation, we must invert $[1 + M^{q'}]$ in the restricted space spanned by $\eta_i^{q'\dagger}$.

The expression for $B(x)$ can be obtained in the following way. Substituting Eqs.(41) and (47) into Eq.(37) and setting $x = 1$, we find

$$B = \tau^{qq'\dagger}(1 + M^q)^{-1} \tan\theta^q \tau^{qq'} R(1). \tag{55}$$

Consequently, the elements of the three generalized density matrices take the form

$$< \Phi_q \mid b_i^{q'\dagger} b_j^q \mid \Phi_{q'} >=< \Phi_q \mid \Phi_{q'} > ([1 + M^{q'}]^{-1} M^{q'})_{ji}, \tag{56}$$

$$< \Phi_q \mid b_i^{q'} b_j^{q'} \mid \Phi_{q'} >= - < \Phi_q \mid \Phi_{q'} > ([1 + M^{q'}]^{-1} \tan\theta^{q'})_{ij}, \tag{57}$$

$$< \Phi_q \mid b_i^{q'\dagger} b_j^{q'\dagger} \mid \Phi_{q'} > = < \Phi_q \mid \Phi_{q'} > (r^{qq'\dagger}[1+M^q]^{-1} \tan\theta^q r^{qq'})_{ji}. \tag{58}$$

The elements of the generalized density matrices enter into the calculation of the kernel through the effective Hamiltonian. In the next section, we show the explicit dependence of the Hamiltonian on these matrix elements. In particular, we apply the formalism developed in this section to the calculation of one- and two-body operators.

4 Evaluation of the matrix $< \Phi_q \mid \mathcal{H} \mid \Phi_{q'} >$

The interaction between nucleons will be assumed to be a two-body effective potential so that the expression for the Hamiltonian takes the form

$$\mathcal{H} = \sum_{\alpha\beta} < \alpha \mid \mathcal{T} \mid \beta > a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} < \alpha\beta \mid \mathcal{V} \mid \widetilde{\gamma\delta} > a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \tag{59}$$

In the above equation, $\mathcal{T}$ denotes the kinetic energy (one-body) operator and $< \alpha\beta \mid \mathcal{V} \mid \widetilde{\gamma\delta} >$ is the antisymmetrized matrix elements of $\mathcal{V}$:

$$< \alpha\beta \mid \mathcal{V} \mid \widetilde{\gamma\delta} > = < \alpha\beta \mid \mathcal{V} \mid \gamma\delta > - < \alpha\beta \mid \mathcal{V} \mid \delta\gamma > . \tag{60}$$

Since the states $\phi_i^{q'}$, defined in Appendix A, provides a complete basis, it is convenient to express $\mathcal{H}$ in this representation, *i.e.* write $\mathcal{H}$ as

$$\mathcal{H} = \sum_{ij} < iq' \mid \mathcal{T} \mid jq' > b_i^{q'\dagger} b_j^{q'} + \frac{1}{4} \sum_{ijkl} < iq'jq' \mid \mathcal{V} \mid \widetilde{kq'lq'} > b_i^{q'\dagger} b_j^{q'\dagger} b_k^{q'} b_l^{q'}. \tag{61}$$

Using Wick's theorem established in Sec.3.1, we can express the matrix elements of $\mathcal{H}$ between the two states $\mid \Phi_q >$ and $\mid \Phi_{q'} >$ as

$$\begin{aligned} < \Phi_q \mid \mathcal{H} \mid \Phi_{q'} > = < \Phi_q \mid \Phi_{q'} > \{ & \sum_{ij} < iq' \mid \mathcal{T} \mid jq' > S_{ji} \\ & + \frac{1}{2} \sum_{ijkl} < iq'jq' \mid \mathcal{V} \mid \widetilde{kq'lq'} > S_{ki} S_{lj} \\ & + \frac{1}{4} \sum_{ijkl} < iq'\bar{j}q' \mid \mathcal{V} \mid \widetilde{kq'\bar{l}q'} > T_{ij} Y_{lk} \}. \end{aligned} \tag{62}$$

The matrices S, T and Y are related to the generalized density matrices according to the relations

$$S_{ji} = \frac{< \Phi_q \mid b_i^{q'\dagger} b_j^{q'} \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >}, \tag{63}$$

$$T_{i\bar{j}} = \frac{< \Phi_q \mid b_i^{q'\dagger} b_{\bar{j}}^{q'\dagger} \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >}, \tag{64}$$

$$Y_{i\bar{j}} = \frac{< \Phi_q \mid b_i^{q'} b_{\bar{j}}^{q'} \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >}, \tag{65}$$

and their properties are presented in details in Appendix D.

In Eq.(62), we can exclude summation over the time-reversed states ($\bar{i}$ and $\bar{j}$) by using the fact that the interaction $\mathcal{V}$ is real, *i.e.*

$$< \bar{i}q'\bar{j}q' \mid \mathcal{V} \mid \bar{k}q'\bar{l}q' >=< iq'jq' \mid \mathcal{V} \mid kq'lq' >^* . \tag{66}$$

Furthermore, using the properties of S, Y and T (given in Appendix D), we find

$$\begin{aligned} < \Phi_q \mid \mathcal{N} \mid \Phi_{q'} >=< \Phi_q \mid \Phi_{q'} > \Re\{2 \sum_{ij} < iq' \mid \mathcal{T} \mid jq' > S_{ji} \\ + \sum_{ijkl>} [(< iq'jq' \mid \mathcal{V} \mid \widetilde{kq'lq'} > + < \bar{i}q'jq' \mid \mathcal{V} \mid \widetilde{\bar{k}q'lq'} >) S_{ki} S_{lj} \\ + < iq'\bar{j}q' \mid \mathcal{V} \mid \widetilde{kq'\bar{l}q'} > T_{i\bar{j}} Y_{lk}]\}. \end{aligned} \tag{67}$$

As shown in Appendix D, it is convenient to define the new matrices

$$\rho = (1 + M^{q'})^{-1} \tan\theta^{q'} \tau^{qq'\dagger} \tan\theta^q, \tag{68}$$

$$K^q = (1 + M^q)^{-1} \tan\theta^q, \tag{69}$$

$$K^{q'} = (1 + M^{q'})^{-1} \tan\theta^{q'}, \tag{70}$$

and express $< \Phi_q \mid \mathcal{N} \mid \Phi_{q'} >$ in terms of matrix elements between the two sets of single-particle states $\phi_i^{q'}$ and ϕ_i^q. The result is

$$\begin{aligned} < \Phi_q \mid \mathcal{N} \mid \Phi_{q'} >=< \Phi_q \mid \Phi_{q'} > \Re\{2 \sum_{ij} < iq \mid \mathcal{T} \mid jq' > \rho_{ji} \\ + \sum_{ijkl>} [(< iqjq \mid \mathcal{V} \mid \widetilde{kq'lq'} > + < \bar{i}qjq \mid \mathcal{V} \mid \widetilde{\bar{k}q'lq'} >) \rho_{ki} \rho_{lj} \\ + < iq\bar{j}q \mid \mathcal{V} \mid \widetilde{kq'\bar{l}q'} > K_{j\bar{i}}^q K_{lk}^{q'}]\}. \end{aligned} \tag{71}$$

We now have all the quantities needed to calculate the kernel $K(q, q')$.

5 Practical considerations

For a given nucleus, we can define a Fermi level i_F as the highest (last) occupied level in the absence of pairing. The behavior of u_i and v_i in actual calculation is shown in fig.1. For very deep levels, $v_i = 1$ and $u_i = 0$ which means that $\tan\theta_i = v_i/u_i \simeq \infty$ and, consequently, all the quantities defined in Eqs.(68)-(70) are singular. Our purpose in the following subsections is to rewrite them in a non-singular form.

5.1 Overlap

According to Eq.(51) in Sec.3.2.1, the overlap is

$$< \Phi_q \mid \Phi_{q'} >= \prod_{i>} u_i^q \prod_{j>} u_j^{q'} \det[1 + M^q], \tag{72}$$

which can be rewritten as

$$< \Phi_q \mid \Phi_{q'} >= \det(u^q)\det(u^{q'})\det[1 + \frac{v^q}{u^q} r^{qq'} \frac{v^{q'}}{u^{q'}} r^{qq'\dagger}]. \tag{73}$$

Using the well-known properties of determinants such as $\det(A)\det(B) = \det(AB)$, $\det(\tilde{A}) = \det(A)$, etc, it is easily seen that

$$< \Phi_q \mid \Phi_{q'} >= \det(r^{qq'})\det[u^{q'}(r^{qq'})^{-1}u^q + v^{q'} r^{qq'\dagger} v^q]. \tag{74}$$

As mentioned in Sec.3.2, the dimensions at collective variable q and q' are determined by the number of $\tan\theta^q$ and $\tan\theta^{q'}$ which are non-zero. Let us call these dimensions N_q and $N_{q'}$, respectively. If $N_q \geq N_{q'}$, then Eq.(73) is correct. In fact, in the original definition of the determinant, the overlap matrix r occurs in a combination like $r^{qq'}(v^{q'}/u^{q'})r^{qq'\dagger}$ and, consequently, we can complete the space at q' with states for which $v^{q'} = 0$, so that we can build the square matrix of dimension $N_q \times N_q$. We can then safely perform the different manipulations leading to Eq.(73). On the other hand, if $N_{q'} \geq N_q$, we have to use Eq.(73) with q and q' interchanged. This is easily understood if we note that $< \Phi_q \mid \Phi_{q'} >=< \Phi_{q'} \mid \Phi_q >$.

As will be apparent in the following subsections, it is convenient to define here the quantity

$$\mathcal{Z}^{qq'} = u^q(r^{qq'\dagger})^{-1}u^{q'} + v^q r^{qq'} v^{q'}, \tag{75}$$

which is nothing but the Hermitian conjugate of the second determinant in Eq.(74). Then the overlap becomes

$$< \Phi_q \mid \Phi_{q'} >= \det(\tau^{qq'}) \det(Z^{qq'\dagger}), \tag{76}$$

or, according to a property of the determinant,

$$< \Phi_q \mid \Phi_{q'} >= \det(\tau^{qq'}) \det(Z^{qq'}). \tag{77}$$

Parenthetically, we remark that $\tau^{qq'\dagger} \neq (\tau^{qq'})^{-1}$ when one does not use the complete basis, as is the case in actual calculation. Furthermore, in the Hartree-Fock limit $u_{i<i_F} = 0$, $v_{i<i_F} = 1$ and $u_{i>i_F} = 1$, $v_{i>i_F} = 0$ and we fall back onto the expression $|\det(v^q \tau^{qq'} v^{q'})|^2$. The square of the determinant occurs because the contribution of time-reversed states is taken into account in Eq.(73).

5.2 Matrices K^q and $K^{q'}$

Let us first consider K^q. By definition [Eq.(69)]

$$K^q = (1 + M^q)^{-1} \tan\theta^q, \tag{78}$$

where, according to Eq.(43),

$$M^q = \frac{v^q}{u^q} \tau^{qq'} \frac{v^{q'}}{u^{q'}} \tau^{qq'\dagger}. \tag{79}$$

It is clear that

$$1 + M^q = \frac{1}{u^q} [u^q (\tau^{qq'\dagger})^{-1} u^{q'} + v^q \tau^{qq'} v^{q'}] \frac{1}{u^{q'}} \tau^{qq'\dagger}. \tag{80}$$

Therefore, according to the definition of $Z^{qq'}$,

$$(1 + M^q)^{-1} = (\tau^{qq'\dagger})^{-1} u^{q'} (Z^{qq'})^{-1} u^q. \tag{81}$$

Thus,

$$K^q_{ij} = \{(\tau^{qq'\dagger})^{-1} u^{q'} (Z^{qq'})^{-1} v^q\}_{ij}. \tag{82}$$

The same demonstration applies to $K^{q'}$ and we obtain its expression by making the substitutions $u^q \rightleftharpoons u^{q'}$, $v^q \rightleftharpoons v^{q'}$ and $\tau^{qq'} \rightleftharpoons \tau^{qq'\dagger}$ in the equation for K^q:

$$K^{q'}_{ij} = \{(\tau^{qq'})^{-1} u^q [(Z^{qq'})^T]^{-1} v^{q'}\}_{ij}. \tag{83}$$

5.3 Matrix ρ

By definition [Eq.(68)], ρ is given by

$$\rho = (1 + M^{qq'})^{-1} \tan\theta^{qq'} r^{qq'\dagger} \tan\theta^{q}, \tag{84}$$

which is also equivalent to

$$\rho = [1 + (M^{qq'})^{-2}]^{-1} (M^{qq'})^{-1} \tan\theta^{qq'} r^{qq'\dagger} \tan\theta^{q}. \tag{85}$$

But

$$(M^{qq'})^{-1} \tan\theta^{qq'} r^{qq'\dagger} \tan\theta^{q} = (r^{qq'})^{-1}. \tag{86}$$

Hence,

$$\rho = [1 + (M^{qq'})^{-1}]^{-1} (r^{qq'})^{-1}. \tag{87}$$

By using the expression

$$[1 + (M^{qq'})^{-1}]^{-1} = v^{qq'} (Z^{qq'})^{-1} v^{q} r^{qq'}, \tag{88}$$

we can recast ρ in the form

$$\rho = v^{qq'} (Z^{qq'})^{-1} v^{q}. \tag{89}$$

6 Application to a non-zero finite range interaction

We present here the calculation of $< \Phi_q \mid \mathcal{H} \mid \Phi_{q'} >$ for a non-zero finite range interaction. Such an interaction allows us to calculate without ambiguities all the quantities associated with pairing, in contrast to that of Skyrme forces[17] with an *ad hoc* prescription for pairing.

We choose an interaction of the form[18]

$$\mathcal{V}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1}^{2} (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) e^{-|\mathbf{r}_1 - \mathbf{r}_2|^2/\mu_i^2}$$

$$+ t_0 (1 + x_0 P_\sigma) \rho^{\alpha} (\frac{1}{2}[\mathbf{r}_1 + \mathbf{r}_2]) \delta(\mathbf{r}_1 - \mathbf{r}_2) + V_{LS}, \tag{90}$$

where $P_\sigma = \frac{1}{2}(1 + \vec{\sigma}_1.\vec{\sigma}_2)$ and $P_\tau = \frac{1}{2}(1 + \vec{\tau}_1.\vec{\tau}_2)$ are the usual spin and isospin exchange operators, respectively. In order to calculate $< \Phi_q \mid \mathcal{H} \mid \Phi_{q'} >$, we define the following three quantities:

$$\rho^t(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q*}_{it}(x,\sigma)\phi^{q'}_{jt}(x',\sigma')\rho^t_{ji}, \tag{91}$$

$$K^{tq}(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q*}_{it}(x,\sigma)\phi^{q*}_{\bar{j}t}(x',\sigma')K^{tq}_{j\bar{i}}, \tag{92}$$

$$K^{tq'}(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q'}_{it}(x,\sigma)\phi^{q'}_{\bar{j}t}(x',\sigma')K^{tq'}_{j\bar{i}}. \tag{93}$$

The summation is performed also over the time-reversed states, and the quantities $K^{tq}_{j\bar{i}}$, $K^{tq'}_{j\bar{i}}$ and ρ^t are defined in Eqs.(82), (83) and (87), respectively, except that the index t is now used to distinguish between orbits of neutrons and protons. For instance, since ρ is diagonal in isospin space, we use the notation $\rho_{ij} = \rho^t_{ij}$ and the indices do not contain anymore the isospin label. Using the properties of K^q, $K^{q'}$, ρ (see Appendix D) and the definition of time-reversed states, it is shown in Appendix E that

$$\rho^t(x,\sigma;x',\sigma') = \sigma\sigma'\rho^{t*}(x,-\sigma;x',-\sigma'), \tag{94}$$

$$K^{tq(q')}(x,\sigma;x',\sigma') = \sigma\sigma' K^{tq(q')*}(x,-\sigma;x',-\sigma'), \tag{95}$$

$$K^{tq(q')}(x,\sigma;x',\sigma') = -K^{tq(q')}(x',\sigma';x,\sigma). \tag{96}$$

It is now possible to express $< \Phi_q \mid \mathcal{H} \mid \Phi_{q'} >$ in the following way:

$$\begin{aligned}
< \Phi_q \mid \mathcal{H} \mid \Phi_{q'} > = & \sum_{ij,t} < itq \mid \mathcal{T} \mid jtq' > \rho^t_{ij} + \sum_i \int\int e^{-|\mathbf{x}-\mathbf{x}'|^2/\mu_i^2} d^3x d^3x' \\
& \times \{ \sum_{tt'} [(W_i - H_i\delta_{tt'})2\rho^t_R(x,\sigma;x,\sigma)\rho^{t'}_R(x',\sigma;x',\sigma) \\
& + (B_i - M_i\delta_{tt'})([\rho^t(x,\sigma;x,\sigma)\rho^{t'}(x',\sigma;x',\sigma)]_R - [\rho^t(x,\sigma;x,-\sigma)\rho^{t'}(x',\sigma;x',-\sigma)]_R) \\
& + (M_i - B_i\delta_{tt'})2\rho^t_R(x,\sigma;x',\sigma)\rho^t_R(x',\sigma;x,\sigma) \\
& + (H_i - W_i\delta_{tt'})([\rho^t(x,\sigma;x',\sigma)\rho^{t'}(x',\sigma;x,\sigma)]_R - [\rho^t(x,\sigma;x',-\sigma)\rho^{t'}(x',\sigma;x,-\sigma)]_R)] \\
& + (W_i - H_i + B_i - M_i)\sum_t ([K^{tq}(x,\sigma;x',\sigma)K^{tq'}(x,\sigma;x',\sigma)]_R \\
& + [K^{tq}(x,\sigma;x',-\sigma)K^{tq'}(x,\sigma;x',-\sigma)]_R) - (B_i - M_i) \\
& \times \sum_t ([K^{tq}(x,\sigma;x',\sigma)K^{tq'}(x',\sigma;x,\sigma)]_R + [K^{tq}(x,\sigma;x',-\sigma)K^{tq'}(x',\sigma;x,-\sigma)]_R)\}
\end{aligned}$$

$$+t_0 \int d^3x \sum_{tt'} \{(1 - x_0\delta_{tt'}) 2\rho^t_R(x,\sigma;x,\sigma)\rho^{t'}_R(x,\sigma;x,\sigma)$$

$$+(x_0 - \delta_{tt'})([\rho^t(x,\sigma,x,\sigma)\rho^{t'}(x,\sigma,x,\sigma)]_R$$

$$-[\rho^t(x,\sigma;x,-\sigma)\rho^{t'}(x,-\sigma;x,-\sigma)]_R)\}[2\rho(x,\sigma;x,\sigma)]^a_R. \quad (97)$$

In the above equation, we have suppressed the summation over the spin variables and expressed $< \Phi_q \mid \mathcal{H} \mid \Phi_{q'} >$ in terms of the real (subscript R) parts of ρ^t, K^{tq} and $K^{tq'}$. Furthermore, x_0 is always equal to one and, consequently, the density dependent part never contributes to the pairing.

7 Hill-Wheeler kernel with the Skyrme interaction

As a further application of the formalism developed in the preceeding sections, we present here the calculation of the kernel for the Skyrme interaction. The parametrization of this interaction in terms of δ-functions helps in reducing the number of integrations and to express the matrix elements as functions of various densities.

The Skyrme interaction can be written as[2,17]

$$\mathcal{V}(\mathbf{r}_1,\mathbf{r}_2) = t_0(1 + x_0P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2}t_1[\delta(\mathbf{r}_1 - \mathbf{r}_2)\,\vec{\nabla}^2_{12}$$

$$+ \overleftarrow{\nabla}^2_{12}\,\delta(\mathbf{r}_1 - \mathbf{r}_2)] + t_2\,\overleftarrow{\nabla}_{12}\,\delta(\mathbf{r}_1 - \mathbf{r}_2)\,\vec{\nabla}_{12}$$

$$+iW_0(\vec{\sigma}_1 + \vec{\sigma}_2).\,\overleftarrow{\nabla}_{12} \times \delta(\mathbf{r}_1 - \mathbf{r}_2)\,\vec{\nabla}_{12} + t_3\rho^\alpha(\frac{1}{2}[\mathbf{r}_1 + \mathbf{r}_2])\delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (98)$$

where

$$\overleftrightarrow{\nabla}_{12} = \frac{1}{2i}(\overrightarrow{\nabla}_1 - \overrightarrow{\nabla}_2). \quad (99)$$

The direction of the arrow indicates on which side (left or right) the operator acts.

The calculation of the kernel with the Skyrme interaction requires the evaluation of

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > \sum_{ijkl,tt'} < iqt, jqt' \mid \mathcal{V} \mid kq't, lq't' > \rho^t_{ki}\rho^{t'}_{lj},$$

which can be recast in the form

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > \sum_{ijkl,tt'} < iqt, jqt' \mid \mathcal{V}(1 - P_xP_\sigma P_\tau) \mid kq't, lq't' > \rho^t_{ki}\rho^{t'}_{lj}.$$

In the latter expression, we took into account the antisymmetrization by introducing the operator $P_x P_\sigma P_\tau$, which exchanges particle 1 and particle 2 in the configuration, spin and isospin spaces, *i.e.*

$$P_x \mid \mathbf{r}_1, \mathbf{r}_2 > = \mid \mathbf{r}_2, \mathbf{r}_1 >, \tag{100}$$

$$P_\sigma \mid \vec{\sigma}_1, \vec{\sigma}_2 > = \frac{1}{2}(1 + \vec{\sigma}_1.\vec{\sigma}_2) \mid \vec{\sigma}_1, \vec{\sigma}_2 > = \mid \vec{\sigma}_2, \vec{\sigma}_1 >, \tag{101}$$

$$P_\tau \mid t_1, t_2 > = \frac{1}{2}(1 + \vec{\tau}_1.\vec{\tau}_2) \mid t_1, t_2 > = \mid t_2, t_1 > . \tag{102}$$

Because of the δ-functions, it is easy to see that P_x is $+1$ or -1 depending on the different terms present in the expression for $\mathcal{V}(\mathbf{r}_1, \mathbf{r}_2)$. In fact, it is clear that for the terms t_0, t_1 and t_3, the two-body wave function must be symmetric in the configuration space and, consequently, $P_x = +1$ for them. For the other two terms, namely t_2 and W_0, the wave function must be antisymmetric and $P_x = -1$. It is also obvious that we can replace P_τ by $\delta_{tt'}$.

7.1 Contribution of t_0

If we use the property $P_\sigma^2 = 1$ and take into account the previous two remarks, then the contribution of the t_0 term is

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > t_0 \sum_{ijkl,\sigma\sigma',tt'} [(1 - x_0\delta_{tt'}) \int d^3x \phi_{it}^{q*}(x,\sigma)\phi_{jt'}^{q*}(x,\sigma')\phi_{kt}^{q'}(x,\sigma)\phi_{lt'}^{q'}(x,\sigma')$$

$$\times \rho_{ki}^{t} \rho_{l;}^{t'} + (x_0 - \delta_{tt'}) \int d^3x \phi_{it}^{q*}(x,\sigma)\phi_{jt'}^{q*}(x,\sigma')\phi_{kt}^{q'}(x,\sigma)\phi_{lt'}^{q'}(x,\sigma')\rho_{ki}^{t}\rho_{lj}^{t'}|.$$

This expression suggests to define the following densities:

$$\rho^t(x) = \sum_{ij,\sigma} \phi_{it}^{q*}(x,\sigma)\phi_{jt}^{q'}(x,\sigma)\rho_{ji}^{t}, \qquad \rho(x) = \sum_t \rho^t(x), \tag{103}$$

$$\rho^t(x,\sigma,\sigma') = \sum_{ij} \phi_{it}^{q*}(x,\sigma)\phi_{jt}^{q'}(x,\sigma')\rho_{ji}^{t}, \qquad \rho(x,\sigma,\sigma') = \sum_t \rho^t(x,\sigma,\sigma'). \tag{104}$$

The contribution of the t_0 term can now be expressed as

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > t_0 \int d^3x \{[\rho^2(x) - x_0(\rho^{p^2}(x) + \rho^{n^2}(x))]$$

$$+(x_0 - \delta_{tt'}) \sum_{\sigma\sigma'} \rho^t(x,\sigma,\sigma')\rho^{t'}(x,\sigma',\sigma)\}.$$

The term containing $\rho^t(x,\sigma,\sigma')$ can be simplified with the aid of Eq.(169) given in Appendix E. The result is

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > t_0 \int d^3x \{\Re[\rho^2(x) - x_0(\rho^{p^2}(x) + \rho^{n^2}(x))$$

$$+2(x_0\rho^2(x,\sigma) - \rho^{p^2}(x,\sigma) - \rho^{n^2}(x,\sigma))]$$

$$-x_0 \mid \rho(x,\sigma,-\sigma) \mid^2 + \mid \rho^p(x,\sigma,-\sigma) \mid^2 + \rho^n(x,\sigma,-\sigma) \mid^2\}.$$

7.2 Contribution of t_1

We first restrict ourself to the calculation of the direct matrix element and take into account the fact that both the terms present in t_1 give contribution which are Hermitian conjugate of each other. Therefore, we just consider the term

$$-\frac{1}{16} < \Phi_q \mid \Phi_{q'} > t_1 \sum_{ijkl,tt'} < iqt, jqt' \mid \delta(\mathbf{r}_1 - \mathbf{r}_2)(\vec{\nabla}_1 - \vec{\nabla}_2)^2 \mid kq't, lq't' > \rho^t_{ki}\rho^{t'}_{lj}$$

which, due to the symmetry between coordinates 1 and 2, is equal to

$$-\frac{1}{8} < \Phi_q \mid \Phi_{q'} > t_1 \sum_{ijkl,tt'} < iqt, jqt' \mid \delta(\mathbf{r}_1 - \mathbf{r}_2)(\nabla^2 - \vec{\nabla}_1.\vec{\nabla}_2) \mid kq't, lq't' > \rho^t_{ki}\rho^{t'}_{lj}.$$

This expression can be rewritten in the configuration space as

$$-\frac{1}{8} < \Phi_q \mid \Phi_{q'} > t_1 \sum_{ijkl,\sigma\sigma',tt'} \int d^3x \{\phi^{q*}_{it}(x,\sigma)\phi^{q'}_{kt}(x,\sigma)\phi^{q*}_{jt'}(x,\sigma')\nabla^2\phi^{q'}_{lt'}(x,\sigma')$$

$$-\phi^{q*}_{it}(x,\sigma)\vec{\nabla}\phi^{q'}_{kt}(x,\sigma).\phi^{q*}_{jt'}(x,\sigma')\vec{\nabla}\phi^{q'}_{lt'}(x,\sigma')\}\rho^t_{ki}\rho^{t'}_{lj}.$$

It is now natural to define

$$\kappa^{qq'}_t(x) = \sum_{ij,\sigma} \phi^{q*}_{it}(x,\sigma)\nabla^2\phi^{q'}_{jt}(x,\sigma)\rho^t_{ji}, \qquad \kappa^{qq'}(x) = \sum_t \kappa^{qq'}_t(x), \tag{105}$$

$$\Gamma^{qq'}_t(x) = \sum_{ij,\sigma} \phi^{q*}_{it}(x,\sigma)\vec{\nabla}\phi^{q'}_{jt}(x,\sigma)\rho^t_{ji}, \qquad \Gamma^{qq'} = \sum_t \Gamma^{qq'}_t(x), \tag{106}$$

so that the contribution of t_1 takes the form

$$-\frac{1}{8} < \Phi_q \mid \Phi_{q'} > t_1 \int d^3x \{[\kappa^{qq'}(x) + \bar{\kappa}^{q'q}(x)]\rho(x)$$

$$-[\Gamma^{qq'}(x).\Gamma^{qq'}(x) + \bar{\Gamma}^{q'q}(x).\bar{\Gamma}^{q'q}(x)]\},$$

where $\bar{\kappa}$ and $\bar{\Gamma}$ are defined in Eqs.(174) and (177) (Appendix E), respectively. If we define an additional quantity

$$\Lambda_t^{qq'}(x) = \sum_{ij,\sigma} \vec{\nabla}\phi_{it}^{q*}(x,\sigma).\vec{\nabla}\phi_{jt}^{q'}(x,\sigma)\rho_{ji}^t, \quad \Lambda^{qq'}(x) = \sum_t \Lambda_t^{qq'}(x), \tag{107}$$

and use Eqs.(176) and (179) of Appendix E, then the contribution of t_1 becomes

$$-\frac{1}{4} < \Phi_q \mid \Phi_{q'} > t_1 \int d^3x[\rho(x)\nabla^2\rho(x) - \Lambda^{qq'}(x)\rho(x)$$

$$+\Gamma^{qq'}(x).\vec{\nabla}\rho(x) - \Gamma^{qq'}(x).\Gamma^{qq'}(x)].$$

The derivation of the exchange term is quite straightforward since one has only to set equal t and t' and to permute the spins σ and σ'. By noting that

$$\Gamma_t^{qq'}(x,\sigma,\sigma') = \sum_{ij} \phi_{it}^{q*}(x,\sigma)\vec{\nabla}\phi_{jt}^{q'}(x,\sigma')\rho_{ji}^t, \tag{108}$$

$$\Lambda_t^{qq'}(x,\sigma,\sigma') = \sum_{ij} \vec{\nabla}\phi_{it}^{q*}(x,\sigma).\vec{\nabla}\phi_{jt}^{q'}(x,\sigma')\rho_{ji}^t, \tag{109}$$

the exchange term becomes

$$\frac{1}{4} < \Phi_q \mid \Phi_{q'} > t_1 \sum_{\sigma,t} \int d^3x\{\rho^t(x,\sigma,\sigma')\nabla^2\rho^t(x,\sigma',\sigma) - \Lambda_t^{qq'}(x,\sigma,\sigma')\rho^t(x,\sigma',\sigma)$$

$$+\Gamma_t^{qq'}(x,\sigma,\sigma').\vec{\nabla}\rho^t(x,\sigma',\sigma) - \Gamma_t^{qq'}(x,\sigma,\sigma').\Gamma_t^{qq'}(x,\sigma',\sigma)\}.$$

As shown in Appendix E, all the quantities, $\rho^t(x,\sigma',\sigma)$, $\Lambda_t^{qq'}(x,\sigma,\sigma')$ and $\Gamma_t^{qq'}(x,\sigma,\sigma')$, have the property

$$A(x,\sigma',\sigma) = \sigma\sigma' A^*(x,-\sigma,-\sigma'), \quad (\sigma = \pm 1). \tag{110}$$

We can, therefore, perform the summation over spin and rewrite the exchange term in the following form:

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > t_1 \Re \sum_t \int d^3x\{\rho^t(x,\sigma,\sigma)\nabla^2\rho^t(x,\sigma,\sigma)$$

$$-\rho^{t*}(x,\sigma,-\sigma)\nabla^2\rho^t(x,\sigma,-\sigma) - [\Lambda_t^{qq'}(x,\sigma,\sigma)\rho^t(x,\sigma,\sigma)$$

$$-\Lambda_t^{qq'}(x,\sigma,-\sigma)\rho^{t*}(x,\sigma,-\sigma)] + [\Gamma_t^{qq'}(x,\sigma,\sigma).\vec{\nabla}\rho^t(x,\sigma,\sigma)$$

$$-\Gamma_t^{qq'}(x,\sigma,-\sigma).\vec{\nabla}\rho^{t*}(x,\sigma,-\sigma)] - [\Gamma_t^{qq'}(x,\sigma,\sigma).\Gamma_t^{qq'}(x,\sigma,\sigma)$$

$$-\Gamma_t^{qq'}(x,\sigma,-\sigma).\Gamma_t^{qq'}(x,\sigma,-\sigma)]\}.$$

In the above expression, we can choose either $\sigma = +1$ or $\sigma = -1$.

7.3 Contribution of t_2

The derivation for the contribution of the t_2 term is very similar to that of t_1. Hence, we shall not describe the details of the calculation but rather give the final result which is

$$< \Phi_q \mid \Phi_{q'} > t_2\{\frac{1}{4}\int d^3x[A^{qq'}(x)\rho(x) + \Gamma^{qq'}(x).\Gamma^{qq'}(x)$$

$$-\Gamma^{qq'}(x).\vec{\nabla}\rho(x)] + \frac{1}{2}\Re\sum_t\int d^3x([A_t^{qq'}(x,\sigma,\sigma)\rho^t(x,\sigma,\sigma)$$

$$-A_t^{qq'}(x,\sigma,-\sigma)\rho^{t*}(x,\sigma,-\sigma)] - [\Gamma_t^{qq'}(x,\sigma,\sigma).\vec{\nabla}\rho^t(x,\sigma,\sigma)$$

$$-\Gamma_t^{qq'}(x,\sigma,-\sigma).\vec{\nabla}\rho^{t*}(x,\sigma,-\sigma)] + [\Gamma_t^{qq'}(x,\sigma,\sigma).\Gamma_t^{qq'}(x,\sigma,\sigma)$$

$$-\Gamma_t^{qq'}(x,\sigma,-\sigma).\Gamma_t^{qq'}(x,\sigma,-\sigma)]]\}.$$

All the quantities appearing in the above expression have been defined earlier.

7.4 Contribution of W_0

The presence of the spin operator $(\vec{\sigma}_1 + \vec{\sigma}_2)$ simplifies considerably the calculation of the exchange term. In fact, it is easy to convince oneself that this operator acts on triplet $(S = 1)$ states only so that $P_\sigma = 1$. Thus, recalling that $P_x = -1$ in the spin-orbit case, we get $P_x P_\sigma P_r = -\delta_{tt'}$ so that the total contribution of the direct and exchange terms is

$$\frac{iW_0}{8} < \Phi_q \mid \Phi_{q'} > \sum_{ijkl,tt'} < iqt, jqt' \mid [\tilde{\nabla}_{12}\,\delta(\mathbf{r}_1 - \mathbf{r}_2)\times \vec{\nabla}_{12}].(\vec{\sigma}_1 + \vec{\sigma}_2)$$

$$\times \mid kq't, lq't' > \rho^t_{ki}\rho^{t'}_{lj}.$$

There is an obvious symmetry between 1 and 2 which allows us to rewrite the spin-orbit term as

$$2iW_0[(\vec{\nabla}_1' \times \vec{\nabla}_1).\vec{\sigma}_2 + \vec{\nabla}_1'.(\vec{\nabla}_1 \times \vec{\sigma}_1) - (\vec{\nabla}_1' \times \vec{\nabla}_2).\vec{\sigma}_1 - \vec{\nabla}_2'.(\vec{\nabla}_1 \times \vec{\sigma}_1)].$$

Furthermore, after carrying out different integrations by parts, it can be shown that the above expression reduces to the simple form

$$4iW_0[(\vec{\nabla}_1' \times \vec{\nabla}_1).\vec{\sigma}_2 - (\vec{\nabla}_2 + \vec{\nabla}_2').(\vec{\nabla}_1 \times \vec{\sigma}_1)].$$

If we now define

$$\Pi_t^{qq'}(x) = \sum_{ij,\sigma} \vec{\nabla}\phi_{it}^{q*}(x,\sigma) \times \vec{\nabla}\phi_{jt}^{q'}(x,\sigma)\rho_{ji}^t, \quad \Pi^{qq'}(x) = \sum_t \Pi_t^{qq'}(x), \tag{111}$$

$$\vec{\sigma}_t^{qq'}(x) = i \sum_{ij,\sigma\sigma'} \phi_{it}^{q*}(x,\sigma) < \sigma \mid \vec{\sigma} \mid \sigma' > \phi_{jt}^{q'}(x,\sigma')\rho_{ji}^t, \quad \vec{\sigma}^{qq'}(x) = \sum_t \vec{\sigma}_t^{qq'}(x), \tag{112}$$

$$\mathbf{J}_t^{qq'}(x) = -i \sum_{ij,\sigma\sigma'} \phi_{it}^{q*}(x,\sigma)\vec{\nabla}\phi_{jt}^{q'}(x,\sigma') \times < \sigma \mid \vec{\sigma} \mid \sigma' > \rho_{ji}^t, \quad \mathbf{J}^{qq'}(x) = \sum_t \mathbf{J}_t^{qq'}(x), \tag{113}$$

then the contribution of the spin-orbit term is given by

$$\frac{1}{2}W_0 \int d^3x \{[\mathbf{\Pi}^{qq'}(x).\vec{\sigma}^{qq'}(x) + \vec{\nabla}\rho(x).\mathbf{J}^{qq'}(x)]$$

$$+ \sum_t [\mathbf{\Pi}_t^{qq'}(x).\vec{\sigma}_t^{qq'}(x) + \vec{\nabla}\rho^t(x).\mathbf{J}_t^{qq'}(x)]\}.$$

7.5 Contribution of t_3

In the first parametrization of the Skyrme interaction proposed by Vautherin and Brink[2], there was a three-body contact term $t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3)$. Later on, however, different authors[19] introduced a density-dependent two-body interaction term

$$t_3\rho^\alpha(\frac{1}{2}[\mathbf{r}_1 + \mathbf{r}_2])\delta(\mathbf{r}_1 - \mathbf{r}_2).$$

In the following, we shall consider both the cases.

7.5.1 Three-body interaction

We have to calculate

$$\frac{t_3}{36} \sum_{ijklmn,tt't''} < iq't, jq't', kq't'' \mid \nu(123) \mid lq't, mq't'', nq't'' >$$

$$\times < \Phi_q \mid b_{it}^{q't} b_{jt'}^{q't'} b_{kt''}^{q't''} b_{nt''}^{q'} b_{mt'}^{q'} b_{lt}^{q'} \mid \Phi_{q'} >,$$

where the matrix element is antisymmetrized with respect to the three particles. According to Wick's theorem described in Sec.3.1, we can express the above contraction in terms of the quantities S, T and Y defined in Eqs.(63)-(65). Since, to our knowledge, the Skyrme interaction is never used directly to calculate pairing correlations, we shall only keep the normal contractions associated with S. As we did with two-body interactions, we can express the contractions in terms of the generalized density matrix. We only give here the result which is

$$\frac{1}{6} < \Phi_q \mid \Phi_{q'} > t_3 \sum_{ijklmn,tt't''} < iqt, jqt', kqt'' \mid \nu(123) \mid lq't, mq't', nq't'' >$$

$$\times \rho^{t''}_{nk} \rho^{t'}_{mj} \rho^{t}_{li}.$$

Due to the presence of the δ-functions in the definition of $\nu(123)$, the wave function must be symmetric in the configuration space and, consequently, antisymmetric in the spin-isospin space. We shall denote the corresponding antisymmetrizer as $P_{\sigma\tau}$ which will allow us to rewrite the above expression as

$$\frac{1}{6} < \Phi_q \mid \Phi_{q'} > t_3 \sum_{ijklmn,tt't''} < iqt, jqt', kqt'' \mid \nu(1,2,3) P_{\sigma\tau} \mid lq't, mq't', nq't'' >$$

$$\times \rho^{t''}_{nk} \rho^{t'}_{mj} \rho^{t}_{li}.$$

Taking into account the obvious symmetries between particles 1, 2 and 3, and relabelling the indices in the summation, it can be shown that

$$P_{\sigma\tau} = 1 + 2P_\sigma(12)P_\sigma(23)P_\tau(12)P_\tau(23) - 3P_\sigma(12)P_\tau(12), \tag{114}$$

where P_σ and P_τ have been defined in Eqs.(101) and (102). After substituting this form of $P_{\sigma\tau}$ in the expression just given above, we obtain

$$\frac{1}{6} < \Phi_q \mid \Phi_{q'} > t_3 \Re \int d^3x [\rho^3(x) - \sigma\rho(x)(\rho^{p^2}(x,\sigma) + \rho^{n^2}(x,\sigma)$$

$$- \mid \rho^p(x,\sigma,\sigma) \mid^2 - \mid \rho^n(x,\sigma,\sigma) \mid^2) + 4\{(\rho^{p^3}(x,\sigma)$$

$$-3\rho^p(x,\sigma)\rho^{p^2}(x,\sigma,-\sigma)) + (\rho^{n^3}(x,\sigma) - 3\rho^n(x,\sigma)\rho^{n^2}(x,\sigma,-\sigma))\}].$$

7.5.2 Density-dependent interaction

Clearly, only the diagonal elements

$$\frac{1}{4} t_3 \int < \Phi_q \mid \delta(\mathbf{r}_1 - \mathbf{r}_2)\rho^\alpha(\frac{1}{2}[\mathbf{r}_1 + \mathbf{r}_2]) \mid \Phi_{q'} > d^3r_1 d^3r_2$$

are unambiguously defined when using a density-dependent interaction. In order to extend its definition to the non-diagonal case, we make the substitution

$$\rho(\mathbf{r}) \rightarrow \mid \sum_\sigma < \Phi_q \mid \Psi^\dagger(\mathbf{r},\sigma)\Psi(\mathbf{r},\sigma) \mid \Phi_{q'} > \mid,$$

which reduces to the density $\rho(r)$ when $q = q'$. Then the contribution of such an interaction is simply given by

$$\frac{1}{2} < \Phi_q \mid \Phi_{q'} > t_3 \int d^3x \{\rho^2(x) - 2\Re[\rho^{p^2}(x,\sigma) + \rho^{n^2}(x,\sigma)]$$

$$+ \mid \rho^p(x,\sigma,-\sigma) \mid^2 + \mid \rho^n(x,\sigma,-\sigma) \mid^2\} \rho^\alpha(x).$$

It is clear that we have different ways of extending the definition of this interaction. In particular, we could have substituted in place of ρ any combination of $\rho(x)$, $\rho(x,\sigma,\sigma)$ and $\rho(x,\sigma,-\sigma)$.

Finally, we mention that when $q = q'$, we have

$$\rho^t(x,\sigma,-\sigma) = 0, \tag{115}$$

$$\rho^t(x,\sigma,\sigma) = \frac{1}{2}\rho^t(x), \tag{116}$$

and the expression for the Skyrme interaction reduces to the well-known Hartree-Fock form[19].

8 Conclusions

This paper has detailed the methodology requisite for calculating the kernel, or matrix element, of the Hill-Wheeler equation. In this, the first of a series, the methodology has been developed and illustrated for the normal, *i.e.* non-pairing, part of zero-range, *i.e.* Skyrme-like forces. It has also been developed for the normal part of a finite range interaction, the Gogny form. Application to the finite range case will be reserved for a subsequent paper.

We have also developed the methodology for the abnormal part of the force, *i.e.* the pairing force, only for the finite range case[1], although its illustration too will await a subsequent paper. We have not touched upon the delicate question of a *unique definition* of the Hill-Wheeler kernel, or matrix element, for density dependent forces. While this presents no ambiguity for diagonal terms, an arbitrary prescription has been introduced for off diagonal matrix elements. The presumed, *modest uncertainty* this will introduce into numerical examples must await future illustration and illumination.

[1] The structure of the Skyrme force does not permit its direct application to the pairing matrix elements. Pairing is always added to the Skyrme Hamiltonian in an *ad hoc* manner.

Appendix A: Notations and conventions

As already mentioned in Sec.3, the Bloch-Messiah theorem[15] allows us to write the most general Bogoliubov transformation[16] in the form of the so-called BCS transformation:

$$\begin{pmatrix} \xi_i^{q\dagger} \\ \xi_i^q \end{pmatrix} = \begin{pmatrix} u_i^q & -v_i^q \\ v_i^q & u_i^q \end{pmatrix} \begin{pmatrix} b_i^{q\dagger} \\ b_i^q \end{pmatrix}, \tag{117}$$

with the condition that $v_i^2 + v_i^2 = 1$. As long as we are only interested in the construction of the vacuum $\mid \Phi_q >$, then $\xi \equiv \eta$. In that case, we can neglect the third transformation (outlined in Sec.3.1). The operators $b_i^{q\dagger}$ create a particle in a state ϕ_i^q which is defined as

$$\phi_i^q(x,\sigma) =< x\sigma \mid b_i^{q\dagger} \mid 0 >, \qquad (\sigma : \textit{spin variable}). \tag{118}$$

We mention here that in the Hartree-Fock + BCS theory[10-12], the states ϕ_i^q are assumed to be Hartree-Fock states.

(i) Time-reversed states

The states ϕ_i^q can be grouped by pairs $(\phi_i^q, \phi_{\bar{i}}^q)$ which are in correspondence via the time-reversal operator T by

$$\phi_{\bar{i}}^q = \mathsf{T}\phi_i^q. \tag{119}$$

Using the conventions of ref.[19], this correspondence in the (x,σ) space is such that

$$\phi_{\bar{i}}^q(x,\sigma) = \sigma\phi_i^{q*}(x,-\sigma), \qquad (\sigma = \pm 1). \tag{120}$$

(ii) Single-particle overlap matrix

If we assume the two sets ϕ^q and $\phi^{q'}$ to form a complete basis, we can expand one in terms of the other as

$$\phi_j^{q'}(x,\sigma) = \sum_i r_{ij}^{qq'}\phi_i^q(x,\sigma), \tag{121}$$

where

$$r_{ij}^{qq'} = \sum_\sigma \int \phi_i^{q*}(x,\sigma)\phi_j^{q'}(x,\sigma)dx. \tag{122}$$

The same expression holds true for the operators $b^{q\dagger}$ and $b^{q'\dagger}$, *i.e*

$$b_j^{q'\dagger} = \sum_i r_{ij}^{qq'} b_i^{q\dagger}, \tag{123}$$

so that the anticommutator

$$\{b_j^{q'\dagger}, b_i^q\} = r_{ij}^{qq'}. \tag{124}$$

This relation is frequently used in Appendix B. It is easy to establish the relations

$$r_{ij}^{qq'} = r_{ij}^{qq'*}, \tag{125}$$

$$r_{ij}^{qq'} = r_{ij}^{q'q\dagger}. \tag{126}$$

Appendix B: Coupled equations satisfied by $A(x)$ and $B(x)$

In this appendix, we derive the equations for $A(x)$ and $B(x)$ whose definitions are

$$A_{ij}(x) = \frac{< \Phi_q, x \mid b_j^q b_i^q \mid \Phi_{q'} >}{< 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >}, \tag{127}$$

$$B_{ij}(x) = \frac{< \Phi_q, x \mid b_j^{q'\dagger} b_i^{q'\dagger} \mid \Phi_{q'} >}{< 0 \mid \Phi_{q'} >< \Phi_q \mid 0 >}. \tag{128}$$

An equivalent definition of $A_{ij}(x)$ is

$$A_{ij}(x) =< \Phi_q, x \mid e^{X_{q'}} e^{-X_{q'}} b_j^q b_i^q e^{X_{q'}} \mid 0 >, \tag{129}$$

where X is defined in Eq.(32). Starting from Eq.(129), we expand in a well-known manner the quantity $e^{-X_{q'}} b_j^q b_i^q e^{X_{q'}}$ in terms of commutators. The result is

$$e^{-X_{q'}} b_j^q b_i^q e^{X_{q'}} = b_j^q b_i^q - [X_{q'}, b_j^q b_i^q] + \frac{1}{2}[X_{q'}, [X_{q'}, b_j^q b_i^q]] + \cdots. \tag{130}$$

Evaluation of the first and second commutators gives

$$[X_{q'}, b_j^q b_i^q] = \sum_{k_>} \tan\theta_k^{q'} (r_{jk}^{qq'} b_k^{q'\dagger} b_i^q + r_{ik}^{qq'} b_k^{q'\dagger} b_j^q - r_{ik}^{qq'} r_{jk}^{qq'}), \tag{131}$$

$$[X_{q'}, [X_{q'}, b_j^q b_i^q]] = -2 \sum_{k_> l_>} \tan\theta_k^{q'} \tan\theta_l^{q'} r_{il}^{qq'} r_{jk}^{qq'} b_k^{q'\dagger} b_l^{q'\dagger}. \tag{132}$$

As a consequence, the expansion ends after the second commutator. Substitution of Eqs. (130)-(132) into Eq.(129) leads to

$$A(x) = r^{qq'} \tan\theta^{q'} r^{qq'\dagger} R(x) - r^{qq'} \tan\theta^{q'} B(x) \tan\theta^{q'} r^{qq'\dagger}, \tag{133}$$

where $R(x)$ is defined by Eq.(28). In deriving Eq.(133), we have used the property $r_{ij}^{qq'} = r_{ij}^{qq'*}$. (See Appendix A.) The notation $\tan\theta^{q'}$ means the matrix whose elements are $(\tan\theta^{q'})_{ij} = \delta_{ij} \tan\theta_i^{q'}$.

The equation for $B(x)$ is easily obtained from the one for $A(x)$ by noting that if we exchange $q \rightleftharpoons q'$ and replace $\tan\theta^q$ by $x \tan\theta^q$, then $B(x) = A^\dagger(x)$. Thus taking the Hermitian conjugate of Eq.(133) and using the property $r^{qq'\dagger} = r^{qq'}$, we obtain

$$B(x) = x\tau^{qq'\dagger}\tan\theta^q\tau^{qq'}R(x) - x^2\tau^{qq'\dagger}\tan\theta^q A(x)\tan\theta^q\tau^{qq'}. \tag{134}$$

Appendix C: Evaluation of the generalized density matrix

It is convenient to write the element $< \Phi_q \mid b_i^{q'\dagger}b_j^{q'} \mid \Phi_{q'} >$ in the form

$$< \Phi_c \mid b_i^{q'\dagger}b_j^{q'} \mid \Phi_{q'} >=< 0 \mid \Phi_{q'} >< \Phi_q \mid e^{X_{q'}}e^{-X_{q'}}b_i^{q'\dagger}b_j^{q'}e^{X_{q'}} \mid 0 >, \tag{135}$$

and expand $e^{-X_{q'}}b_i^{q'\dagger}b_j^{q'}e^{X_{q'}}$ in terms of commutators. The expansion is given by Eq.(130). However, all the commutator terms in the expansion except the first one are zero. Therefore,

$$< \Phi_q \mid b_i^{q'\dagger}b_j^{q'} \mid \Phi_{q'} >=< 0 \mid \Phi_{q'} >< \Phi_q \mid e^{X_{q'}}(b_i^{q'\dagger}b_j^{q'} - [X_{q'}, b_i^{q'\dagger}b_j^{q'}]) \mid 0 >, \tag{136}$$

where

$$[X_{q'}, b_i^{q'\dagger}b_j^{q'}] = -\sum_{k>}\tan\theta_k^{q'}(\delta_k^{q'\dagger}b_i^{q'\dagger} + b_i^{q'\dagger}b_k^{q'\dagger})\delta_{kj}. \tag{137}$$

Using now the definition of B [Eq.(35)], Eq.(136) can be written as

$$< \Phi_q \mid b_i^{q'\dagger}b_j^{q'} \mid \Phi_{q'} >= \tan\theta_j^{q'}B_{ji} < 0 \mid \Phi_{q'} >< \Phi_q \mid 0 > . \tag{138}$$

Finally, using Eqs.(51) and (53), we get

$$< \Phi_q \mid b_i^{q'\dagger}b_j^{q'} \mid \Phi_{q'} >=< \Phi_q \mid \Phi_{q'} > ([1 + M^{q'}]^{-1}M^{q'})_{ji}. \tag{139}$$

To calculate the element $< \Phi \mid b_i^{q'}b_j^{q'} \mid \Phi_{q'} >$, we proceed as before and note that only the first two commuttor terms are non-zero. Hence,

$$< \Phi_q \mid b_i^{q'}b_j^{q'} \mid \Phi_{q'} >=< 0 \mid \Phi_{q'} >< \Phi_q \mid e^{X_{q'}}(b_i^{q'}b_j^{q'} - [X_{q'}, b_i^{q'}b_j^{q'}]$$

$$+\frac{1}{2}[X_{q'}, [X_{q'}, b_i^{q'}b_j^{q'}]]) \mid 0 >, \tag{140}$$

where

$$[X_{q'}, b_i^{q'}b_j^{q'}] = -\tan\theta_j^{q'}b_j^{q'\dagger}b_i^{q'} - \tan\theta_i^{q'}(b_i^{q'\dagger}b_j^{q'} - \delta_{ij}), \tag{141}$$

$$[X_{q'}, [X_{q'}, b_i^{q'}b_j^{q'}]] = 2\tan\theta_i^{q'}\tan\theta_j^{q'}b_j^{q'\dagger}b_i^{q'\dagger}. \tag{142}$$

Substituting Eqs.(141) and (142) into Eq.(140) and then using Eqs.(35), (51) and (53), we obtain

$$< \Phi_q \mid b_i^{q'}b_j^{q'} \mid \Phi_{q'} >= - < \Phi_q \mid \Phi_{q'} > ([1 + M^{q'}]^{-1}\tan\theta^{q'})_{ij}. \tag{143}$$

The expression for $< \Phi_q \mid b_i^{q'\dagger} b_j^{q'\dagger} \mid \Phi_{q'} >$ is, by definition, directly connected to B and is

$$< \Phi_q \mid b_i^{q'\dagger} b_j^{q'\dagger} \mid \Phi_{q'} >= B_{ji} < 0 \mid \Phi_{q'} >< \Phi_q \mid 0 > . \tag{144}$$

Using Eqs.(53) and (55), Eq.(144) can be reduced to

$$< \Phi_q \mid b_i^{q'\dagger} b_j^{q'\dagger} \mid \Phi_{q'} >=< \Phi_q \mid \Phi_{q'} > (\tau^{qq'\dagger}[1+M^q]^{-1} \tan\theta^q \tau^{qq'})_{ji}. \tag{145}$$

Appendix D: Matrices S, T, Y, K and ρ

(I) Properties of S, T and Y

(a) $S_{\bar{i}\bar{j}} = S_{ij}$

Proof: Using the definition of S [Eq.(63)], we can write

$$S_{\bar{i}\bar{j}} = \frac{< \Phi_q \mid b_j^{q'\dagger} b_i^{q'} \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >}, \tag{146}$$

where

$$b_i^\dagger = \mathsf{T}^\dagger b_i^\dagger \mathsf{T}, \tag{147}$$

$$b_{\bar{i}}^\dagger = -\mathsf{T}^\dagger b_i^\dagger \mathsf{T}, \tag{148}$$

and T is the time-reversal operator. Furthermore, $\mid \Phi_q >$ as well as $\mid \Phi_{q'} >$ are even under application of the time-reversal operator, *i.e.* $\mathsf{T} \mid \Phi_q >= \mid \Phi_q >$, and the overlap $< \Phi_q \mid \Phi_{q'} >$ is real. Therefore,

$$\begin{aligned} S_{\bar{i}\bar{j}} &= \frac{< \Phi_q \mid \mathsf{T}^\dagger b_j^{q'\dagger} b_i^{q'} \mathsf{T} \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >} \\ &= \frac{< \Phi_q \mid b_j^{q'\dagger} b_i^{q'} \mid \Phi_{q'} >^*}{< \Phi_q \mid \Phi_{q'} >^*} \\ &= S_{ij}^*. \end{aligned} \tag{149}$$

But S is real. So,

$$S_{\bar{i}\bar{j}} = S_{ij}. \quad QED$$

(b) $Y_{\bar{i}j} = -Y_{i\bar{j}} = Y_{\bar{j}i}$

Proof: Using Eqs.(63), (147) and (148), we can write $Y_{\bar{i}j}$ as

$$Y_{ij} = -\frac{< \Phi_q \mid b_i^{q'} b_j^{q'} \mid \Phi_{q'} >}{< \Phi_q \mid \Phi_{q'} >}$$

$$= -\cdot \frac{< \Phi_q \mid \mathsf{T}^\dagger b_i^{q'} b_j^{q'} \mathsf{T} \mid \Phi_{q'} >^*}{< \Phi_q \mid \Phi_{q'} >^*}$$

$$= -Y_{ij}^* = -Y_{ij}. \tag{150}$$

Hence,

$$Y_{ij} = -Y_{ij} = Y_{ji}. \quad QED$$

(c) $T_{ij} = -T_{ij} = T_{ji}$

Proof: The proof is the same as that in (b).

(ii) Definition of ρ and K

Let us first calculate $\sum_{ij} S_{ij} < jq' \mid$, where S_{ij}, according to Eqs.(63) and (139), can be written as

$$S_{ij} = ([1 + M^{q'}]^{-1} M^{q'})_{ij}. \tag{151}$$

We now express $\sum_j M_{kj}^{q'} < jq' \mid$ as

$$\sum_{mj} (\tan\theta^{q'} \tau^{qq'\dagger} \tan\theta^q)_{km} \tau_{mj}^{qq'} < jq' \mid .$$

It is obvious that

$$\sum_j \tau_{mj}^{qq'} < jq' \mid = < mq \mid . \tag{152}$$

Thus,

$$\sum_{ij} S_{ij} < jq' \mid = \sum_{ij} ([1 + M^{q'}]^{-1} \tan\theta^{q'} \tau^{qq'\dagger} \tan\theta^q)_{ij} < jq \mid, \tag{153}$$

which leads us to define

$$\rho_{ij} = ([1 + M^{q'}]^{-1} \tan\theta^{q'} \tau^{qq'\dagger} \tan\theta^q)_{ij}, \tag{154}$$

so that we have the relation

$$\sum_{ij} S_{ij} < jq' \mid = \sum_{ij} \rho_{ij} < jq \mid . \tag{155}$$

To define K, we look at the quantity $\sum_{ij} T_{ij} < iq' \bar{j} q' \mid$, where T_{ij}, according to Eqs.(64) and (145), can be expressed in the form

$$T_{i\bar{j}} = (r^{qq'}[1 + M^q]^{-1} \tan\theta^q r^{qq'})_{j\bar{i}}. \tag{156}$$

Using the identity

$$\sum_j r^{qq'\dagger}_{jm} < \bar{j}q' \mid = < \bar{m}q \mid, \tag{157}$$

we find that

$$\sum_{ij} T_{i\bar{j}} < iq'\bar{j}q' \mid = \sum_{ij} ([1 + M^q]^{-1} \tan\theta^q)_{ij} < j\bar{q}\bar{i}q' \mid . \tag{158}$$

If we set

$$K^q_{i\bar{j}} = ([1 + M^q]^{-1} \tan\theta^q)_{ij}, \tag{159}$$

we get the relation

$$\sum_{ij} T_{i\bar{j}} < iq'\bar{j}q' \mid = \sum_{ij} K^q_{i\bar{j}} < j\bar{q}\bar{i}q' \mid . \tag{160}$$

Furthermore, from the definition of Y [Eq.(65)] and Eq.(143),

$$Y_{i\bar{j}} = -([1 + M^{q'}]^{-1} \tan\theta^{q'})_{ij}, \tag{161}$$

so that by comparing with Eq.(159), we get the following identity:

$$K^{q'}_{i\bar{j}} = -Y_{i\bar{j}}. \tag{162}$$

(iii) Properties of ρ, K^q and $K^{q'}$

According to Eqs.(155$\bar{j}$), (160) and (162), ρ has the same properties as S, K^q as T and $K^{q'}$ as Y. In particular, ρ, K^q and $K^{q'}$ are real. Furthermore,

$$\rho_{i\bar{j}} = \rho_{\bar{i}j}, \tag{163}$$

$$K^q_{i\bar{j}} = -K^q_{\bar{i}j} = K^q_{j\bar{i}}, \tag{164}$$

$$K^{q'}_{i\bar{j}} = -K^{q'}_{\bar{i}j} = K^q_{j\bar{i}}. \tag{165}$$

Appendix E: Properties of ρ^t, K^{tq}, $\kappa^{qq'}_t$ and $\Gamma^{qq'}_t$

The quantities $\rho^t(x,\sigma;x',\sigma')$, $K^{tq}(x,\sigma;x',\sigma')$, $\kappa^{qq'}_t(x)$ and $\Gamma^{qq'}_t(x)$ satisfy a number of relations which we shall derive in this appendix.

(i) $\rho^t(x,\sigma;x',\sigma') = \sigma\sigma'\rho^{t*}(x,-\sigma;x',-\sigma')$

We start from the definition of ρ^t which is [Eq.(91)]

$$\rho^t(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q*}_{it}(x,\sigma)\phi^{q'}_{jt}(x',\sigma')\rho^t_{ji}, \tag{166}$$

where the summation runs over the time-reversed states also. We can, therefore, also write Eq.(166) as

$$\rho^t(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q*}_{i\bar{t}}(x,\sigma)\phi^{q'}_{j\bar{t}}(x',\sigma')\rho^{\bar{t}}_{ji}. \tag{167}$$

Using Eqs.(120) and (163) in Eq.(167), we get

$$\rho^t(x,\sigma;x',\sigma') = \sigma\sigma'[\sum_{ij} \phi^{q*}_{it}(x,-\sigma)\phi^{q'}_{jt}(x',-\sigma')\rho^t_{ji}]^*, \tag{168}$$

which is simply the identity

$$\rho^t(x,\sigma;x',\sigma') = \sigma\sigma'\rho^{t*}(x,-\sigma;x',-\sigma'). \tag{169}$$

(ii) $K^{tq}(x,\sigma;x',\sigma') = \sigma\sigma' K^{tq*}(x,-\sigma;x',-\sigma')$

The definition of K^{tq} is [Eq.(92)]

$$K^{tq}(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q*}_{it}(x,\sigma)\phi^{q*}_{j\bar{t}}(x',\sigma')K^{tq}_{j\bar{i}}, \tag{170}$$

which can also be rewritten as

$$K^{tq}(x,\sigma;x',\sigma') = \sum_{ij} \phi^{q*}_{i\bar{t}}(x,\sigma)\phi^{q*}_{jt}(x',\sigma')K^{tq}_{\bar{j}i}. \tag{171}$$

Again, using Eq.(120) and the property of K given by Eq.(164), we obtain

$$K^{tq}(x,\sigma;x',\sigma') = \sigma\sigma'[\sum_{ij} \phi^{q*}_{it}(x,-\sigma)\phi^{q*}_{j\bar{t}}(x',\sigma')K^{tq}_{j\bar{i}}]^*, \tag{172}$$

which is nothing but the relation

$$K^{tq}(x,\sigma;x',\sigma') = \sigma\sigma' K^{tq*}(x,-\sigma;x',-\sigma'). \tag{173}$$

The property given by Eq.(96) is easily derived by using the fact that $K_{ij} = -K_{\bar{j}\bar{i}}$.

(iii) Properties of $\kappa^{qq'}_t(x)$ and $\Gamma^{qq'}_t(x)$

The definition of $\bar{\kappa}^{q'q}_t(x)$ is [Eq.(105)

$$\bar{\kappa}^{q'q}_t(x) = \sum_{ij,\sigma} [\nabla^2\phi^{q*}_{it}(x,\sigma)]\phi^{q'}_{jt}(x,\sigma)\rho^t_{ji}. \tag{174}$$

It is obvious that

$$\bar{\kappa}^{q'q}_t(x) + \kappa^{qq'}_t(x) = \nabla^2[\sum_{ij,\sigma} \phi^{q*}_{it}(x,\sigma)\phi^{q'}_{jt}(x,\sigma)\rho^t_{ji}] - 2\sum_{ij,\sigma} \vec{\nabla}\phi^{q*}_{it}(x,\sigma).\vec{\nabla}\phi^{q'}_{jt}(x,\sigma)\rho^t_{ji}. \tag{175}$$

Hence, we have the identity

$$\bar{\kappa}_t^{q'q}(x) + \kappa_t^{qq'}(x) = \nabla^2 \rho^t(x) - 2A_t^{qq'}(x), \tag{176}$$

where $A_t^{qq'}(x)$ is given by Eq.(107).

The definition of $\bar{\Gamma}_t^{q'q}(x)$ is [Eq.(106)]

$$\bar{\Gamma}_t^{q'q}(x) = \sum_{ij,\sigma} [\vec{\nabla}\phi_{it}^{q*}(x,\sigma)]\phi_{jt}^{q'}(x,\sigma)\rho_{ji}^t, \tag{177}$$

which is also equivalent to

$$\bar{\Gamma}_t^{q'q}(x) = \vec{\nabla}[\sum_{ij,\sigma} \phi_{it}^{q*}(x,\sigma)\phi_{jt}^{q'}(x,\sigma)\rho_{ji}^t] - \sum_{ij,\sigma} \phi_{it}^{q*}(x,\sigma)\vec{\nabla}\phi_{jt}^{q'}(x,\sigma)\rho_{ji}^t. \tag{178}$$

Hence, we have

$$\bar{\Gamma}_t^{q'q}(x) = \vec{\nabla}\rho^t(x) - \Gamma_t^{qq'}(x). \tag{179}$$

Appendix F: Numerical procedure

In calculating the energy E within the Hill-Wheeler approach, we have discretized the configuration space on a three-dimensional rectangular mesh. The mesh size Δx is the same in the three directions. The integrations were performed using the trapezoidal rule and the single-particle wave functions ϕ (Slater determinants) required in the calculation were obtained with the Hartree-Fock code of Bonche *et al*[19].

The expression for the total energy (kinetic + Skyrme + spin-orbit) depends on the first and second derivatives of the single-particle states. However, the terms involving the second derivatives can be expressed in terms of the first derivative as

$$\int \phi^* \nabla^2 \phi d^3x = -\int \vec{\nabla}\phi^* . \vec{\nabla}\phi d^3x. \tag{180}$$

To achieve good accuracy for all the terms in the energy, it is important that the gradients be computed with high precision. We have used the approximation

$$\frac{\partial f}{\partial x} = \frac{1}{\Delta x} \sum_{\lambda=-n}^{n} \omega_\lambda f(x + \lambda\Delta x) + O(\Delta x^{2n+2}), \tag{181}$$

where $2n+1$ is the number of points to be used in the approximation. We have done the calculations with the 7-point ($n = 3$) as well as the 9-point ($n = 4$) approximations and, as expected, found that the latter gives results with the desirable accuracy. The coefficients ω_λ are given in Table 1 and an example of the accuracy for the kinetic energy of ^{16}O with

spherical oscillator functions is shown in Table 2. In Table 3, we compare the Skyrme energy (SkIII interaction of Beiner *et al*[20]) given by the 9-point approximation with that of the Hartree-Fock calculation[19].

The numerical precision of the present calculation is further demonstrated in Table 4 where we present the nuclear binding energy of ^{16}O for $\Delta x = 1$ fm at finite quadrupole deformations $q = q' = 130$ fm^2. We notice a difference of about 2 MeV in the Skyrme energy given by the Hill-Wheeler and Hartree-Fock methods. This is because the Hartree-Fock method uses the 7-point approximation to calculate the first derivatives appearing in the expression for the Skyrme energy. If we use the 7-point approximation, we get -351.252 MeV which is very close to the Hartree-Fock result. However, the relative difference in the total energy calculated with the two methods is less that 0.2%.

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Table 1: Values of the coefficients ω_i.

Approximation	ω_0	$\omega_{\pm 1}$	$\omega_{\pm 2}$	$\omega_{\pm 3}$	$\omega_{\pm 4}$
7-point	0	$\pm 45/60$	$\mp 9/60$	$\pm 1/60$	-
9-point	0	$\pm 672/840$	$\mp 168/840$	$\pm 32/840$	$\mp 3/840$

Table 2: Accuracy on the kinetic energy (in MeV) of ^{16}O. The Slater determinant is built from harmonic oscillator functions (given by the Hartree-Fock code[19]) with β=0.275 fm^{-2}. The Hartree-Fock calculations used a 9-point Laplacian.

Mesh size (in fm)	1.0	0.8	0.5
Hartree-Fock	192.425	192.452	192.458
Hill-Wheeler			
a) 7-point	191.382	192.036	192.496
b) 9-point	192.154	192.398	192.456

Table 3: Skyrme energy (in MeV) of ^{16}O. The Hill-Wheeler results are obtained with the 9-point approximation.

Mesh size (in fm)	1.0	0.8	0.5
Hartree-Fock	−323.795	−323.555	−323.459
Hill-Wheeler	−323.711	−323.509	−323.455

Table 4: Nuclear binding energy (in MeV) of ^{16}O for $q = q' = 130$ fm^2. The Hill-Wheeler results are obtained with the 9-point approximation and a mesh size of 1 fm.

Energy	Hill-Wheeler	Hartree-Fock
Kinetic	246.613	247.959
Skyrme	−349.564	−351.549
Spin-Orbit	−22.589	−22.191
Total	−125.540	−125.781

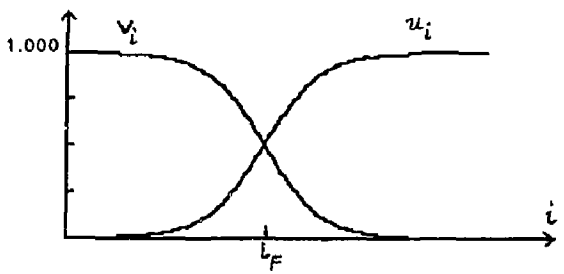

Figure 1: u_i and v_i as functions of i. i_F denotes the Fermi level.