Number-conserving random phase approximation with analytically integrated matrix elements

M. Kyotoku

Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, D-7400 Tübingen, Federal Republic of Germany and Departamento de Física, Universidade Federal da Paraiba, 5800 João Pessoa, Paraíba, Brazil

K. W. Schmid

Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, D-7400 Tübingen, Federal Republic of Germany

F. Grümmer

Institut für Theoretische Physik II, Universität Bochum, Postfach 102148, D-4630 Bochum, Federal Republic of Germany

Amand Faessler

Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, D-7400 Tübingen, Federal Republic of Germany (Received 10 April 1989)

In the present paper a number conserving random phase approximation is derived as a special case of the recently developed random phase approximation in general symmetry projected quasiparticle mean fields. All the occurring integrals induced by the number projection are performed analytically after writing the various overlap and energy matrices in the random phase approximation equation as polynomials in the gauge angle. In the limit of a large number of particles the well-known pairing vibration matrix elements are recovered. We also present a new analytically number projected variational equation for the number conserving pairing problem.

I. INTRODUCTION

In a recent paper a method to derive the random phase approximation (RPA) in general symmetryprojected quasiparticle mean fields was developed. In that paper the symmetries were restored by the VAMP procedure² (variation after mean field projection in realistic model spaces. This has been called the VAMPIR procedure in other publications.) In this rather sophisticated method one considers general Hartree-Fock-Bogoliubov (HFB) transformations breaking parity, charge number, mass number, and angular momentum conservation. Instead of considering this general case, we shall restrict ourselves in the present paper to the very simple case of a seniority zero system. Then the basic building blocks consist out of pairs of particles coupled to angular momentum zero, and consequently our system has fixed total angular momentum and parity $I^{\pi}=0^+$. Since we also consider only one type of particles (neutrons or protons), our system has a definite charge, too. Thus the only broken symmetry remaining is the nonconservation of the number of particles. The main purpose of the present paper is to use this simple seniority zero model as a testing ground for the general VAMP-RPA formalism.

Recently, by transforming both the energy as well as the overlap kernels into polynomial forms,3 the wellknown integral of number-projected Bardeen-Cooper-Schieffer (BCS) theory⁴ could be performed analytically. In the present paper we extend this procedure to the overlap and energy matrix elements that appear in the RPA formalism. This kind of extension is neither obvious nor trivial, since in these matrix elements there occur additional pairs of quasiparticles.

In the VAMP-RPA formalism a general symmetry projection is performed before the variation. Here we consider as broken symmetry only the particle number. Thus the general VAMP procedure can be replaced by the well-known FBCS (Ref. 5) prescription (BCS with fixed number of particles). In the present paper we shall take the opportunity to rederive the corresponding variational equation using the generalized form of Thouless' theorem⁶ and perform the occurring integrals analytically. This new FBCS equation gets a very simple form, and can be used later on to simplify part of the numberprojected matrix elements of the RPA scheme. Here we can see one of the advantages of the analytical integration revealing some nontrivial connections between the projected RPA and FBCS. This fact suggests some possible simplifications in the treatment of the general VAMP-RPA, too.

Via the transformation of overlaps and energy matrix elements into polynomials, we obtain a binomial type of distribution. Taking the Gaussian limit of this distribution. i.e., the limit for a large number of particles, we can test the consistency of our procedure. Indeed, in this limit not only the usual BCS-variational equation is regained, but also some well-known expressions from the standard RPA (Ref. 7) in the seniority model are recovered. Thus the VAMP-RPA formalism is soundly based, and it seems worthwhile to study some less restrictive versions of it than the present one in the future.

From a more restricted point of view, we present here

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one more of several alternative ways to deal with the pairing collective model, 8 which still 9 attracts some attention, mainly as a testing ground for nuclear many-body theories. In this context it should be stressed that the present approach is symmetry conserving and thus does not encounter the typical breakdown of the usual quasiparticle RPA. The number-conserving RPA scheme presented here allows the extension of the BCS and RPA theories, in which the physical interpretation is very transparent, across the so-called phase transition region.

The present paper is organized as follows: in the next section we derive the analytical number-conserving BCS variational equation (FBCS equation). In Sec. III then the number-conserving Tamm-Dancoff approximation (TDA) and RPA approaches are presented. Performing the number projection analytically, all the occurring matrix elements are represented in closed form in Sec. IV. The Gaussian limit of these expressions is then obtained in Sec. V, and, finally, some conclusions are drawn in Sec. VI.

II. ANALYTICAL FBCS EQUATION

Let us start by defining the creation and annihilation operators in the spherical shell model basis as c_{jm}^{\dagger} and c_{jm} , respectively. We then introduce BCS-type quasiparticle creation and annihilation operators via

$$\begin{bmatrix}
a_{jm}^{\dagger}(\Delta) \\
a_{jm}(\Delta)
\end{bmatrix} = F^{T}(\Delta) \begin{bmatrix}
c_{jm}^{\dagger}(\Delta) \\
c_{jm}(\Delta)
\end{bmatrix},$$
(2.1)

with $a_{j\bar{m}}$ being the usual time-reversed operators defined as

$$a_{i\overline{m}} \equiv (-)^{j-m} a_{j-m}$$

and

$$F(\Delta) \equiv \begin{bmatrix} u_j(\Delta) & v_j(\Delta) \\ -v_i(\Delta) & u_i(\Delta) \end{bmatrix} . \tag{2.2}$$

This is the well-known Bogoliubov-Valatin¹⁰ transformation. The parameter Δ is here explicitly indicated in order to distinguish between different BCS transformations. The vacuum $|F(\Delta)\rangle$ of the annihilation operators in (2.1) has the form

$$|F(\Delta)\rangle = \left\{\prod_{im} a_{jm}(\Delta)\right\}|0\rangle.$$
 (2.3)

Let us now assume that a particular vacuum $|F(\Delta_0)\rangle$ of the above form is known. Using the generalized Thouless' theorem⁶ one can then write any other BCS vacuum $|F(\Delta)\rangle$, which is not orthogonal to $|F(\Delta_0)\rangle$, as

$$|F(\Delta)\rangle = c(\Delta) \exp\left[\sum_{j} \sqrt{\Omega_{j}} d_{j} \mathcal{A}_{j}^{\dagger}\right] |F(\Delta_{0})\rangle$$
, (2.4)

with $\mathcal{A}_{i}^{\dagger}$ being defined in Appendix A (A17) and

$$c(\Delta) = \langle F(\Delta_0) | F(\Delta) \rangle$$
, while $\Omega_j = j + \frac{1}{2}$. (2.5)

The parameters d_j in the formula (2.4) connect the BCS transformation coefficients related to the different vacua

 Δ and Δ_0 . These parameters, and further properties of this representation were discussed in Ref. 2 for the general case of angular momentum and number projection, and it is redundant to repeat this discussion here.

Obviously the BCS-type vacuum (2.3) or (2.4) violates the conservation of the particle number. In order to restore it we have to use the projection operator⁴

$$\hat{P}_{N} = \frac{1}{2\pi} \int_{0}^{2\pi} \exp\left[-i\frac{\theta}{2}(N - \hat{N})\right] d\theta$$

$$\equiv \frac{1}{2\pi} \int_{0}^{2\pi} \exp\left[-i\frac{N}{2}\theta\right] \hat{S} d\theta , \qquad (2.6)$$

where N is the total number of particles of the system and $\hat{N} = \sum c_{jm}^{\dagger} c_{jm}$ the particle number operator.

The expectation value of the usual pure pairing force Hamiltonian (this Hamiltonian and its quasiparticle representation are presented in Appendix A) within the number projected vacuum (2.4) is then given by

$$E_0^N = \frac{I_E}{I_O} \ , \tag{2.7}$$

where

$$I_{O} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{-i(N/2)\theta} \langle F | \hat{S} \exp \left[\sum_{j} \sqrt{\Omega_{j}} d_{j} \mathcal{A}_{j}^{\dagger} \right] | F_{0} \rangle d\theta ,$$
(2.8)

and

$$I_{E} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{-i(N/2)\theta} \langle F | \hat{H} \hat{S} \exp \left[\sum_{j} \sqrt{\Omega_{j}} d_{j} \mathcal{A}_{j}^{\dagger} \right] | F_{0} \rangle d\theta$$
(2.9)

The variation of the functional (2.7) with respect to the d_j yields then

$$\frac{\partial E_0^N}{\partial d_i} = 0 = g_j(\Delta) , \qquad (2.10)$$

with

$$g_{j}(\Delta) = \frac{1}{2\pi} \int_{0}^{2\pi} e^{-i(N/2)\theta} \sqrt{\Omega_{j}} \langle F | (\hat{H} - E_{0}^{N}) \hat{S} \mathcal{A}_{j}^{\dagger} | F \rangle d\theta .$$

$$(2.11)$$

The evaluation of general matrix elements with rotated and nonrotated quasiparticles using a sort of generalized Wick's theorem was discussed in Ref. 11 for the case of general HFB quasiparticle transformations. For the simple case of pairs of quasiparticles coupled to total angular momentum zero [see expression (A17)] considered here one can also use the prescriptions presented in Ref. 12. We simply show the final result for the overlap between a rotated two quasiparticle and the zero quasiparticle state. The derivation is given in the reference mentioned above. We obtain

$$\langle F|\widehat{S}\mathcal{A}_{j}^{\dagger}|F\rangle = n(\theta)\sqrt{\Omega_{j}}k_{j}(\theta)$$
, (2.12)

with

$$n(\theta) = \prod_{p} (u_{p}^{2} + v_{p}^{2} e^{i\theta})^{\Omega_{p}} , \qquad (2.13)$$

and

$$k_{j}(\theta) = \frac{\sqrt{\Omega_{j}} u_{j} v_{j} (e^{i\theta} - 1)}{(u_{i}^{2} + v_{i}^{2} e^{i\theta})} . \tag{2.14}$$

The prescription for the derivation of the energy matrix elements in (2.11) is very similar. Some details can be found in Appendix B. For nucleons in a spherical mean field, ϵ_j , subject to a residual pure pairing force G, the energy matrix elements in (2.11) are

$$\langle F | \hat{H} \hat{S} \mathcal{A}_{j}^{\dagger} | F \rangle = \frac{n(\theta)}{\sqrt{\Omega_{j}}} \left[\frac{2\mathcal{E}_{j} \Omega_{j} u_{j} v_{j} e^{i\theta}}{u_{j}^{2} + v_{j}^{2} e^{i\theta}} - G \frac{\Omega_{j} (u_{j}^{2} - v_{j}^{2})}{u_{j}^{2} + v_{j}^{2} e^{i\theta}} \sum_{p} \frac{\Omega_{p} \tilde{\delta}(pj) u_{p} v_{p} e^{i\theta}}{u_{p}^{2} + v_{p}^{2} e^{i\theta}} \right]$$

$$+ \frac{n(\theta)}{\Omega_{j}} k_{j}(\theta) \left[\sum_{p} \frac{2\mathcal{E}_{p} \Omega_{j} \Omega_{p} v_{p}^{2} e^{i\theta}}{u_{p}^{2} + v_{p}^{2} e^{i\theta}} \tilde{\delta}(pj) - G \sum_{pq} \frac{\Omega_{p} \Omega_{q} \tilde{\delta}(pq) \tilde{\delta}(qj^{2}) u_{p} v_{p} u_{q} v_{q} e^{i\theta}}{(u_{p}^{2} + v_{p}^{2} e^{i\theta}) (u_{q}^{2} + v_{p}^{2} e^{i\theta})} \right],$$

$$(2.15)$$

where

$$\mathcal{E}_j \equiv \epsilon_j - \frac{G}{2} , \qquad (2.16)$$

$$\widetilde{\delta}(pj) \equiv 1 - \frac{\delta_{pj}}{\Omega_p}$$
, (2.17)

$$\widetilde{\delta}(qj^2) \equiv 1 - 2\frac{\delta_{qj}}{\Omega_p} \ . \tag{2.18}$$

One should mention that the shifting term G/2 in (2.16) appears as a counterpart to the term (2.17) in the formula (2.15), and can be interpreted as an overall shift in the single-particle levels. However, in the case of a more realistic force, to which our scheme can easily be generalized, the diagonal matrix elements yield state-dependent shifts of the corresponding single-particle levels. The last of the preceding three formulas (2.18) appears as a connection between h_0 and h_{02}^{\dagger} , which are given in Appendix B by Eqs. (B5) and (B6), respectively.

Now the overlaps (2.12) and the energy matrix elements (2.15) can be expanded into polynomials in the variable $e^{i\theta}$ after successively using Newton's binomial formula in (2.13). Here the expressions (2.17) and (2.18) play an essential role, since both factors, $\Omega_p \tilde{\delta}(pj)$ and $\Omega_p \Omega_q \tilde{\delta}(pq) \tilde{\delta}(qj^2)$, cancel the terms, which cannot be expressed by a polynomial form. The prescription how to transform overlaps into polynomial forms was formulated

in Ref. 3, and hence will not be repeated here. However we mention that the standard binomial distribution of the type

$$B_{p} = \begin{bmatrix} \Omega_{p} \\ l_{p} \end{bmatrix} (u_{p}^{2})^{\Omega_{p} - l_{p}} (v_{p}^{2})^{l_{p}} , \qquad (2.19)$$

appears clearly isolated from the other terms and the polynomial resembles the expression (2.12) and (2.15). This separation is not so obvious because of the existence of terms like $(u_p^2 + v_p^2 e^{i\theta})^n$, with n an integer, in the denominator, however, using some identities for binomial coefficients and a convenient renumeration of the l_p , it is possible to obtain the polynomial form, which we are looking for.

After having the overlaps and the energy matrix elements in the polynomial form, we can easily perform the integration over the gauge angle θ , and we obtain the following very simple number-projected variational equation (FBCS equation):

$$\left[I_O \hat{I}_E - I_E \hat{I}_O\right] (l_j - \Omega_j v_j^2) = 0 \tag{2.20}$$

with

$$I_O = \sum_{(I=N/2)} \left(\prod_p B_p \right) \tag{2.21}$$

and

$$I_E = \sum_{(l=N/2)} \left[\left[\prod_p B_p \right] \left[\sum_q 2\mathcal{E}_q l_q - G \sum_{qr} \frac{u_r v_q}{u_q v_r} (\Omega_q - l_q) l_r \right] \right], \tag{2.22}$$

where the sums run over all l_p $(p=1,\ldots,M)$ with M being the number of spherical basis orbits) with the constraints that $l=\sum l_p=N/2$ and $0 \le l_p \le \Omega_p$. The aforementioned "hat" symbols \widehat{I}_E and \widehat{I}_O indicate that the corresponding expressions (2.22) and (2.21) have to be multiplied with the additional factor $(l_j-\Omega_j v_j^2)$ before the sums are performed. Obviously the factor $\Omega_j v_j^2$ does

not contribute in (2.20), and hence we could drop it. However, we shall keep it here for additional discussions and approximations in Sec. V. The expressions (2.21) and (2.22) are, respectively, the analytically projected BCS energy and overlap kernels and were obtained from Eqs. (2.8) and (2.9) in Ref. 3. The energy kernel (2.22) I_E is presented here in an even simpler form than in this refer-

ence.

As one can easily see, the structure of the integrated FBCS equation (2.20) is different from the usual BCS equation, where one part proportional to $(u_j^2 - v_j^2)$ and another to $u_j v_j$ is obtained. However, if we approximate the binomial distribution (2.19) by a Gaussian form and the sums over the l's by integrals, as will be shown in Sec. V, the usual BCS equation is recovered. Thus the FBCS equation (2.20) is related to the well-known gap equation in spite of the fact that the gap parameter (Δ) from the BCS theory does not appear here as transparently as in the broken-symmetry variational equation.

In practical calculations, the solution of the FBCS equation (2.20) is as easy as that of the normal gap equation. One needs as input only the parameters (ϵ_p , G, Ω_p , and N) provided by the problem and can then determine the u_p and v_p with the condition $u_p^2 + v_p^2 = 1$ after performing adequately the summation over the l_1, l_2, \ldots, l_M . As already mentioned, the factor $\Omega_j v_j^2$ does not contribute to Eq. (2.20) and can hence be ignored in such a calculation. Finally, we would like to mention already at this place that Eq. (2.20) can be used later on to simplify part of the matrix elements occurring in the FBCS-TDA and FBCS-RPA approaches discussed later. This is another advantage of the analytically integrated equation presented here.

Last but not least, it is worthwhile to note that Eq. (2.20) can be rederived from the standard variational scheme, i.e., obtaining first the projected functional in analytical form and then performing the variation such that

$$\left[\frac{\partial}{\partial v_j} - \frac{v_j}{u_i} \frac{\partial}{\partial u_i}\right] E_0^N \equiv \nabla(v_j, u_j) E_0^N = 0 . \qquad (2.23)$$

Using (2.7), (2.21), (2.22), and the binomial distribution (2.19) we can easily get the variational equation (2.20), because of the identity

$$\sum_{(l=N/2)} \left[\prod_{p} B_{p} \right] \left[\sum_{j \neq p} \left[\frac{u_{p}}{u_{j}^{3} v_{p}} (\Omega_{j} - l_{j}) l_{p} - \frac{v_{p}}{u_{j} v_{j}^{2} u_{p}} (\Omega_{p} - l_{p}) l_{j} \right] \right] = 0 ,$$

$$(2.24)$$

which is easy to verify, if one writes the product $(\prod_p B_p)$ as $(\prod_{q\neq p\neq j} B_q) B_p B_j$. The term in inner square brackets in (2.24) is the result of the differentiation

$$\nabla(v_j, u_j) \sum_{pq} \frac{u_q u_p}{u_p v_q} (\Omega_p - l_p) l_q , \qquad (2.25)$$

while factor $(l_j - \Omega_j v_j^2)$ in (2.20) is obtained by the differentiation

$$\nabla(v_j, u_j) B_j = \frac{2(l_j - \Omega_j v_j^2)}{u_i^2 v_j} B_j . \qquad (2.26)$$

Because of the vanishing right-hand side of Eq. (2.23) the term $2/u_j^2 v_j$ can be dropped, and the number-projected variational equation is obtained as

$$I_{O}\nabla(v_{i},u_{i})I_{E}-I_{E}\nabla(v_{i},u_{i})I_{O}=0$$
, (2.27)

with the $\nabla(v_j, u_j)$ given by (2.23) and the differentiation in I_E to be performed over the binomial distribution B_j . The additional differentiation gives zero, as can be seen from the expression (2.24).

In the present section we have derived in two alternative ways a number-projected variational equation in order to obtain the Bogoliubov transformation coefficients, u_p and v_p , which will be essential in what follows.

III. FBCS-TDA AND FBCS-RPA

Solving the number-projected variational equation (2.2) one obtains the minimum of the functional (2.7). The next step is to consider vibrations around this minimum, i.e., to obtain a corresponding TDA or RPA. For the seniority zero system, the TDA formulation in the number-conserving scheme was proposed long ago, ¹³ however, even for this very simple case the RPA is yet to be done, and therefore this is one of the main purposes of the present paper.

Recently we proposed a method to incorporate vibrational excitations in a general symmetry-projected variational method (VAMP approach). In that paper a symmetry-conserving RPA equation (VAMP-RPA) was derived. Now, if we consider that all the particle pairs are coupled to total angular momentum zero (seniority zero), the formalism of the VAMP-RPA is reduced to the case of FBCS-RPA, or in other words, we present an application of the formalism previously developed to the case of projection of only the particle number. We furthermore simplify the problem by choosing a pure pairing force. This choice is not essential for the derivation, but since no additional qualitative information is obtained in considering a general force, we prefer to restrict ourselves to the most simple one available.

Since the FBCS-TDA and FBCS-RPA are contained in the VAMP-TDA and VAMP-RPA, we present here only those features of the latter approximations that are essential for the full understanding of the present paper. Further details and additional discussions can be found in Ref. 1.

A. FBCS-TDA

Let us start with a configuration space consisting out of the number-projected zero and two quasiparticle states:

$$\zeta_N \equiv \left[\hat{P}_N | F_N \rangle \equiv |0_N \rangle; \; \hat{P}_N \mathcal{A}_j^{\dagger} | F_N \rangle \equiv |j_N \rangle \; \right] .$$
(3.1)

Here $|F_N\rangle$ means that the coefficients of the Bogoliubov transformation (2.2) have been determined through the FBCS equation (2.20) for a specific nucleus with N particles. This procedure determines the projected zero quasiparticle state $|0_N\rangle$ (the FBCS solution).

Because of the number projection operator, the aforementioned states (3.1) are not anymore orthogonal. They can, however, be orthogonalized by the Gram-Schmidt procedure via

$$|(j)_N\rangle = |j_N\rangle - |0_N\rangle \mathcal{N}_{0:i} , \qquad (3.2)$$

where

$$\mathcal{N}_{0:i} = \langle 0_N | j_N \rangle = \langle F_N | \hat{P}_N \mathcal{A}_i^{\dagger} | F_N \rangle , \qquad (3.3)$$

is the overlap between the number-projected zero and two quasiparticle states. Obviously, (3.2) is by construction orthogonal to $|0_N\rangle$. Furthermore, because of Eqs. (2.10) and (2.11) we obtain

$$\langle 0_N | \hat{H} | (j)_N \rangle = \langle 0_N | \hat{H} | j_N \rangle$$

$$-E_0 \mathcal{N}_{0,j} = g_j(\Delta) = 0.$$
(3.4)

The overlap matrix between the number-projected orthogonalized states (3.2) then has the form

$$C_{ii}^{N} \equiv \langle (i)_{N} | (j)_{N} \rangle \equiv \mathcal{N}_{i:i} - \mathcal{N}_{0:i}^{*} \mathcal{N}_{0:i} , \qquad (3.5)$$

with

$$\mathcal{N}_{i \cdot i} \equiv \langle F_N | \mathcal{A}_i \hat{P}_N \mathcal{A}_i^{\dagger} | F_N \rangle . \tag{3.6}$$

The corresponding energy matrix elements can be written as

$$\langle (i)_N | \hat{H} | (j)_N \rangle = A_{ii}^N + E_0^N C_{ii}^N,$$
 (3.7)

where E_0^N is the FBCS energy given by (2.7), while

$$A_{ij}^{N} = H_{i;j} - E_{0}^{N} \mathcal{N}_{i;j} , \qquad (3.8)$$

and, finally,

$$H_{i:i} = \langle F_N | \mathcal{A}_i \hat{H} \hat{P}_N \mathcal{A}_i^{\dagger} | F_N \rangle . \tag{3.9}$$

The next step is then to diagonalize the overlap matrix (3.5). Since C^N is symmetric and positive definite, there exists an orthogonal transformation matrix X_N such that

$$X_N^T C^N X_N = 1_n \lambda_N$$
,

and thus

$$\lambda_N^{-1/2} X_N^T C^N X_N \lambda_N^{-1/2} = 1_m . {(3.10)}$$

Keeping only the $m \le n$ linear independent solutions (with $\lambda_N \ne 0$)

$$|\mu_N\rangle = \sum_j (\lambda_N^{-1/2} X_N)_{j\mu} |(j)_N\rangle, \quad \mu = 1, \dots m ,$$
 (3.11)

we obtain an m-dimensional, orthonormal basis for the subsequent diagonalization of the Hamiltonian. Defining

$$(H_{\text{TDA}}^{N})_{\mu\nu} \equiv \langle \mu_{N} | \hat{H} | \nu_{N} \rangle - E_{0}^{N} \langle \mu_{N} | \nu_{N} \rangle$$

$$\equiv (\lambda_{N}^{-1/2} X_{N}^{T} A^{N} X_{N} \lambda_{N}^{1/2})_{\mu\nu}$$

$$\equiv A_{\mu\nu}^{N} , \qquad (3.12)$$

the diagonalization

$$Y_{\text{TDA}}^{N^T} H_{\text{TDA}}^N Y_{\text{TDA}}^N = 1_m \hbar \omega^{\text{TDA}} , \qquad (3.13)$$

vields then a set of m eigenstates

$$|\omega_N^{\text{TDA}}\rangle = \sum_{\mu=1}^m |\mu_N\rangle Y_{\text{TDA}}^N , \qquad (3.14)$$

with eigenvalues

$$\hbar\omega^{\text{TDA}} = E_{\omega}^{N} - E_{0}^{N} . \tag{3.15}$$

The present subsection establishes once more the FBCS-TDA scheme as well as the main quantities, which are needed to be derived through a sort of generalized Wick's theorem, subsequently transformed into a polynomial, and finally to be integrated.

B. FBCS-RPA

The extension of the earlier approach to an RPA-like model is now straightforward. We start be defining the creation operators

$$b_{\mu}^{\dagger} = \sum_{j} (\lambda_{N}^{-1/2} X_{N}^{T})_{\mu j} (\mathcal{A}_{j}^{\dagger} - \mathcal{N}_{0;j}) , \qquad (3.16)$$

in terms of which of the orthonormalized numberprojected 2qp configurations (3.11) may be written as

$$|\mu_N\rangle = \hat{P}_N b_\mu^\dagger |F_N\rangle \ . \tag{3.17}$$

Similarly, we can introduce number-projected 4qp configurations via

$$|\mu_N \nu_N\rangle = \hat{P}_N b_\mu^{\dagger} b_\nu^{\dagger} |F_N\rangle , \qquad (3.18)$$

however, these states are neither orthogonal to the FBCS state $|0_N\rangle$ nor the configuration (3.17). Thus, we proceed by defining

$$|(\mu\nu)_N\rangle = \hat{S}_{\mathbf{Z}}\hat{P}_{\mathbf{N}}b_{\mu}^{\dagger}b_{\nu}^{\dagger}|F_N\rangle \tag{3.19}$$

with

$$\hat{S}_{Z} \equiv 1 - |0_{N}\rangle\langle 0_{N}| - \sum_{\mu} |\mu_{N}\rangle\langle \mu_{N}| , \qquad (3.20)$$

being a mathematical projector ensuring the required orthogonality. Now, we can construct a generating function

$$|\phi_{N}(z')\rangle = |0_{N}\rangle + \sum_{\mu} |\mu_{N}\rangle z_{\mu}^{\prime*} + \frac{1}{2} \sum_{\mu\nu} |(\mu\nu)_{N}\rangle z_{\mu}^{\prime*} z_{\nu}^{\prime*} + O(|z'^{*}|^{3}), \quad (3.21)$$

and then, following Jancovici and Schiff¹⁴ and Holzwarth,¹⁵ make a GCM (Ref. 16) ansatz

$$|\Psi_N(z')\rangle = \int |\phi_N(z')\rangle \mathcal{F}_N(z')dz', \qquad (3.22)$$

for the total wave function. Minimizing the normalized energy expectation value E in this wave function, with respect to variations of the weight function $\mathcal{F}(z')$, one gets the well-known Griffin-Hill-Wheeler (GHW) integral equation. Using the generating function (3.21) the overlap kernel of the GHW equation now approximately takes a Gaussian shape. Expanding the quotient of energy and overlap kernel of the GHW equation only up to second order, and with the help of the transformed function G_N defined as

$$G_N(z) \equiv \int \exp \left[\sum_{\mu} z_{\mu} z_{\nu}^{\prime *} \right] \mathcal{F}_N(z^{\prime}) dz^{\prime} , \qquad (3.23)$$

it is possible to transform the GHW integral equation into a system of coupled partial differential equations for

 $G_N(z)$ of the form

$$\sum_{\mu\nu} \left[A_{\mu\nu}^{N} z_{\mu} \frac{\partial}{\partial z_{\nu}} + \frac{1}{2} B_{\mu\nu}^{N} z_{\mu} z_{\nu} + \frac{1}{2} B_{\mu\nu}^{N} \frac{\partial^{2}}{\partial z_{\mu} \partial z_{\nu}} - (E - E_{0}^{N}) \right] G_{N}(z) = 0 .$$

$$(3.24)$$

Here $A_{\mu\nu}^N$ is given by (3.12). Because of the nonorthonormality between the projected zero 2 and 4qp states, the matrix elements of $B_{\mu\nu}^N$ are more complicated than in the standard case. They can be obtained through the expressions (3.16) and (3.19) as

$$B_{\mu\nu}^{N} \equiv \langle 0_{N} | \hat{H} | (\mu\nu)_{N} \rangle$$

$$\equiv \sum_{ij} (\lambda_{N}^{-1/2} X_{N}^{T})_{\mu i} B_{ij}^{N} (X_{N} \lambda_{N}^{-1/2})_{j\nu} , \qquad (3.25)$$

where

$$B_{ii}^{N} \equiv H_{0:ii} - E_{0}^{N} N_{0:ii}$$
 (3.26)

with

$$\begin{bmatrix}
N_{0;ij} \\
H_{0;ij}
\end{bmatrix} = \left\langle F_N \middle| \begin{cases} 1 \\ \widehat{H} \end{cases} \widehat{P}_N \mathcal{A}_i^{\dagger} \mathcal{A}_j^{\dagger} \middle| F_N \right\rangle.$$
(3.27)

The differential equations (3.24) are the well-known representation of the Schrödinger equation with a quadratic Hamiltonian for bosons

$$\hat{H}_{q} = E_{0}^{N} + \sum_{\mu\nu} A_{\mu\nu}^{N} b_{\mu}^{\dagger} b_{\nu} + \frac{1}{2} \sum_{\mu\nu} B_{\mu\nu}^{N} (b_{\nu}^{\dagger} b_{\nu}^{\dagger} + b_{\mu} b_{\nu}) , \quad (3.28)$$

being one of the few many-body Hamiltonians that can be solved exactly. It can be diagonalized with the help of a Bogoliubov transformation for bosons, yielding the standard RPA equation, which subsequently can be rewritten after suitable manipulations of the matrix C^N (3.5) and the matrix transformation X_N . This leads to a number-projected RPA equation of the form

$$\begin{bmatrix} A^{N} & B^{N} \\ B^{N} & A^{N} \end{bmatrix} \begin{bmatrix} \tilde{Y}^{N} \\ \tilde{Z}^{N} \end{bmatrix} = \hbar \omega^{\text{RPA}} \begin{bmatrix} C^{N} & 0 \\ 0 & -C^{N} \end{bmatrix} \begin{bmatrix} \tilde{Y}^{N} \\ \tilde{Z}^{N} \end{bmatrix} . \quad (3.29)$$

This form of the RPA equation is well known in theoretical chemistry. The matrix elements A^N and B^N can be calculated through (3.8) and (3.26), after the determination of the coefficients u_p and v_p through the variational equation (2.20). The column matrix $(\frac{\tilde{Y}^N}{\tilde{Z}^N})$ is related to the original RPA column matrix $(\frac{Y^N}{Z^N})$ via

$$\begin{bmatrix} \widetilde{Y}^{N} \\ \widetilde{Z}^{N} \end{bmatrix} = \begin{bmatrix} X_{N} \lambda_{N}^{-1/2} & 0 \\ 0 & X_{N} \lambda_{N}^{-1/2} \end{bmatrix} \begin{bmatrix} Y^{N} \\ Z^{N} \end{bmatrix}.$$
 (3.30)

In the next section we are evaluating the matrix elements out of (3.29) by an analytical integration over the gauge angle.

IV. ANALYTICALLY INTEGRATED QUASIPARTICLE OVERLAPS AND ENERGY MATRIX ELEMENTS

In the present section we shall perform the numberprojection integrals analytically, in a similar way as we did to derive the FBCS equation in Sec. II. We obtain the various overlaps and energy matrix elements derived in the last section and summarized in the eigenvalue equation (3.29) in terms of the Bogoliubov transformation coefficients (2.2) and the fixed parameters of our problem $(\epsilon_p, G, \Omega_p, \text{ and } N)$.

A. Analytically integrated overlaps

The first overlap expression (3.3) that appears in Sec. III was already defined by (2.12). The corresponding analytically integrated expression is

$$\mathcal{N}_{0;j} = \frac{1}{\sqrt{\sigma_i}} \hat{I}_O(l_j - \Omega_j v_j^2) , \qquad (4.1)$$

where I_O is given in (2.21) [see discussion following (2.21) for the explanation of \hat{I}_O] and

$$\sigma_i \equiv \Omega_i u_i^2 v_i^2 \ . \tag{4.2}$$

The second overlap to be calculated is the expression (3.6) with two rotated quasiparticles on one side, and another two quasiparticle state on the other side. This overlap was derived for the rotations in the Euler and gauge angles in Ref. 11. For our restricted case we obtain

$$\langle F_N | \mathcal{A}_i \hat{S} \mathcal{A}_i^{\dagger} | F_N \rangle = n(\theta) n_{ij}(\theta) ,$$
 (4.3)

with

$$n_{ij}(\theta) = \frac{\delta_{ij}}{X_i^2(\theta)} + k_i(\theta)k_j(\theta) , \qquad (4.4)$$

where $k_i(\theta)$ is given by (2.14) and

$$X_{j}(\theta) \equiv u_{j}^{2} e^{-(i/2)\theta} + v_{j}^{2} e^{(i/2)\theta}$$
 (4.5)

In order to perform the analytical integration over the expression (4.3) we need to rewrite it as a polynomial. For this purpose we use the simple identities

$$\frac{1}{u_i^2 + v_i^2 e^{i\theta}} \begin{bmatrix} e^{i\theta} \\ 1 \end{bmatrix} = 1 \pm \frac{(e^{i\theta} - 1)}{u_i^2 + v_i^2 e^{i\theta}} \begin{bmatrix} u_i^2 \\ v_i^2 \end{bmatrix}, \tag{4.6}$$

to rewrite the expression (4.4) as

$$n_{ij}(\theta) = \delta_{ij} \frac{v_i^2 + u_i^2 e^{i\theta}}{u_i^2 + v_i^2 e^{i\theta}} + \tilde{\delta}(ij)k_i(\theta)k_j(\theta) . \tag{4.7}$$

As in (2.15) the factor $\tilde{\delta}(ij)$ cancels here all the terms, which cannot be represented in polynomial form. After obtaining the polynomial form we can perform the integration for both the $i\neq j$ and i=j cases. The final results are

$$\mathcal{N}_{i;j} = \frac{1}{\sqrt{\sigma_i \sigma_j}} \hat{I}_O L_{ij}^{(1)} , \qquad (4.8)$$

with

$$L_{ii}^{(1)} \equiv (l_i - \Omega_i v_i^2)(l_i - \Omega_i v_i^2) . \tag{4.9}$$

Inserting (4.8) and (4.1) in (3.5) we get

$$C_{ij}^{N} = \frac{1}{\sqrt{\sigma_{i}\sigma_{j}}} \{ \hat{I}_{O}L_{ij}^{(1)} - [\hat{I}_{O}(l_{i} - \Omega_{i}v_{i}^{2})] \times [\hat{I}_{O}(l_{j} - \Omega_{j}v_{j}^{2})] \}, \qquad (4.10)$$

which can be diagonalized according to (3.10), yielding the transformation matrix X_N needed to orthonormalize the wave functions (3.11).

Finally, following the same techniques used up to here, we can obtain the last integrated overlap with four rotated quasiparticles on one side and zero quasiparticles on the other side (3.27). Here one derives

$$\mathcal{N}_{0;ij} = \frac{1}{\sqrt{\sigma_i \sigma_i}} \hat{I}_O L_{ij} , \qquad (4.11)$$

with

$$L_{ii} \equiv L_{ii}^{(1)} + L_{ii}^{(2)} , \qquad (4.12)$$

where $L_{ij}^{(1)}$ was given by (4.9), and $L_{ij}^{(2)}$ is the diagonal matrix element

$$L_{ii}^{(2)} \equiv \delta_{ii} [v_i^2 (l_i - \Omega_i v_i^2) - l_i u_i^2] . \tag{4.13}$$

B. Analytical energy matrices

We now proceed by deriving the energy matrix elements. Following the systematic order of Sec. III, the first to be evaluated ought to be (3.9) and the second one is (3.27). We begin with (3.27) being

$$H_{0;ij} = \frac{1}{2\pi} \int_0^{2\pi} \langle F_N | \hat{H} \hat{S} \mathcal{A}_i^{\dagger} \mathcal{A}_j^{\dagger} | F_N \rangle d\theta . \qquad (4.14)$$

This matrix element is discussed in some detail in Appendix B. We obtain, dropping the angle θ from the notation

$$\langle F_{N}\hat{H}\hat{S}\mathcal{A}_{i}^{\dagger}\mathcal{A}_{j}^{\dagger}|F_{N}\rangle = \tilde{\delta}(ij) \left[k_{i}k_{j}h_{0} + \frac{k_{i}}{X_{j}^{2}}h_{02}^{i} + \frac{k_{j}}{X_{i}^{2}}h_{02}^{j} + \frac{2n(\theta)}{X_{i}^{2}X_{j}^{2}}H_{40}^{ij} \right],$$
(4.15)

where $\tilde{\delta}(ij)$ was defined by (2.17) and h_0 and h_{02}^i (or h_{02}^j) can be rewritten from (B5) and (B6) as

$$h_{0} = n(\theta) \left[\sum_{p} \frac{2\mathcal{E}_{p} v_{p}^{2} e^{i\theta}}{u_{p}^{2} + v_{p}^{2} e^{i\theta}} - G \sum_{pq} \frac{\Omega_{q} \Omega_{p} \tilde{\delta}(pq) u_{p} v_{p} u_{q} v_{q} e^{i\theta}}{(u_{p}^{2} + v_{p}^{2} e^{i\theta})(u_{q}^{2} + v_{q}^{2} e^{i\theta})} \right]$$
(4.16)

and

$$h_{02}^{i} = n(\theta) \left[2\mathcal{E}_{i} \Omega_{i} u_{i} v_{i} - G(u_{i}^{2} - v_{i}^{2} e^{i\theta}) \sum_{p} \frac{\Omega_{p} \widetilde{\delta}(pi) u_{p} v_{p}}{u_{p}^{2} + v_{p}^{2} e^{i\theta}} \right], \quad (4.17)$$

respectively. The H_{40}^{ij} are given by (A13). Finally, the definition of X_i and k_i can be found in (4.5) and (2.14), respectively. The term $\delta(ij)$ can be interpreted as a functional manifestation of the Pauli principle, since if i=j and $\Omega_i=1$ we get $\delta(ij)=0$, i.e., no more than one pair of quasiparticles is allowed for this particular case.

Using the identities (4.6) and additionally

$$\frac{u_i^2 - v_i^2 e^{i\theta}}{u_i^2 + v_i^2 e^{i\theta}} = (u_i^2 - v_i^2) - \frac{2u_i^2 v_i^2 (e^{i\theta} - 1)}{u_i^2 + v_i^2 e^{i\theta}} , \qquad (4.18)$$

we can transform the energy matrix elements (4.15) into

$$\begin{split} \langle F_N | \hat{H} \hat{S} \mathcal{A}_i^{\dagger} \mathcal{A}_j^{\dagger} | F_N \rangle &= n(\theta) \tilde{\delta}(ij) \left[\frac{G \sqrt{\Omega_i \Omega_j} (u_i^2 v_j^2 + v_i^2 u_j^2) e^{i\theta}}{(u_i^2 + v_i^2 e^{i\theta}) (u_j^2 + v_j^2 e^{i\theta})} \right. \\ &+ k_i \left[\frac{2 \mathcal{E}_j \sqrt{\Omega_j} u_j v_j e^{i\theta}}{u_j^2 + v_j^2 e^{i\theta}} - \frac{G \sqrt{\Omega_j} e^{i\theta}}{u_j^2 + v_j^2 e^{i\theta}} \sum_{pq} \frac{(u_q^2 - v_q^2) u_p v_p}{u_p^2 + v_p^2 e^{i\theta}} \Omega_p \tilde{\delta}(pqi) \delta_{qj} \right] \\ &+ k_j \left[\frac{2 \mathcal{E}_i \sqrt{\Omega_i} u_i v_i e^{i\theta}}{u_i^2 + v_i^2 e^{i\theta}} - \frac{G \sqrt{\Omega_i} e^{i\theta}}{u_i^2 + v_i^2 e^{i\theta}} \sum_{pq} \frac{(u_q^2 - v_q^2) u_p v_p}{u_p^2 + v_p^2 e^{i\theta}} \Omega_p \tilde{\delta}(pqj) \delta_{qi} \right] \\ &+ k_i k_j \left[\sum_p \frac{2 \mathcal{E}_p v_p^2 e^{i\theta}}{u_p^2 + v_p^2 e^{i\theta}} \tilde{\delta}(pij) - G \sum_{pq} \frac{[\Omega_p \Omega_q \tilde{\delta}(pq) \tilde{\delta}(qi^2j^2) + 2 \delta_{pi} \delta_{qj}] u_p v_p u_q v_q e^{i\theta}}{(u_p^2 + v_p^2 e^{i\theta}) (u_q^2 + v_q^2 e^{i\theta})} \right] \right], \end{split}$$

where

$$\widetilde{\delta}(pqi) \equiv 1 - \frac{\delta_{pq}}{\Omega_p} - \frac{\delta_{pi}}{\Omega_p} , \qquad (4.20)$$

$$\widetilde{\delta}(qi^2j^2) \equiv 1 - 2\frac{\delta_{qi}}{\Omega_a} - 2\frac{\delta_{qj}}{\Omega_a} \ . \tag{4.21}$$

The last two formulas (4.20) and (4.21) are obvious exten-

sions of (2.17) and (2.18), respectively. Together with

$$[\widetilde{\delta}(pq)\widetilde{\delta}(qi^2j^2) + 2\delta_{pi}\delta_{qj}], \qquad (4.22)$$

they always appear in energy matrix elements such as (4.19) or (2.15) and cancel just those terms, which cannot be represented by a polynomial. This feature obviously should have some interpretation. The main reason seems to be the functional manifestation of the Pauli principle

as discussed in the expression (4.15). This can be seen, for example, by calculating the term $\langle F_N | \hat{H}_{40} \mathcal{A}_i^{\dagger} \mathcal{A}_j^{\dagger} | F_N \rangle$. However, the ultimate reason for the existence of factors such as (4.22) is not always clear. They appear also as a result of algebraic manipulations with the help of the identities (4.6) and (4.8). The most trivial example for this case is (4.7), which was derived from (4.4), and the factor $\delta(ij)$ appears quite naturally without any clear physical meaning.

After obtaining a polynomial the integration is straightforward though lengthy. We finally obtain

$$H_{0;ij} = \frac{1}{\sqrt{\sigma_i \sigma_j}} \hat{I}_E L_{ij} , \qquad (4.23)$$

where L_{ij} and I_E are given by (4.12) and (2.22), respectively. There the explanation for the symbol (\hat{I}_E) can also be found. As in (2.26) one notes that the factor

$$(l_i - \Omega_i v_i^2)(l_i - \Omega_i v_i^2)$$

in (4.23) originates from the differentiation of B_p first with respect to $\nabla(u_j, v_j)$ and afterwards to $\nabla(u_i, v_i)$. However, the origin of the term

$$\delta_{ij}[v_i^2(l_i - \Omega_i v_i^2) - u_i^2 l_i]$$

is not so easy to be interpreted. Here the factor $\tilde{\delta}(ij)$ plays an important role.

Inserting the expressions (4.23), (4.11), and (2.7) in (3.26) we obtain

$$B_{ij}^{N} = \frac{I_O \hat{I}_E - I_E \hat{I}_O}{\sqrt{\sigma_i \sigma_i} I_O} L_{ij} . \tag{4.24}$$

This is actually a very simple expression for the RPA matrix (3.26). However, from the new FBCS equation (2.20), we immediately see that

$$\delta_{ii}(I_O \hat{I}_E - I_E \hat{I}_O)[v_i^2 (l_i - \Omega_i v_i^2) - l_i u_i^2] = 0 , \qquad (4.25)$$

and thus our B_{ii}^{N} will have the even simpler form

$$B_{ij}^{N} = \frac{I_{O}\hat{I}_{E} - I_{E}\hat{I}_{O}}{\sqrt{\sigma_{i}\sigma_{i}}I_{O}} (l_{i} - \Omega_{i}v_{i}^{2})(l_{j} - \Omega_{j}v_{j}^{2}) . \tag{4.26}$$

Again the terms $\Omega_i v_i^2$ and $\Omega_j v_j^2$ do not contribute here and could hence be dropped. However, as in Sec. II, we shall keep them here for further discussions in Sec. V. It is worth to emphasize that the FBCS equation (4.25) could be used here to obtain the simple expression (4.26). This fact shows the power of the present scheme using closed forms obtained by analytical integration, suggesting clearly that it is worthwhile to try to treat less restricted models than the present one in a similar way. This nontrivial interconnection between the RPA matrix elements and the number-projected variational equation is one of the most interesting consequences of the present work.

In order to get the A_{ij}^N we need to calculate the most complicated energy matrix elements. These matrix elements (3.9) involve two quasiparticles on each side of the Hamiltonian

$$H_{i;j} = \frac{1}{2\pi} \int_0^{2\pi} \langle F_N | \mathcal{A}_i \widehat{H} \widehat{S} \mathcal{A}_j^{\dagger} | F_N \rangle d\theta , \qquad (4.27)$$

and are also obtained in some detail in Appendix B. Inserting (4.7), (A12), (A13), and (A14) in (B18) we get, after some straightforward manipulations

$$\langle F_{N} | \mathcal{A}_{i} \hat{H} \hat{S} \mathcal{A}_{j}^{\dagger} | F_{N} \rangle = \tilde{\delta}(ij) \left[k_{i} k_{j} h_{0} + \frac{k_{i}}{X_{j}^{2}} h_{02}^{i} + \frac{k_{j}}{X_{i}^{2}} h_{02}^{j} + \frac{2n(\theta)}{X_{i}^{2} X_{j}^{2}} H_{40}^{ij} \right] + \left[2k_{i} k_{j} h_{11}^{i} - \frac{v_{i}^{2} + u_{i}^{2} e^{i\theta}}{u^{2} + v_{i}^{2} e^{i\theta}} k_{j} h_{02}^{i} + k_{j} h_{22}^{i} \right]$$

$$+ \delta_{ij} \left[\frac{v_{i}^{2} + u_{i}^{2} e^{i\theta}}{u_{i}^{2} + v_{i}^{2} e^{i\theta}} h_{0} + \frac{2}{X_{i}^{2}} h_{11}^{i} + n(\theta) \frac{G(u_{i}^{4} + v_{i}^{4}) e^{i\theta}}{(u_{i}^{2} + v_{i}^{2} e^{i\theta})^{2}} \right] - \tilde{\delta}(ij) \left[\frac{n(\theta) G \sqrt{\Omega_{i} \Omega_{j}} e^{i\theta}}{(u_{i}^{2} + v_{i}^{2} e^{i\theta}) (u_{i}^{2} + v_{i}^{2} e^{i\theta})} \right], \quad (4.28)$$

with h_{11}^i and h_{22}^i being defined in Appendix B by the formulas (B19) and (B20), respectively. They can be represented as

$$h_{11}^{i} = n(\theta) \left[\epsilon_{i} (u_{i}^{2} - v_{i}^{2}) + G v_{i}^{4} + G u_{i} v_{i} \sum_{p} \frac{\tilde{\delta}(pi) u_{p} v_{p} (e^{i\theta} + 1)}{u_{p}^{2} + v_{p}^{2} e^{i\theta}} \right]$$

$$(4.29)$$

and

$$h_{22}^{i} = n(\theta)\sqrt{\Omega_{i}} \left[(\epsilon_{i} - Gv_{i}^{2})2u_{i}v_{i} - G(u_{i}^{2}e^{i\theta} - v_{i}^{2}) \sum_{p} \frac{\Omega_{p}u_{p}v_{p}}{u_{p}^{2} + v_{p}^{2}e^{i\theta}} \right]. \tag{4.30}$$

Let us call the first term in (4.28) $\langle F_N | \mathcal{A}_i \hat{H} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle_1$. This is the same expression as (4.14). The integrated expression of this term $(H_{i;j}^1)$, was already obtained in (4.23). The second term of (4.18) $(H_{i;j}^2)$ is zero. This one can easily verify, since

$$h_{22}^{i} = -2k_{i}h_{11}^{i} + \frac{v_{i}^{2} + u_{i}^{2}e^{i\theta}}{u_{i}^{2} + v_{i}^{2}e^{i\theta}}h_{02}^{i} . \tag{4.31}$$

Now we need to obtain the integrated form of the third term $(H_{i;j}^3)$. Let us rewrite this term in the form

$$\langle F_{N} | \mathcal{A}_{i} \widehat{H} \widehat{S} \mathcal{A}_{j}^{\dagger} | F_{N} \rangle_{3} = \delta_{ij} \left[-h_{0} + n(\theta) \left[\frac{2\mathcal{E}_{i} \Omega_{i} e^{i\theta}}{u_{i}^{2} + v_{i}^{2} e^{i\theta}} + \sum_{p} \frac{2\mathcal{E}_{p} \Omega_{p} \widetilde{\delta}(pi) v_{p}^{2} e^{i\theta}(e^{i\theta} + 1)}{(u_{i}^{2} + v_{i}^{2} e^{i\theta})(u_{p}^{2} + v_{p}^{2} e^{i\theta})} \right. \\ \left. + G \sum_{pq} \frac{\Omega_{p} \Omega_{q} \widetilde{\delta}(pq) \widetilde{\delta}(qi^{2}) u_{p} v_{p} u_{q} v_{q} e^{i\theta}(e^{i\theta} + 1)}{(u_{i}^{2} + v_{i}^{2} e^{i\theta})(u_{p}^{2} + v_{p}^{2} e^{i\theta})(u_{q}^{2} + v_{q}^{2} e^{i\theta})} \right] \right] .$$
 (4.32)

The last and fourth term will be left as in (4.28). Now transforming the third term (4.32) and the fourth term in polynomials and performing the analytical intergration we get

$$H_{i;j}^{3} = -\frac{1}{\sigma_{i}} \left[\hat{I}_{E} L_{ij}^{(2)} - \delta_{ij} G \hat{I}_{O} \sum_{p} \frac{u_{p} v_{i}}{u_{i} v_{p}} (\Omega_{i} - l_{i}) l_{p} \right]$$
(4.33)

and

$$H_{i;j}^{4} = -\frac{G}{\sqrt{\sigma_{i}\sigma_{j}}} \hat{I}_{O} \frac{u_{j}v_{i}}{u_{i}v_{j}} (\Omega_{i} - l_{i})l_{j} , \qquad (4.34)$$

respectively. Adding all the $H_{i;j}$'s, i.e., (4.23), (4.33), and (4.34), we note that the first term of $H_{i;j}^3$ is equal to the last of $H_{i;j}^1$ but with opposite sign. Thus, we get

$$H_{i;j} = \frac{1}{\sqrt{\sigma_i \sigma_j}} \hat{I}_E L_{ij}^{(1)} + A_{ij}^R , \qquad (4.35)$$

with

$$A_{ij}^{R} \equiv \frac{G}{\sqrt{\sigma_{i}\sigma_{i}}} \hat{I}_{O} \sum_{p} \frac{u_{p}}{v_{p}} l_{p} (\delta_{ij} - \delta_{pj}) \frac{v_{i}}{u_{i}} (\Omega_{i} - l_{i}) . \tag{4.36}$$

Inserting now the aformentioned $H_{i;j}$, (4.35), (4.8), and (2.7) in (3.8) we get simply

$$A_{ij}^{N} = B_{ij}^{N} + A_{ij}^{R} . {(4.37)}$$

These are the last energy matrix elements that are needed, and together with B_{ij}^N and C_{ij}^N can be used to obtain the solutions of the number-projected RPA equation (3.29) yielding the numerical eigenvalues of the quadratic Hamiltonian (3.28). These can thus be compared with some exact solutions. ¹⁸ However, in the present paper we shall only check the consistency of our derivation by taking the limit for large N and reproducing the well-known results for pairing vibrations. Numerical results from the FBCS-RPA will be published in a forthcoming paper.

V. GAUSSIAN LIMIT

In the last section we derived the number-projected matrix elements A_{ij}^N and B_{ij}^N , which appear in the number-projected RPA equation. In the present section, using the standard Gaussian limit for the binomial expression (2.19), we shall transform the obtained summations into integrals, which in contrast to the gauge integrals are trivial to be performed, as we shall see. In this way we shall obtain the A_{ij}^N and B_{ij}^N in the well-known form. This illustrates the consistency of our FBCS-RPA equations, since the limit of FBCS-RPA for a large number of particles should be the usual broken-symmetry quasiparticle RPA.

Since this kind of procedure has not been discussed in

the usual number-projected theories, we shall take here the opportunity to rederive the BCS ground-state energy from the analytical number-projected expression. We shall also present the Gaussian limit of the FBCS equation (2.20).

A. BCS approximation

Transforming the binomial distribution (2.19) into Gaussian form is not new in the context of the nuclear pairing model. However, it was not widely used, since the aforementioned procedure was applied to more restricted cases, and, as we shall see, our conclusions are a little bit different from those of Ref. 19. Thus, it is worthwhile to present a few lines about this subject.

Using the Stirling formula for the factorials

$$n! \simeq (2\pi)^{1/2} (n)^{n+1/2} e^{-n}$$

in the binomial distribution (2.19) we get the so-called Moivre-Laplace limit²⁰ for the binomial

$$B_{p} = \left[\frac{\Omega_{p}}{2\pi l_{p}(\Omega_{p} - l_{p})}\right]^{1/2} \left[\frac{\Omega_{p}v_{p}^{2}}{\Omega_{p}}\right]^{l_{p}} \left[\frac{\Omega_{p}u_{p}^{2}}{\Omega_{p} - l_{p}}\right]^{\Omega_{p} - l_{p}}.$$

$$(5.1)$$

Introducing a new variable

$$l_p = \Omega_p v_p^2 + \chi_p \quad , \tag{5.2}$$

in the expression (5.1), passing to the logarithmic form, and subsequently performing a Taylor expansion in $\chi_p/\Omega_p v_p^2$ and $\chi_p/\Omega_p u_p^2$, we obtain after convenient rearrangements the simple Gaussian form

$$B_p \simeq \frac{1}{\sqrt{2\pi}\sigma_p} \exp\left[-\frac{\chi_p^2}{2\sigma_p^2}\right],$$
 (5.3)

where σ_p was given by (4.2).

With the introduction of the new variable (5.2) we get after performing the number projection integral

$$\sum_{p} l_{p} = \sum_{p} \Omega_{p} v_{p}^{2} + \chi_{p} = \frac{N}{2} . \tag{5.4}$$

Considering the number equation from the BCS theory

$$\sum \Omega_n v_n^2 = N/2 , \qquad (5.5)$$

we immediately get

$$\sum_{p} \chi_{p} = 0 . ag{5.6}$$

Therefore, if the sum of all the terms of the new variable is zero, and considering that our system has a large number of particles, then $-\infty < \chi_p < \infty$, and all the summations, for example, in (2.21) can be replaced by a product of standard type Gaussian integrals

$$I_O = \prod_p \left[\frac{1}{\sqrt{2\pi}\sigma_p} \int_{-\infty}^{\infty} \exp\left[-\frac{\chi_p^2}{2\sigma_p^2} \right] d\chi_p \right] = 1 . \quad (5.7)$$

Now we introduce some well-known results involving Gaussian functions, which will be useful later.

$$\langle \chi_p \rangle = \langle \chi_p \chi_q \chi_i \rangle = \frac{1}{\sqrt{2\pi}\sigma_p} \int_{-\infty}^{\infty} \chi_p B_p d\chi_p = 0 , \quad (5.8a)$$

$$\langle \chi_p^n \rangle = \frac{1}{\sqrt{2\pi}\sigma_p} \int_{-\infty}^{\infty} \chi_p^n B_p d\chi_p = 1 \cdot 3 \cdot \cdot \cdot (2n-1)(\sigma_p^2)^n ,$$

$$\sqrt{2\pi O_p}$$
 ω

and

$$\langle \chi_p \chi_q \rangle = \frac{1}{2\pi\sigma_p \sigma_q} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \chi_p \chi_q B_p B_q d\chi_p d\chi_q$$
$$= \sigma_p \delta_{pq} . \tag{5.8c}$$

With these results in mind we can insert (5.2) into (2.22). Using the Gaussian limit in the projected nuclear pairing model we obtain

$$I_{E} = \sum_{p} (2\epsilon_{p} - G)(\Omega_{p}v_{p}^{2} + \langle \chi_{p} \rangle) - G\sum_{pq} \frac{u_{q}v_{p}}{u_{p}v_{q}}(\Omega_{p}\Omega_{q}u_{p}^{2}v_{q}^{2} + \Omega_{p}v_{p}^{2}\langle \chi_{q} \rangle - \Omega_{q}v_{q}^{2}\langle \chi_{p} \rangle - \langle \chi_{p}\chi_{q} \rangle) , \qquad (5.9)$$

where the integrals of the type (5.7) have already been performed.

Using (5.8) in (5.9) we get trivially

$$I_{\text{BCS}} = \sum_{p} (2\epsilon_{p} - \lambda - Gv_{p}^{2})\Omega_{p}v_{p}^{2} - G\sum_{pq} \Omega_{p}\Omega_{q}u_{p}u_{q}v_{p}v_{q} , \qquad (5.10)$$

which is the standard BCS expression for the ground-state energy of a seniority zero system. Transforming the binomial distribution into Gaussian form we thus get back the BCS ground-state energy and recover the broken-symmetry result. Here we need to introduce the Lagrange multiplier λ in order to conserve at least the average number of particles, which is assured by the number equation (5.5). This conclusion is different from that of Ref. 19, where an additional correction term in the two level case was obtained, but it is also not new. In fact the Gaussian limit for a binomial distribution means that we have the limit of number of particles $N \to \infty$, i.e., $\Omega_i \to \infty$. In this limit Bayman⁴ recovered the BCS approximation long ago by transforming the overlap integrals (2.8) and (2.9) in a Darwin-Fowler type of integral.

B. Gaussian limit for the FBCS equation

The simple prescription described in the previous section can also be applied to the FBCS equation (2.20). Inserting (5.2) in (2.20) and using $\hat{I}_O \langle \chi_i \rangle = 0$ and $I_O = 1$ we derive

$$\sum_{p} (2\epsilon_{p} - \lambda - G)(\Omega_{p}v_{p}^{2}\langle\chi_{i}\rangle + \langle\chi_{p}\chi_{i}\rangle) - G\sum_{pq} \frac{u_{q}v_{p}}{u_{p}v_{q}} \left[\Omega_{p}\Omega_{q}u_{p}^{2}v_{q}^{2}\langle\chi_{i}\rangle + \Omega_{p}u_{p}^{2}\langle\chi_{q}\chi_{i}\rangle - \Omega_{q}v_{q}^{2}\langle\chi_{p}\chi_{i}\rangle - \langle\chi_{p}\chi_{q}\chi_{i}\rangle\right] = 0.$$

$$(5.11)$$

With the help of (5.8) this yields immediately

$$(2\epsilon_i - \lambda - G)u_i v_i - G(u_i^2 - v_i^2) \sum_p \Omega_p u_p v_q = 0.$$
 (5.12)

This is the BCS equation if $G \rightarrow 2Gv_p^2$. This small difference is due to the fact that the Gaussian approximation to the integral of the second term in (2.15) is not zero, providing a small difference between the preceding result and the BCS equation.

C. Broken-symmetry RPA

We shall now apply the Gaussian limit to the RPA equation. Using

$$\mathcal{N}_{0;j} = \frac{1}{\sqrt{\sigma_j}} \langle \chi_j \rangle = 0 , \qquad (5.13)$$

$$\mathcal{N}_{i;j} = \frac{1}{\sqrt{\sigma_i \sigma_j}} \langle \chi_i \chi_j \rangle = \delta_{ij} , \qquad (5.14)$$

and

$$\mathcal{N}_{0;ij} = \frac{1}{\sqrt{\sigma_i \sigma_j}} \{ \langle \chi_i \chi_j \rangle - \delta_{ij} [(u_i^2 - v_i^2) \langle \chi_i \rangle + \Omega_i u_i^2 v_i^2] \} = 0 , \qquad (5.15)$$

we obtain for (3.5) $C_{i:j} = \delta_{ij}$. Therefore the matrix X_N in (3.10) is the unit matrix with the eigenvalues $\lambda_N = 1$. Conse-

quently (3.11) has the form

$$|\mu_N\rangle = \sum_j \delta_{j\mu} |(j)_N\rangle . \tag{5.16}$$

These approximations mean that $\hat{P}_N = 1$, and we are again left with the broken-symmetry case. Equation (3.29) now becomes a standard RPA equation with B_{ij}^N and A_{ij}^N , given by (4.26) and (4.37), respectively. Using the Gaussian approximation and inserting (5.2) into (4.26) we get

$$B_{ij} = \frac{1}{\sqrt{\sigma_i \sigma_j}} \left[\sum_{p} (2\epsilon_p - \lambda - G) \Omega_p v_p^2 \langle \chi_i \chi_j \rangle - G \sum_{pq} \frac{u_q v_p}{u_p v_q} (\Omega_p \Omega_q u_p^2 v_q^2 \langle \chi_i \chi_j \rangle - \langle \chi_p \chi_q \chi_i \chi_j \rangle) - I_{BCS} \langle \chi_i \chi_j \rangle \right]. \tag{5.17}$$

Let us first consider the case $i \neq j$. Here the outcome is obvious, since $\langle \chi_i \chi_j \rangle$ is zero according to Eq. (5.8c) and the only term to be calculated is $\langle \chi_p \chi_q \chi_i \chi_j \rangle$. After some trivial manipulations one obtains finally

$$B_{ij} = -\frac{G}{2} \sqrt{\Omega_i \Omega_j} (u_i^2 - v_i^2) (u_j^2 - v_j^2) + \frac{G}{2} \sqrt{\Omega_i \Omega_j} ,$$
(5.18)

which is identical to the result obtained long ago in Ref. 7, except for the term $(G/2)\sqrt{\Omega_i\Omega_j}$, responsible for the spurious pairing vibration modes. For the case i=j, the BCS-like term appears twice, canceling each other. The term different from zero comes partially from the term $\langle \chi_i^4 \rangle$, partially from $\langle \chi_i^2 \rangle \langle \chi_i^2 \rangle$, yielding the same expression as above now with i=j.

The last expression to be approximated is A_{ij}^N out of Eq. (4.37). We have already partially studied this case and need only to analyze A_{ij}^R (4.36). In this case the nonzero terms are

$$A_{ij}^{R} = \frac{G}{u_i v_j} \delta_{ij} \sum_{p} \Omega_p u_p v_p - G \sqrt{\Omega_i \Omega_j} . \qquad (5.19)$$

If we take the FBCS equation

$$\frac{(u_i^2 - v_i^2)}{u_i v_i} (I_O \hat{I}_E - I_E \hat{I}_O) (l_i - \Omega_i v_i^2) = 0$$
 (5.20)

in the Gaussian limit and add the expression (5.19), we finally get

$$A_{ij} = 2\delta_{ij}H_{11}^{i} - \frac{G}{2}\sqrt{\Omega_{i}\Omega_{j}}(u_{i}^{2} - v_{i}^{2})(u_{j}^{2} - v_{j}^{2}) - \frac{G}{2}\sqrt{\Omega_{i}\Omega_{j}}.$$
(5.21)

Here H_{11}^i is given by (A10) if we replace again G by $2Gv_p^2$. This is again a well-known result: if the Gaussian approximation is applied to the number-projected RPA matrix elements one obtains the usual pairing vibration matrix elements.

VI. CONCLUSIONS

In the present work, using the Thouless' theorem, we obtain the FBCS equation with the overlaps and the energy matrix elements to be integrated. Then, transforming them into polynomials in the gauge angles, we could perform the occurring integrals analytically. The resulting FBCS equation (2.20) is equally simple as the usual BCS equation in spite of the fact the gap parameter (Δ) from

the BCS theory does not appear here in an equally transparent way. The analytical FBCS equation was later rederived using the standard variational procedure over the analytically integrated energy functional.

Considering small-amplitude vibrations around the minimum from the above-mentioned analytically integrated energy functional we have derived, as a particular case of the recently developed VAMP-RPA, using the well-known technique developed by Jancovici and Schiff and later generalized by Holzwarth, a number-projected RPA equation (3.29). This RPA equation is known in theoretical chemistry and resembles the standard RPA eigenvalue equation. Here the matrices A^N , B^N , as well as the matrix C^N , which appears additionally in the present scheme, are obtained from number-projected wave functions.

It should be noted that the VAMP-RPA, though using a similar formalism, is conceptually somewhat different from the broken pair model recently reviewed by Allaart et al.21 While in the latter the shell model configuration space is truncated according to a generalized seniority scheme, in the VAMP approach and its recent extensions (see, e.g., Ref. 22, and references therein) the selection of the relevant configurations is entirely left to the dynamics of the considered system and achieved by various chains of variational calculations. Nevertheless, it would be interesting to see whether the broken pair model could be extended to general symmetry-breaking mean fields of the VAMP type and to compare the resulting truncation to the small-amplitude approximation made here and in Ref. 1. For this purpose, however, the techniques discussed in Ref. 21 are not yet sufficient.

Transforming the overlaps as well as the energy matrix elements occurring in the above-mentioned number-projected RPA equation into polynomials, we could obtain the matrix elements A_{ij}^N , B_{ij}^N , and C_{ij}^N , Eqs. (4.37), (4.26), and (4.10), respectively, in a closed form after performing the integrals analytically. The final expressions for the earlier matrices are so simple and practical as the FBCS equation. One of the interesting aspects of the present procedure is that the analytical FBCS equation (2.20) could be used to simplify part of the diagonal elements of the matrices A^N and B^N .

In order to test the validity of the present approach we considered the limit of a large number of particles. As expected, in this limit we obtain the well-known pairing vibration matrix elements as well as the BCS expression for the ground state and the BCS gap equation. Therefore we could establish once again, this time in a more

practical way, the general method to obtain a RPA on the basis of general symmetry-projected quasiparticle mean fields. Thus it may be worthwhile to pursue less restricted versions of this approach than the one studied in the present paper in spite of all the limitations of the RPA itself, which were discussed in detail in Ref. 1.

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APPENDIX A

Using the quasiparticle transformation (2.2) one can represent the usual pairing Hamiltonian

$$\hat{H} = \sum_{pm} \epsilon_p c_{pm}^{\dagger} c_{pm} - \frac{G}{4} \sum_{pqmn} c_{pm}^{\dagger} c_{p\overline{m}}^{\dagger} c_{q\overline{n}} c_{qn}$$
 (A1)

in terms of the quasiparticle creation a_{pm}^{\dagger} and annihilation operators a_{pm} in many different ways. We write this Hamiltonian in the quasiparticle representation as

$$\hat{H} = H_0 + \hat{H}_{11} + \hat{H}_{20} + \hat{H}_{22} + \hat{H}_{40} + \hat{H}_{31} + \hat{H}_{22}'$$
, (A2)

with

$$H_{0} = \sum_{p} (2\epsilon_{p} - Gv_{p}^{2})\Omega_{p}v_{p}^{2} - G\sum_{pq} \Omega_{p}\Omega_{q}u_{p}u_{p}v_{q}v_{q} , \quad (A3)$$

$$\hat{H}_{11} = \sum_{a} H_{11}^{p} \mathcal{N}_{p}$$
, (A4)

$$\hat{H}_{20} = \sum_{p} H_{20}^{p} (\mathcal{A}_{p}^{\dagger} + \mathcal{A}_{p}) ,$$
 (A5)

$$\hat{H}_{22} = \sum_{p} H_{22}^{pq} \mathcal{A}_{p}^{\dagger} \mathcal{A}_{q} , \qquad (A6)$$

$$\hat{H}_{40} = \sum_{pq} H_{40}^{pq} (\mathcal{A}_{p}^{\dagger} \mathcal{A}_{p}^{\dagger} + \mathcal{A}_{p} \mathcal{A}_{q}) , \qquad (A7)$$

$$\hat{H}_{31} = \sum_{pq} H_{31}^{pq} (\mathcal{A}_p^{\dagger} \mathcal{N}_q + \mathcal{N}_p \mathcal{A}_q) , \qquad (A8)$$

$$\hat{H}'_{22} = \sum_{pq} \tilde{H}^{pq}_{22} (\mathcal{N}_p \mathcal{N}_q - \delta_{pq} \mathcal{N}_p) , \qquad (A9)$$

where

$$H_{11}^{p} = (\epsilon_{p} - Gv_{p}^{2})(u_{p}^{2} - v_{p}^{2}) + \left[G\sum_{q}\Omega_{q}u_{q}v_{q}\right]2u_{p}v_{p} , \tag{A10} \label{eq:A10}$$

$$\begin{split} H_{20}^p = & (\epsilon_p - G v_p^2) \sqrt{\Omega_p} \, 2 u_p v_p \\ & - \sqrt{\Omega_p} \left[G \sum_q \Omega_q u_q v_q \right] (u_p^2 - v_p^2) \ , \end{split} \tag{A11}$$

$$H_{22}^{pq} = -G\sqrt{\Omega_p\Omega_q}(u_p^2u_q^2 + v_p^2v_q^2) , \qquad (A12)$$

$$H_{40}^{pq} = \frac{1}{2}G\sqrt{\Omega_{p}\Omega_{q}}(u_{p}^{2}v_{q}^{2} + v_{p}^{2}u_{q}^{2}), \qquad (A13)$$

$$H_{31}^{pq} = G\sqrt{\Omega_n}(u_n^2 - v_n^2)v_n u_n , \qquad (A14)$$

$$\tilde{H}_{23}^{pq} = -Gu_n v_a u_a v_a , \qquad (A15)$$

and the operators \mathcal{N}_{n} , $\mathcal{A}_{n}^{\dagger}$, and \mathcal{A}_{n} are given by

$$\mathcal{N}_p = \sum_m a_{pm}^{\dagger} a_{pm} \ , \tag{A16}$$

$$\mathcal{A}_{p}^{\dagger} = \frac{1}{\sqrt{\Omega_{p}}} \sum_{m>0} a_{pm}^{\dagger} a_{p\overline{m}}^{\dagger} , \qquad (A17)$$

$$\mathcal{A}_{p} = (\mathcal{A}_{p}^{\dagger})^{\dagger} , \qquad (A18)$$

respectively. These operators obey the commutation relations

$$[\mathcal{A}_{p}, \mathcal{A}_{q}^{\dagger}] = \delta_{pq} \left[1 - \frac{\mathcal{N}_{p}}{\Omega_{p}} \right], \qquad (A19)$$

$$[\mathcal{N}_{p}, \mathcal{A}_{q}^{\dagger}] = 2\delta_{pq} \mathcal{A}_{p} . \tag{A20}$$

APPENDIX B

With the help of a generalized Wick's theorem and the commutation relations given in Appendix A we can derive the energy matrix elements occurring in the main text.

For the rotated two quasiparticle energy matrix we obtain

$$\langle F_N | H_0 \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = H_0 k_j(\theta) n(\theta) ,$$
 (B1)

$$\langle F_N | \hat{H}_{20} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) \left[\frac{1}{X_j^2} H_{20}^J + k_j \sum_p H_{20}^p k_p \right],$$
(B2)

$$\langle F_N | \hat{H}_{40} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) \left[\frac{2}{X_j^2} \sum_p H_{40}^{pj} k_p \tilde{\delta}(pj) \right]$$

$$+k_{J}\sum_{pq}H_{40}^{pq}k_{p}k_{q}\tilde{\delta}(pq)$$
, (B3)

where $n(\theta)$, $k_j(\theta)$, and $X_j(\theta)$ are given by Eqs. (2.13), (2.14), and (4.5), respectively, and $\tilde{\delta}(pq)$ is defined in (2.17). The other energy matrix terms of the Hamiltonian (A2) are obviously zero.

Defining

$$\tilde{H}_{40}^{p} \equiv \sum_{q} H_{40}^{pq} k_{q} \tilde{\delta}(pq) , \qquad (B4)$$

$$h_0 \equiv n(\theta) \left[H_0 + \sum_{p} (H_{20}^p + \tilde{H}_{40}^p) k_p \right],$$
 (B5)

$$h_{02}^{J} \equiv n(\theta)(H_{20}^{J} + 2\tilde{H}_{40}^{J}),$$
 (B6)

we get

$$\langle F_N | \hat{H} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = \left[k_j h_0 + \frac{1}{X_j^2} h_{02}^j \right] . \tag{B7}$$

Now we can calculate the four quasiparticle energy matrix elements. We obtain

$$\langle F_N | H_0 \hat{S} \mathcal{A}_i^{\dagger} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) H_0 k_i k_j \tilde{\delta}(ij) , \qquad (B8)$$

$$\langle F_N | \hat{H}_{20} \hat{S} \mathcal{A}_i^{\dagger} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) \tilde{\delta}(ij) \left[\left[\frac{k_j}{X_i^2} H_{20}^i + \frac{k_i}{X_j^2} H_{20}^j \right] + k_i k_j \sum_p H_{20}^p k_p \right], \tag{B9}$$

$$\langle F_{N} | \hat{H}_{40} \hat{S} \mathcal{A}_{i}^{\dagger} \mathcal{A}_{j}^{\dagger} | F_{N} \rangle = n(\theta) \tilde{\delta}(ij) \left[\frac{2H_{40}^{ij}}{X_{i}^{2} X_{j}^{2}} + \frac{2k_{i}}{X_{j}^{2}} \tilde{H}_{40}^{j} + \frac{2k_{j}}{X_{i}^{2}} \tilde{H}_{40}^{i} + k_{i} k_{j} \sum_{p} \tilde{H}_{40}^{p} k_{p} \right]. \tag{B10}$$

Obviously all the other terms are again zero. Adding all the preceding terms we get the expression (4.15) of the main text. The last term to be calculated is

$$\langle F_N | \mathcal{A}_i H_0 \hat{S} \mathcal{A}_i^{\dagger} | F_N \rangle = n(\theta) n_{ii}(\theta) H_0 , \qquad (B11)$$

$$\langle F_N | \mathcal{A}_i \hat{H}_{11} \hat{S} \mathcal{A}_i^{\dagger} | F_N \rangle = 2n(\theta) n_{ii}(\theta) H_{11}^i , \qquad (B12)$$

$$\langle F_N | \mathcal{A}_i \hat{H}_{20} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) \left[k_j H_{20}^i + \frac{k_i}{X_j^2} \tilde{\delta}(ij) H_{20}^j + n_{ij}(\theta) \sum_p H_{20}^p k_p \tilde{\delta}(pi) \right], \tag{B13}$$

$$\langle F_N | \mathcal{A}_i \hat{H}_{40} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) \left[\tilde{\delta}(ij) \frac{2k_i}{X_i^2} \left[\tilde{H}_{40}^i - \frac{k_i}{\Omega_i} H_{40}^{ij} \right] + n_{ij}(\theta) \left[\sum_p \tilde{H}_{40}^p k_p - 2 \frac{k_i}{\Omega_i} \tilde{H}_{40}^i \right] \right], \tag{B14}$$

$$\langle F_N | \mathcal{A}_i \widehat{H}_{31} \widehat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = 2n(\theta) \left[\frac{k_i}{X_j^2} \widetilde{\delta}(ij) H_{31}^{ji} + n_{ij}(\theta) \sum_p H_{31}^{pi} k_p \widetilde{\delta}(pi) \right], \tag{B15}$$

$$\langle F_N | \mathcal{A}_i \hat{H}_{22} \hat{S} \mathcal{A}_j^{\dagger} | F_N \rangle = n(\theta) \left[\frac{H_{22}^{ij}}{X_j^2} + k_j \sum_p H_{22}^{pi} k_p \right], \tag{B16}$$

$$\langle F_N | \mathcal{A}_i \hat{H}_{22}^i \hat{S} \mathcal{A}_i^{\dagger} F_N \rangle = n(\theta) n_{ii}(\theta) \tilde{H}_{22}^{ii}$$
(B17)

where $n_{ii}(\theta)$ is defined by Eq. (4.4).

Assembling all the preceding terms we finally obtain

$$\langle F_{N} | \mathcal{A}_{i} \hat{H} \hat{S} \mathcal{A}_{j}^{\dagger} | F_{N} \rangle = n(\theta) \left[n_{ij}(\theta) \left[h_{0} - \frac{k_{i}}{\Omega_{i}} h_{02}^{i} + 2h_{11}^{i} \right] + \frac{k_{i}}{X_{i}^{2}} \tilde{\delta}(ij) \left[h_{02}^{j} + 2n(\theta) H_{31}^{\mu} - 2n(\theta) \frac{k_{i}}{\Omega_{i}} H_{40}^{ij} \right] + \left[\frac{n(\theta)}{X_{i}^{2}} H_{22}^{ij} + k_{j} h_{22}^{i} \right] \right],$$
(B18)

$$h_{11}^{i} \equiv n(\theta) \left[H_{11}^{i} + \tilde{H}_{22}^{i} + \sum_{p} H_{31}^{pi} k_{p} \tilde{\delta}(pi) \right] , \tag{B19}$$

$$h_{22}^{i} \equiv n(\theta) \left[H_{20}^{i} + \sum_{p} H_{22}^{pi} k_{p} \right] .$$
 (B20)

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