PHYSICAL REVIEW C **75**, 024306 (2007)

Quasiparticle time blocking approximation within the framework of generalized Green function formalism

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(Received 1 August 2006; published 20 February 2007)

The problem of the microscopic description of excited states of the even-even open-shell atomic nuclei is considered. A model is formulated which allows one to go beyond the quasiparticle random phase approximation. The physical content of the model is determined by the quasiparticle time blocking approximation (QTBA) which enables one to include contributions of the two-quasiparticle and the two-phonon configurations, while excluding (blocking) more complicated intermediate states. In addition, the QTBA ensures consistent treatment of ground state correlations in the Fermi systems with pairing. The model is based on the generalized Green function formalism (GGFF) in which the normal and the anomalous Green functions are treated in a unified way in terms of the components of generalized Green functions in a space that is double the size of the usual single-particle space. Modification of the GGFF is considered in the case when the many-body nuclear Hamiltonian contains two-, three-, and other many-particle effective forces.

DOI: 10.1103/PhysRevC.75.024306 PACS number(s): 21.60.−n, 74.20.−z

I. INTRODUCTION

One of the most widely used approaches applied to the description of excitations of the even-even atomic nuclei is the random phase approximation (RPA, see, e.g., Ref. [1]). Within this approximation, the nuclear excitations are treated as the one-phonon states which are superpositions of the one-particle–one-hole (1p1h) configurations. However, this approach is applicable only in the case when pairing correlations are not essential, i.e., strictly speaking, only for magic nuclei. Generalization of the RPA taking into account pairing correlations explicitly is the quasiparticle RPA (QRPA), in which the excited states (phonons) are expanded in the two-quasiparticle (2q) configurations. Thereby the QRPA extends the range of the RPA to the open-shell (nonmagic) nuclei. Nevertheless, despite the significant success of both the RPA and the QRPA, there are several reasons to develop models that go beyond these approximations.

First of all, description of the nuclear excitations in terms of the one-phonon wave functions is justified only for low-lying states. At higher excitation energies, fragmentation of the one-phonon states becomes important. This means that in addition to the 1p1h or 2q configurations, more complex configurations should be incorporated (see Ref. [2]). The role of the effects related to the complex configurations is well manifested, for example, in the theory of giant multipole resonances (GMRs). It is well known (see, e.g., Ref. [3]) that RPA and QRPA enable one to describe the centroid energies and total strengths of the GMRs. However, both models fail to reproduce the total widths of the resonances and their fine structure. The reason is that these characteristics of the GMRs are significantly affected by the complex (mainly 2p2h or 4q) configurations which form the spreading width of the resonance.

Another direction for developing a nuclear structure theory is associated with the models in which ground state correlations (GSC) beyond those in the RPA and QRPA are taken into account (see Refs. [3–7]). It has been shown that the GSC caused by complex configurations play an important role in the theoretical description of the experimental data. In what follows, we will refer to these GSC as GSC2 in order to distinguish them from the GSC1 included in the RPA and QRPA. In some cases, the GSC2 can strongly affect the transition strengths and can even lead to the appearance of new transitions that are absent in calculations that include complex configurations in the excited states only, i.e., in calculations neglecting this type of GSC and using a restricted basis (see Refs. [3,5]).

A variety of models have been developed to study the effects of complex configurations on the structure of excited states of the even-even atomic nuclei (in addition to the aforementioned papers, see also Refs. [8–14] and references therein). Nevertheless, until recently (see Refs. [13,14]), the quasiparticle-phonon model (QPM, Ref. [2]) developed by Soloviev and co-workers was the only working approach that consistently treated the complex configurations and the pairing correlations on an equal footing. It is no surprise that comprehensive studies of the excitations of the open-shell nuclei taking into account complex (mainly two-phonon) configurations at the microscopic level have been carried out only within the QPM. In view of this, the development of other approaches in this direction is particularly important.

The principal goal of the present paper is to generalize the model of Ref. [11] by including the pairing correlations. This model was developed to describe the excited states of the even-even doubly magic nuclei taking into account 2p2h (more precisely, 1p1h $\otimes$ phonon) configurations. The model is based on the Green function (GF) formalism. The GSC2 were completely included within the model approximations. In the framework of this model, the calculations of the GMRs in magic stable and unstable nuclei have been performed. Some of the results are presented in Refs. [3,11]. In these calculations, reasonable agreement has been obtained with the experimental data for the integral characteristics of GMRs,

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including the total resonance widths. Thus, one can expect that the extension of the model [11] to the open-shell nuclei will also give reasonable results.

The second goal of the paper is to provide a modification of the GF formalism for Fermi systems with pairing which is most suitable for solving the problem under consideration. To this aim, the generalized Green function formalism (GGFF) is presented, in which normal and anomalous GFs are treated in a unified way in terms of the components of generalized GFs in a space that is double the size of the usual single-particle space. Modification of the GGFF is considered in the case when the many-body nuclear Hamiltonian contains two-, three-, and other many-particle effective forces.

The paper is divided into two main parts. The first part (Sec. II) reviews the basic formulas and equations of the GGFF and introduces the single-quasiparticle basis functions, which provide suitable representation of the model equations. The second part (Sec. III) contains the formulation of the model in which pairing correlations, 2q, 2q $\otimes$ phonon, and two-phonon configurations are included. The model is analyzed within the sum rule approach. A subtraction procedure is introduced to eliminate spurious states and to avoid double counting of the complex configurations within the model. The conclusions are given Sec. IV.

II. GENERALIZED GREEN FUNCTION FORMALISM

A. Basic definitions

Let $a^\dagger(x)$ and $a(x)$ be creation and annihilation operators of particles (free fermions) in the coordinate representation of the usual single-particle space. Here symbol $x = \{\boldsymbol{r}, \sigma, \tau\}$ includes the spatial coordinate $\boldsymbol{r}$, spin σ, and isospin τ variables. Considering the Fermi systems with pairing correlations, it is convenient to pass from this single-particle space spanned by the coordinates x to the extended (doubled) space spanned by the coordinates $y = \{x, \chi\}$, where $\chi = \pm 1$ is an additional index introduced for denoting the different components of the single-particle functions in the extended space (see Refs. [1,15] for details). Let us define the operators $b(y) = b(x, \chi)$ by the relations

$$b(x, +) = a(x), \quad b(x, -) = a^\dagger(x). \tag{2.1}$$

From this, it follows that $b^\dagger(y) = b(\bar{y})$, where $\bar{y} = \{x, -\chi\}$. The Heisenberg representation of the b operators (in units where Planck's constant $\hbar = 1$) reads

$$\Psi(z) = e^{iHt} b(y)\, e^{-iHt}. \tag{2.2}$$

Here and in the following, $z = \{t, y\}$, t is the time variable, and H is a many-body Hamiltonian of an interacting fermion system. Obviously, these Ψ operators possess the property

$$\Psi^\dagger(z) = \Psi(\bar{z}), \tag{2.3}$$

where $\bar{z} = \{t, \bar{y}\}$.

We will assume that the motion in the fermion system is determined by the nonrelativistic Hamiltonian H of the form

$$H = H^0 + V, \tag{2.4}$$

where H^0 is a single-particle Hamiltonian including the external anomalous pair potentials

$$H^0 = \int dx_1 dx_1' \big(h^0(x_1, x_1') a^\dagger(x_1) a(x_1') + \tfrac{1}{2}\, \Delta^0(x_1, x_1') \times a^\dagger(x_1)\, a^\dagger(x_1') - \tfrac{1}{2} \Delta^{0*}(x_1, x_1') a(x_1)\, a(x_1') \big), \tag{2.5}$$

and V is an interaction including two-, three-, and other many-particle effective forces

$$V = \sum_{k=2}^{K} V^{(k)}, \tag{2.6}$$

$$V^{(k)} = \frac{1}{k!} \int dx_1 \cdot \ldots \cdot dx_k dx_1' \cdot \ldots \cdot dx_k' \times v^{(k)}(x_1, \ldots, x_k; x_1', \ldots, x_k') \times a^\dagger(x_1) \cdot \ldots \cdot a^\dagger(x_k) a(x_k') \cdot \ldots \cdot a(x_1'). \tag{2.7}$$

Here and in the following equations, $\int dx$ means the space integral over $\boldsymbol{r}$ and the sum over σ and τ indices. Analogously, in the following, $\int dy$ will denote $\int dx$ and the sum over χ, and $\int dz$ will denote $\int dt\, dy$. In case of the exact nuclear Hamiltonian, we have

$$h^0(x, x') = -\left(\frac{\boldsymbol{\nabla}_{\mathbf{r}}^2}{2m} + \mu_\tau \right) \delta(x, x'), \quad \Delta^0(x, x') = 0, \tag{2.8}$$

where $\delta(x, x') = \delta(\boldsymbol{r} - \boldsymbol{r}')\, \delta_{\sigma,\sigma'} \delta_{\tau,\tau'}$, and μ_τ is the chemical potential for the nucleons with the isospin projection τ which is introduced to simplify the following equations. Notice that the Hamiltonian H^0 can be formally rewritten in terms of the b operators as

$$H^0 = \frac{1}{2} \int dy\, dy'\, \mathcal{H}^0(y, y')\, b^\dagger(y)\, b(y') + \epsilon_0, \tag{2.9}$$

where $\epsilon_0 = \frac{1}{2} \int dx\, h^0(x, x)$,

$$\left.\begin{array}{ll} \mathcal{H}^0(x, +, x', +) = h^0(x, x'), & \mathcal{H}^0(x, +, x', -) = \Delta^0(x, x'), \\ \mathcal{H}^0(x, -, x', +) = -\Delta^{0*}(x, x'), & \mathcal{H}^0(x, -, x', -) = -h^{0*}(x, x'). \end{array}\right\} \tag{2.10}$$

Let $|0\rangle$ be the wave function of the ground state of the interacting fermion system. If the Hamiltonian H does not contain the external anomalous pair potentials Δ^0 [e.g., if Eqs. (2.8) are fulfilled], the number of particles is conserved, and $|0\rangle$ is an eigenfunction of the particle-number operator. However, in the general case we will not suppose that $\Delta^0 = 0$ in Eq. (2.5), i.e. , we will not suppose that the condition of the particle-number conservation is fulfilled for $|0\rangle$. Let us define the k-particle generalized GF in the time representation by the formula

$$G^{(k)}(z_1,\ldots,z_k;z'_1,\ldots,z'_k) = i^{-k}\langle 0|\mathrm{T}\Psi(z_1)\cdot\ldots\cdot\Psi(z_k)\,\Psi^{\dagger}(z'_k)\cdot\ldots\cdot\Psi^{\dagger}(z'_1)|0\rangle, \tag{2.11}$$

where T is the time-ordering operator. In particular, for the single-particle GF we have

$$G(z,z') \equiv G^{(1)}(z;z') = -i\langle 0|\mathrm{T}\,\Psi(z)\Psi^{\dagger}(z')|0\rangle. \tag{2.12}$$

The property

$$G(z,z') = -G(\bar{z}',\bar{z}) \tag{2.13}$$

follows from Eqs. (2.3) and (2.12). It can be seen from the definitions (2.1) and (2.2) that the normal and the anomalous GFs are the components of the generalized GFs $G^{(k)}$ corresponding to the different values of the χ indices.

B. Equations of motion for the Green functions

In the case of Fermi systems with pairing, the equations of motion for the many-particle GFs can be obtained with the help of the same technique based on generating functionals depending on auxiliary source fields that is frequently used for the Fermi systems without pairing correlations (see, e.g., Ref [16]). Let us define the generating functional W depending on the source field ξ as

$$W[\xi] = \ln\langle 0|\mathrm{TU}|0\rangle, \tag{2.14}$$

where

$$\mathrm{U} = \exp\left(i\int dz\,dz'\,\xi(z,z')\,\Psi^{\dagger}(z)\Psi(z')\right). \tag{2.15}$$

It follows from Eq. (2.3) that one can consider the equality $\xi(z,z') = -\xi(\bar{z}',\bar{z})$ to be fulfilled. Let us introduce the GFs with a source field ξ:

$$G^{(k)}_{\xi}(z_1,\ldots,z_k;z'_1,\ldots,z'_k) = i^{-k}\frac{\langle 0|\mathrm{T\,U}\Psi(z_1)\cdot\ldots\cdot\Psi(z_k)\,\Psi^{\dagger}(z'_k)\cdot\ldots\cdot\Psi^{\dagger}(z'_1)|0\rangle}{\langle 0|\mathrm{TU}|0\rangle}. \tag{2.16}$$

Obviously, $G^{(k)}_{\xi}$ coincides with $G^{(k)}$ defined by Eq. (2.11) at $\xi = 0$.

It is easy to see that the GFs $G^{(k)}_{\xi}$ can be obtained from the generating functional $W[\xi]$ by a successive differentiation with respect to ξ. In particular, we obtain

$$G_{\xi}(z_1,z_2) \equiv G^{(1)}_{\xi}(z_1;\,z_2) = \frac{\delta W}{\delta\xi(z_2,z_1)}, \tag{2.17}$$

$$L_{\xi}(z_1,z_2;\,z_3,z_4) = \frac{\delta^2 W}{\delta\xi(z_1,z_2)\,\delta\xi(z_4,z_3)} = \frac{\delta G_{\xi}(z_2,z_1)}{\delta\xi(z_4,z_3)}, \tag{2.18}$$

where L_{ξ} is a response function defined as

$$L_{\xi}(z_1,z_2;\,z_3,z_4) = G^{(2)}_{\xi}(z_2,z_3;\,z_1,z_4) - G_{\xi}(z_2,z_1)G_{\xi}(z_3,z_4) \tag{2.19}$$

(notice that this formula differs from the definition in Ref. [16] by the permutation of the arguments of L_{ξ}).

The equation of motion for the single-particle GF is obtained by the differentiation of $G_{\xi}(z_1,z_2)$ with respect to time in analogy to the case of the Fermi systems without pairing correlations (see Ref [16]). It has the form

$$(G^0)^{-1}(z_1,z_2) + \xi(z_1,z_2) - \xi(\bar{z}_2,\bar{z}_1) = G^{-1}_{\xi}(z_1,z_2) + \Sigma_{\xi}(z_1,z_2), \tag{2.20}$$

where

$$(G^0)^{-1}(z_1,z_2) = \left(i\delta(y_1,y_2)\frac{\partial}{\partial t_1} - \mathcal{H}^0(y_1,y_2)\right)\delta(t_1-t_2), \tag{2.21}$$

$\delta(y,y') = \delta_{\chi,\chi'}\delta(x,x')$, and Σ_{ξ} is the mass operator defined by the equations

$$\int dz''\,\Sigma_{\xi}(z,z'')G_{\xi}(z'',z') = \sum_{k=2}^{K}\frac{i^{1-k}}{k\,!\,(k-1)}\int dz'_2\cdot\ldots\cdot dz'_k dz''_1\cdot\ldots\cdot dz''_k \times\mathcal{W}^{(k)}(z,z'_2,\ldots,z'_k;z''_1,\ldots,z''_k) \times G^{(k)}_{\xi}(z''_1,\ldots,z''_k;\,z',z'_2,\ldots,z'_k), \tag{2.22}$$

$$\mathcal{W}^{(k)}(z_1,\ldots,z_k;z'_1,\ldots,z'_k) = \delta_{\chi_1,\chi'_1}\delta(t_1-t'_1-\chi_1\cdot 0) \times\left(\prod_{l=1}^{k-1}\delta_{\chi_l,\chi_{l+1}}\delta_{\chi'_l,\chi'_{l+1}}\delta(t_l-t_{l+1})\delta(t'_l-t'_{l+1})\right) \times\left[\delta_{\chi_1,+1}w^{(k)}(x_1,\ldots,x_k;x'_1,\ldots,x'_k) + \delta_{\chi_1,-1}(-1)^k w^{(k)}(x'_1,\ldots,x'_k;x_1,\ldots,x_k)\right]. \tag{2.23}$$

In Eq. (2.23), $w^{(k)}$ is the antisymmetrized matrix element of the k-particle interaction in the coordinate representation defined through the effective forces $v^{(k)}$ entering Eq. (2.7) and through the generalized antisymmetrized δ functions by the formulas

$$w^{(k)}(x_1,\ldots,x_k;x'_1,\ldots,x'_k) = \frac{1}{k\,!\,(k-2)\,!}\int dx''_1\cdot\ldots\cdot dx''_k dx'''_1\cdot\ldots\cdot dx'''_k \times\delta\begin{pmatrix}x''_1,\ldots,x''_k\\x_1,\ldots,x_k\end{pmatrix}\delta\begin{pmatrix}x'''_1,\ldots,x'''_k\\x'_1,\ldots,x'_k\end{pmatrix} \times v^{(k)}(x''_1,\ldots,x''_k;x'''_1,\ldots,x'''_k), \tag{2.24}$$

where

$$\delta\begin{pmatrix}x'_1,\ldots,x'_k\\x_1,\ldots,x_k\end{pmatrix} = \det\begin{pmatrix}\delta(x_1,x'_1)\ldots\delta(x_1,x'_k)\\ \cdots\quad\cdots\quad\cdots\\ \delta(x_k,x'_1)\ldots\delta(x_k,x'_k)\end{pmatrix}. \tag{2.25}$$

Notice that from Eqs. (2.10), (2.13), (2.20), and (2.21) it follows that

$$\Sigma_{\xi}(z,z') = -\Sigma_{\xi}(\bar{z}',\bar{z}). \tag{2.26}$$

The symmetry property of $\mathcal{W}^{(k)}$ follows from its definition (2.23):

$$\mathcal{W}^{(k)}(z_1,\ldots,z_k;z'_1,\ldots,z'_k) = (-1)^k\,\mathcal{W}^{(k)}(\bar{z}'_1,\ldots,\bar{z}'_k;\bar{z}_1,\ldots,\bar{z}_k). \tag{2.27}$$

To obtain equations for the other (many-particle) GFs, let us perform a change of the functional variable ξ to the G_ξ and consider a Legendre transformation of the functional $W[\xi]$:

$$\Gamma[G_\xi] = 2\,W[\xi] - \int dz_1\,dz_2[\xi(z_2,z_1) - \xi(\bar{z}_1,\bar{z}_2)]G_\xi(z_1,z_2). \tag{2.28}$$

Using Eqs. (2.13) and (2.17), we obtain

$$\frac{\delta\Gamma}{\delta_- G_\xi(z_1,z_2)} = \xi(\bar{z}_1,\bar{z}_2) - \xi(z_2,z_1). \tag{2.29}$$

The notation δ_- means that the variations of the GF G_ξ conserve the property of antisymmetry (2.13). This condition should be taken into account since variations of ξ, which generate the variations of G_ξ, obviously do not lead to the violation of Eq. (2.13). Conservation of the property (2.13) in the variational procedure can be automatically ensured if the following substitution is performed in a G_ξ-dependent functional:

$$G_\xi(z,z') = \tfrac{1}{2}[G_\xi(z,z') - G_\xi(\bar{z}',\bar{z})]. \tag{2.30}$$

In case of the vanishing source field, the Eq. (2.29) leads to the stationarity condition: $\delta\Gamma/\delta_- G(z_1,z_2) = 0$. Using, further, Eq. (2.20), we obtain from Eq. (2.29) the relation

$$\frac{\delta\Sigma_\xi(z_2,z_1)}{\delta_- G_\xi(z_4,z_3)} = \frac{1}{2}\big[G_\xi^{-1}(z_2,z_4)G_\xi^{-1}(z_3,z_1) - G_\xi^{-1}(\bar{z}_1,z_4)G_\xi^{-1}(z_3,\bar{z}_2)\big] - \frac{\delta^2\Gamma}{\delta_- G_\xi(z_1,z_2)\,\delta_- G_\xi(z_4,z_3)}. \tag{2.31}$$

Let us introduce an amplitude of the effective interaction $\mathcal{I}_\xi$ which includes irreducible amplitudes both in the particle-hole (ph) and in the particle-particle (pp) channels (for the sake of simplicity, we do not introduce special terms for the hole-particle and hole-hole channels which are also included):

$$\mathcal{I}_\xi(z_1,z_2;\,z_3,z_4) = i\,\frac{\delta\Sigma_\xi(z_2,z_1)}{\delta_- G_\xi(z_4,z_3)}. \tag{2.32}$$

From Eqs. (2.13) and (2.26), we obtain

$$\mathcal{I}_\xi(z_1,z_2;\,z_3,z_4) = -\mathcal{I}_\xi(\bar{z}_2,\bar{z}_1;\,z_3,z_4) = -\mathcal{I}_\xi(z_1,z_2;\,\bar{z}_4,\bar{z}_3). \tag{2.33}$$

In addition, from Eq. (2.31), it follows that

$$\mathcal{I}_\xi(z_1,z_2;\,z_3,z_4) = \mathcal{I}_\xi(z_4,z_3;\,z_2,z_1). \tag{2.34}$$

Notice that the response function defined by Eq. (2.18) satisfies the analogous equalities

$$L_\xi(z_1,z_2;\,z_3,z_4) = -L_\xi(\bar{z}_2,\bar{z}_1;\,z_3,z_4) = -L_\xi(z_1,z_2;\,\bar{z}_4,\bar{z}_3), \tag{2.35}$$

$$L_\xi(z_1,z_2;\,z_3,z_4) = L_\xi(z_4,z_3;\,z_2,z_1). \tag{2.36}$$

Differentiating Eq. (2.20) with respect to ξ and then using Eqs. (2.18) and (2.32), we obtain the Bethe-Salpeter equation (BSE) for the response function:

$$L_\xi(z_1,z_2;\,z_3,z_4) = G_\xi(\bar{z}_4,z_1)\,G_\xi(z_2,\bar{z}_3) - G_\xi(z_3,z_1)\,G_\xi(z_2,z_4) - i\int dz_5dz_6dz_7dz_8\;G_\xi(z_5,z_1)\,G_\xi(z_2,z_6) \times\mathcal{I}_\xi(z_5,z_6;\,z_7,z_8)L_\xi(z_7,z_8;\,z_3,z_4). \tag{2.37}$$

The equations for the many-particle GFs $G_\xi^{(k)}$ with $k>2$ are obtained by a differentiation of Eq. (2.16) with respect to ξ. Taking into account the relation

$$\frac{\delta}{\delta\xi(z_1,z_2)} = \int dz_3dz_4L_\xi(z_1,z_2;\,z_3,z_4)\frac{\delta}{\delta G_\xi(z_3,z_4)}, \tag{2.38}$$

which follows from Eq. (2.18), we come to the recurrence formula

$$G_\xi^{(k)}(z_1,\ldots,z_k;z'_1,\ldots,z'_k) = \left[G_\xi(z_1,z'_1) + \int dzdz'L_\xi(z'_1,z_1;\,z',z) \times\frac{\delta}{\delta G_\xi(z',z)}\right]G_\xi^{(k-1)}(z_2,\ldots,z_k;z'_2,\ldots,z'_k). \tag{2.39}$$

Notice that in Eqs. (2.38) and (2.39) we have $\delta_- G_\xi = \delta G_\xi$ owing to the presence of the response function satisfying Eqs. (2.35).

Equations (2.19), (2.22), (2.32), (2.37), and (2.39) form the closed system of the functional differential equations of the GGFF. An important feature of these equations is that they do not change their form when the many-particle forces are added to the two-particle interaction in the total Hamiltonian. The exception is Eq. (2.22) for the mass operator in which the many-particle forces enter in the explicit form. This result of the GGFF could be expected, but it needed to be proved. It allows one to extend the standard GF methods developed for the Fermi systems with two-particle interaction to the systems interacting through the many-particle effective forces.

In the final equations, we can set $\xi=0$. So, in what follows, we will omit the ξ indices of the functions, implying the limit at $\xi=0$ and coming back to the GFs without source field defined by Eq. (2.11). The independent functional variable is the single-particle GF G satisfying the Dyson equation which follows from Eq. (2.20), that is,

$$G(z_1,z_2) = G^0(z_1,z_2) + \int dz_3dz_4G^0(z_1,z_3)\Sigma(z_3,z_4)\,G(z_4,z_2). \tag{2.40}$$

In the case of Fermi systems without pairing correlations, when the external anomalous pair potentials vanish in Eq. (2.5), the above equations can be reduced to ones for the normal components of GFs which satisfy the condition

$$\sum_{n=1}^{k}(\chi_n - \chi'_n)G^{(k)}(z_1,\ldots,z_k;z'_1,\ldots,z'_k) = 0. \tag{2.41}$$

These reduced equations will coincide with ones obtained in Ref. [17]. On the other hand, if we restrict consideration of Fermi systems with pairing to the case of two-particle interaction in the Hamiltonian (2.4), i.e., if we assume $H = H^0 + V^{(2)}$, then Eqs. (2.19), (2.22), (2.32), and (2.37) will coincide, up to the permutation of the arguments, with the corresponding equations in Ref. [18].

C. Transformation of the basic equations

For further applications, it is convenient to introduce a nonantisymmetric response function R satisfying the following BSE:

$$R(z_1, z_2;\, z_3, z_4) = R^0(z_1, z_2;\, z_3, z_4) + i \int dz_5 dz_6 dz_7 dz_8 \times R^0(z_1, z_2;\, z_5, z_6)\mathcal{U}(z_5, z_6;\, z_7, z_8) \times R(z_7, z_8;\, z_3, z_4), \tag{2.42}$$

where

$$R^0(z_1, z_2; z_3, z_4) = -G(z_3, z_1)\, G(z_2, z_4), \tag{2.43}$$

and $\mathcal{U}$ is a nonantisymmetric amplitude of the effective interaction defined by

$$\mathcal{U}(z_1, z_2;\, z_3, z_4) = i\, \frac{\delta \Sigma(z_2, z_1)}{\delta G(z_4, z_3)}, \tag{2.44}$$

where the condition (2.13) is not supposed to be fulfilled under variations of G and substitution (2.30) is not applied. The amplitude $\mathcal{U}$ satisfies the equalities

$$\mathcal{U}(z_1, z_2;\, z_3, z_4) = \mathcal{U}(z_4, z_3;\, z_2, z_1) = \mathcal{U}(\bar{z}_2, \bar{z}_1;\, \bar{z}_4, \bar{z}_3), \tag{2.45}$$

but generally $\mathcal{U}$ does not possess the property of antisymmetry (2.33).

It is easy to show that first the equalities

$$R(z_1, z_2;\, z_3, z_4) = R(z_4, z_3;\, z_2, z_1) = R(\bar{z}_2, \bar{z}_1;\, \bar{z}_4, \bar{z}_3) \tag{2.46}$$

hold, while the Eqs. (2.35) do not hold for R. Second, the amplitude $\mathcal{I}$ and the response function L are expressed in terms of $\mathcal{U}$ and R as

$$\mathcal{I}(z_1, z_2;\, z_3, z_4) = \tfrac{1}{2}[\mathcal{U}(z_1, z_2;\, z_3, z_4) - \mathcal{U}(\bar{z}_2, \bar{z}_1;\, z_3, z_4)], \tag{2.47}$$

$$L(z_1, z_2;\, z_3, z_4) = R(z_1, z_2;\, z_3, z_4) - R(\bar{z}_2, \bar{z}_1;\, z_3, z_4). \tag{2.48}$$

Thus, for the determination of the response function L, it is sufficient to solve Eq. (2.42) for the nonantisymmetric function R.

Now, following the method described in Ref. [3], we represent the total mass operator Σ and the total nonantisymmetric amplitude of the effective interaction $\mathcal{U}$ as a sum of two terms

$$\Sigma = \tilde{\Sigma} + \Sigma^e, \quad \mathcal{U} = \tilde{\mathcal{U}} + \mathcal{U}^e, \tag{2.49}$$

where

$$\tilde{\Sigma}(z_1, z_2) = \tilde{\Sigma}(y_1, y_2)\, \delta(t_1 - t_2), \tag{2.50}$$

$$\tilde{\mathcal{U}}(z_1, z_2;\, z_3, z_4) = \tilde{\mathcal{U}}(y_1, y_2;\, y_3, y_4)\, \delta(t_1 - t_2) \times \delta(t_3 - t_4)\delta(t_1 - t_3). \tag{2.51}$$

After transformation to the energy representation (see Sec. II D), the first terms in Eqs. (2.49), $\tilde{\Sigma}$ and $\tilde{\mathcal{U}}$, are found to be energy independent. The term $\tilde{\Sigma}$ corresponds to the mean-field contribution into the mass operator including the pair potentials. The term $\tilde{\mathcal{U}}$ corresponds to the residual energy-independent interaction both in the ph and in the pp channels. The second terms in Eqs. (2.49), Σ^e and $\mathcal{U}^e$, have a strong energy dependence and represent dynamic contributions of complex configurations.

We stress that the quantities $\tilde{\Sigma}$ and $\tilde{\mathcal{U}}$ (and, consequently, Σ^e and $\mathcal{U}^e$) are not defined rigorously by Eqs. (2.49). They will be specified in the following within the framework of the model to be considered. At the moment, only the general properties, which are expressed by Eqs. (2.50) and (2.51), are important. Notice, however, that in the particular case of the self-consistent Hartree-Fock-Bogoliubov (HFB) approximation restricted by the two-particle interaction, we have $\tilde{\Sigma} = \Sigma^{\text{HFB}}$, $\tilde{\mathcal{U}} = \mathcal{U}^{\text{HFB}}$, where

$$\Sigma^{\text{HFB}}(z_1, z_2) = i \int dz_3 dz_4 \left[\mathcal{W}^{(2)}(z_1, z_4;\, z_3, z_2) - \tfrac{1}{2}\mathcal{W}^{(2)}(z_1, \bar{z}_2;\, z_3, \bar{z}_4)\right] \tilde{G}(z_3, z_4), \tag{2.52}$$

$$\mathcal{U}^{\text{HFB}}(z_1, z_2;\, z_3, z_4) = \mathcal{W}^{(2)}(z_2, z_3;\, z_1, z_4) + \tfrac{1}{2}\mathcal{W}^{(2)}(z_2, \bar{z}_1;\, z_4, \bar{z}_3), \tag{2.53}$$

and GF $\tilde{G}$ is a solution of Eq. (2.55) (see below).

Using decompositions (2.49), one can transform both Eqs. (2.40) and (2.42) to the system of two equations. In the symbolic notations we have

$$G = \tilde{G} + \tilde{G}\, \Sigma^e\, G, \tag{2.54}$$

$$\tilde{G} = G^0 + G^0\, \tilde{\Sigma}\, \tilde{G}, \tag{2.55}$$

$$R = R^e + i\, R^e \tilde{\mathcal{U}}\, R, \tag{2.56}$$

$$R^e = R^0 + i\, R^0 \mathcal{U}^e\, R^e. \tag{2.57}$$

Proceeding by the same method as in Refs. [3,11], the last equation can be brought to the form

$$R^e(z_1, z_2;\, z_3, z_4) = \tilde{R}^0(z_1, z_2;\, z_3, z_4) + i \int dz_5 dz_6 dz_7 dz_8 \times \tilde{R}^0(z_1, z_2;\, z_5, z_6)\mathcal{W}^e(z_5, z_6;\, z_7, z_8) \times R^e(z_7, z_8;\, z_3, z_4), \tag{2.58}$$

where

$$\tilde{R}^0(z_1, z_2;\, z_3, z_4) = -\tilde{G}(z_3, z_1)\, \tilde{G}(z_2, z_4), \tag{2.59}$$

$$\mathcal{W}^e(z_1, z_2;\, z_3, z_4) = \mathcal{U}^e(z_1, z_2;\, z_3, z_4) + i\,\Sigma^e(z_3, z_1) \times \tilde{G}^{-1}(z_2, z_4) + i\, \tilde{G}^{-1}(z_3, z_1) \times \Sigma^e(z_2, z_4) - i\, \Sigma^e(z_3, z_1)\, \Sigma^e(z_2, z_4). \tag{2.60}$$

Equation (2.58) is the basic one for building the model which will be considered in the second part of the paper.

D. Single-quasiparticle basis functions and the energy representation

For the following analysis, it is required that we introduce a set of basis functions $\{\psi_1(y)\}$ in the extended space defined previously in Sec. II A. The usual conditions of orthonormality and completeness are supposed to be fulfilled:

$$\int dy\, \psi_1^*(y)\, \psi_{1'}(y) = \delta_{1,1'}, \qquad \sum_1 \psi_1^*(y)\, \psi_1(y') = \delta(y, y'). \tag{2.61}$$

It is convenient to consider $\psi_1(y)$ as the eigenfunctions of the operator

$$\mathcal{H}(y, y') = \mathcal{H}^0(y, y') + \tilde{\Sigma}(y, y'), \tag{2.62}$$

where $\mathcal{H}^0$ defines the single-particle term of the total Hamiltonian according to Eqs. (2.9) and (2.10), and $\tilde{\Sigma}$ is the mean-field contribution into the total mass operator in Eqs. (2.49). Thus, we assume the following equation to be fulfilled:

$$\int dy'\, \mathcal{H}(y, y')\, \psi_1(y') = E_1 \psi_1(y). \tag{2.63}$$

Since $\mathcal{H}$ possesses the same symmetry properties as the operators $\mathcal{H}^0$ and $\tilde{\Sigma}$, i.e.,

$$\mathcal{H}(y, y') = \mathcal{H}^*(y', y) = -\mathcal{H}(\bar{y}', \bar{y}), \tag{2.64}$$

it is not difficult to see that the complete set of the eigenfunctions of $\mathcal{H}$ is divided into two equal parts which are related by the operation of conjugation, that is,

$$\psi_{\bar{1}}(y) = \psi_1^*(\bar{y}). \tag{2.65}$$

For the corresponding eigenvalues, we have $E_{\bar{1}} = -E_1$. So one can denote $1 = \{\lambda_1, \eta_1\}$, $\bar{1} = \{\lambda_1, -\eta_1\}$, where λ_1 is the index of the usual single-particle configuration space (e.g., $\lambda = \{\tau_\lambda, n, l, j, m\}$ for the spherically symmetric system), and $\eta_1 = \pm 1$ is the sign of the eigenvalue E_1, that is, $E_1 = \eta_1 E_{\lambda_1}$, $E_{\lambda_1} = |E_1|$.

In the representation of ψ functions, the b operators defined by Eq. (2.1) have the form

$$b_1 = \int dy\, \psi_1^*(y)\, b(y). \tag{2.66}$$

It is worth noting that the b operators in this representation are simply related to the creation and annihilation operators of the quasiparticles $\alpha_\lambda^\dagger$ and α_λ which are usually introduced in the HFB theory. Namely, we have (see Ref. [15]) $b_{\lambda,+} = \alpha_\lambda$, $b_{\lambda,-} = \alpha_\lambda^\dagger$. So, in what follows we shall refer to functions $\psi_1(y)$ as the single-quasiparticle functions. A more detailed form of functions $\psi_1(y)$ can be obtained using the Bloch-Messiah theorem, see Refs. [1,15,19].

Up to now we have not restricted our analysis to systems in which the number of particles is conserved exactly. The reason is that our aim was to modify the existing general GF formalism for the arbitrary Fermi systems with pairing. However, application of the formalism to the atomic nuclei we are interested in implies that the particle-number conservation law is fulfilled. Thus, in what follows, we assume that the total Hamiltonian H defined by Eqs. (2.4)–(2.7) does not contain the external anomalous pair potentials Δ^0 and that Eqs. (2.8) hold. In that case, the ground state wave function $|0\rangle$ which enters the definition of the GFs (2.11) is an eigenfunction of the particle-number operator. This means that the exact GFs do not contain anomalous components. In particular, the exact single-particle GF satisfies the condition [cf. Eq. (2.41)]

$$(\chi - \chi')\, G(z, z') = 0. \tag{2.67}$$

However, this condition is not fulfilled for the GF $\tilde{G}$ which is the solution of Eq. (2.55) with the operator $\tilde{\Sigma}$ including the pair potentials independently of the Hamiltonian H (e.g., within the HFB approximation). Justification of using such GF $\tilde{G}$ is as follows. It enables one to take into account pairing correlations effectively and should be considered only as an approximation to the exact GF. The latter is found from Eq. (2.54) in which the mass operator Σ^e has to contain all necessary corrections to $\tilde{\Sigma}$, such that the solution of Eq. (2.54) satisfies Eq. (2.67). Of course this scheme should be considered only as a philosophy of the approach, i.e., as an ideal program which is difficult to implement completely in practice.

Let us now define the energy representation of the Green functions and of the related quantities entering the above equations. Making use of the basis $\{\psi_1(y)\}$, let us introduce the following Fourier transformations:

$$G_{12}(\varepsilon) = \int dz_1\, dz_2\, \psi_1^*(y_1)\, \psi_2(y_2)\, \delta(t_2) \times \exp(i\varepsilon\,(t_1 - t_2)) G(z_1, z_2), \tag{2.68}$$

$$\begin{aligned} R_{12,34}(\omega) &= -i \int dz_1\, dz_2\, dz_3\, dz_4\, \psi_1(y_1)\, \psi_2^*(y_2)\, \psi_3^*(y_3)\, \psi_4(y_4) \\ &\quad \times \delta(t_1 - t_2 - 0)\, \delta(t_4 - t_3 - 0)\, \delta(t_4) \\ &\quad \times \exp(i\omega\,(t_3 - t_1)) R(z_1, z_2;\, z_3, z_4), \end{aligned} \tag{2.69}$$

$$\begin{aligned} \mathcal{U}_{12,34}(\omega,\, \varepsilon,\, \varepsilon') &= \int dz_1\, dz_2\, dz_3\, dz_4 \psi_1(y_1)\, \psi_2^*(y_2)\, \psi_3^*(y_3)\, \psi_4(y_4) \\ &\quad \times \delta(t_4) \exp(i\omega\,(t_3 - t_1) + i\varepsilon\,(t_2 - t_1) + i\varepsilon'\,(t_3 - t_4)) \\ &\quad \times \mathcal{U}(z_1, z_2;\, z_3, z_4). \end{aligned} \tag{2.70}$$

The quantities $\tilde{G}_{12}(\varepsilon)$, $\Sigma^e_{12}(\varepsilon)$, $L_{12,34}(\omega)$, $\mathcal{U}^e_{12,34}(\omega,\, \varepsilon,\, \varepsilon')$, and others are defined in analogy to these formulas. In accordance with Eqs. (2.48), (2.65), and (2.69), we have

$$L_{12,34}(\omega) = R_{12,34}(\omega) - R_{\bar{2}\bar{1},34}(\omega). \tag{2.71}$$

Notice that spectral expansion for the response function $L(\omega)$ has the form

$$L_{12,34}(\omega) = -\sum_{\eta=\pm 1} \sum_{n\neq 0} \frac{\eta\, \rho_{12}^{n(\eta)}\, \rho_{34}^{n(\eta)*}}{\omega - \eta\,(\omega_n - i\cdot 0)}, \tag{2.72}$$

which is similar to the analogous formula for Fermi systems without pairing correlations (see, e.g., Ref. [20]). The difference consists in the definition of the transition amplitudes. In

Eq. (2.72), we have

$$\rho_{12}^{n(\eta)} = \delta_{\eta,+1}\langle n|\, b_1^\dagger\, b_2|0\rangle + \delta_{\eta,-1}\,\langle 0|\, b_1^\dagger\, b_2|n\rangle, \quad \omega_n = E_n - E_0, \tag{2.73}$$

where $|n\rangle$, $|0\rangle$, E_n, and E_0 are the eigenfunctions and eigenvalues of the Hamiltonian H. Taking into account definitions (2.1) and (2.66), one can see that even if the ground-state wave function $|0\rangle$ is an eigenfunction of the particle-number operator, the amplitudes $\rho_{12}^{n(\eta)}$ take nonzero values not only for the transitions between the states with the same number of particles, but also for the transitions between the ground state of the N-particle system $|0\rangle$ and the states $|n\rangle$ of the systems consisting of $N \pm 2$ particles. Thus, the spectral expansion (2.72) contains information about excitations of the N-particle system in both the ph and pp channels.

III. QUASIPARTICLE TIME BLOCKING APPROXIMATION

A. General framework

Let us now turn to the question of determining the physical observables and related quantities in this approach, namely, excitation energies ω_n and transition amplitudes $\rho_{12}^{n(\eta)}$. It follows from Eqs. (2.71) and (2.72) that to find these characteristics, we need to know the response function $R(\omega)$, i.e., to solve the system of equations (2.56) and (2.58). The basic difficulty in performing this task is that Eq. (2.58) contains energy-dependent interaction $\mathcal{U}^e$ and mass operator Σ^e. Notice, however, that these energy-dependent quantities arise only in the case when the dynamic contributions of complex configurations are explicitly taken into account. In the energy representation, Eq. (2.58) is an integral equation for the function $R^e(\omega,\ \varepsilon,\ \varepsilon')$ [defined in analogy to Eq. (2.70)] over the energy variable ε, which cannot be, strictly speaking, reduced to the closed equation for $R^e(\omega)$ because of the energy dependence of $\mathcal{U}^e$ and Σ^e. Fortunately, there are methods that allow us to avoid the complicated problem of the exact solution of this equation, making use of certain approximations. One such method will be considered here.

We begin by noting that if we use the eigenfunctions of the operator $\mathcal{H}$, i.e., the set $\{\psi_1(y)\}$, as the basis functions, the single-particle GF $\tilde{G}$ is diagonal, that is,

$$\tilde{G}_{12}(\varepsilon) = \frac{\delta_{12}}{\varepsilon - E_1 + i\,\eta_1 \cdot 0}, \tag{3.1}$$

as follows from Eqs. (2.21), (2.55), (2.62), and (2.63). In the time representation, we have

$$\tilde{G}_{12}(t_1, t_2) = -i\,\eta_1 \delta_{12}\,\theta(\eta_1 t_{12})\,\exp(-i E_1 t_{12}), \tag{3.2}$$

where $t_{12} = t_1 - t_2$, $\theta(\tau)$ is the step function. These expressions are formally identical with analogous formulas for the normal GFs, except that they are written in the extended basis representation. It enables one to apply, practically without changes, the method of chronological decoupling of diagrams (MCDD) to the solution of Eqs. (2.56) and (2.58) which contain the GFs with pairing. The MCDD was developed in Ref. [11] to solve ph-channel BSE in the normal Fermi system including dynamic effects both in the interaction and in the mass operator. The idea of the method is similar to that used in the other methods developed earlier to solve the analogous problems in Refs. [21] (ph-channel BSE) and [22–24] (pp-channel BSE). However, the MCDD differs from the aforementioned methods in some details, in particular concerning the treatment of the GSC2. Almost all the resulting equations obtained by means of this straightforward extension of the MCDD are found to be formally identical with equations for the normal Fermi system in the same sense as Eqs. (3.1) and (3.2). Because derivation of these equations in the latter case was described in detail in Refs. [3,11], we will draw only the main formulas and the final results.

First of all, the function $\tilde{R}^0 = -\tilde{G}\tilde{G}$ entering Eq. (2.58) is divided into two parts, $\tilde{R}^0 = \tilde{R}^{0(a)} + \tilde{R}^{0(b)}$, where

$$\tilde{R}^{0(a)}_{12,34}(t_1, t_2; t_3, t_4) = -\delta_{\eta_1,-\eta_2}\,\theta(\eta_1 t_{41})\,\theta(\eta_1 t_{32}) \times \tilde{G}_{31}(t_3, t_1)\tilde{G}_{24}(t_2, t_4), \tag{3.3}$$

and $\tilde{R}^{0(b)}$ is the remainder term, which is absorbed in part in the renormalization procedure. As compared with the initial function $\tilde{R}^0$ defined by Eq. (2.59), the term $\tilde{R}^{0(a)}$ contains two additional time-dependent step functions and the factor $\delta_{\eta_1,-\eta_2}$ which play a twofold role. On the one hand, they allow one to obtain a closed set of algebraic equations in the energy representation for the main component of the function $R^e(\omega)$ [see Eqs. (3.5), (3.18), and (3.19) below] which is much more simple to solve than the initial Eq. (2.58). On the other hand, owing to these additional θ and δ functions, an approximate solution of Eq. (2.58) obtained in this way contains main contributions of the 2q and 2q $\otimes$ phonon configurations (within the model described in the next subsection), while more complicated intermediate states (e.g., 2q $\otimes$ 2phonon, 2q $\otimes$ 3phonon, and so on) are blocked, in part, in the time representation. So in the following, this scheme will be referred to as the quasiparticle time blocking approximation (QTBA). Examples of the blocked intermediate 2q $\otimes$ 2phonon states are shown later in Fig. 2.

Further, a renormalization procedure is applied to Eq. (2.56) for the response function R, which leads to the following equation for the effective response function R^{eff} in the energy representation:

$$R^{\text{eff}}_{12,34}(\omega) = A_{12,34}(\omega) - \sum_{5678} A_{12,56}(\omega)\mathcal{F}_{56,78}R^{\text{eff}}_{78,34}(\omega), \tag{3.4}$$

where $A(\omega)$ is a joint (ph and pp) correlated propagator, and $\mathcal{F}$ is an amplitude of the effective interaction. The propagator $A(\omega)$ is the main term of the formal decomposition

$$R^e_{12,34}(\omega) = A_{12,34}(\omega) + B_{12,34}. \tag{3.5}$$

It contains (i) the sum of an infinite number of terms to all orders in $\tilde{R}^{0(a)}$ and (ii) the terms linear and quadratic in $\tilde{R}^{0(b)}$ which are related to the GSC2. The term B in Eq. (3.5) is an auxiliary quantity which is supposed to be energy independent. In addition, it is supposed that B contains all the contributions not included explicitly in the propagator $A(\omega)$. The effective interaction $\mathcal{F}$ and the effective charge operator e are defined by

$$\mathcal{F}_{12,34} = \sum_{56} e_{12,56}\, \tilde{\mathcal{U}}_{56,34},$$
$$e_{12,34} = \delta_{13}\,\delta_{24} - \sum_{56} \mathcal{F}_{12,56} B_{56,34} = (e^{\dagger}_{34,12})^{*}. \tag{3.6}$$

In terms of these quantities, the exact response function R is related to the effective response function by the ansatz

$$R_{12,34}(\omega) = \sum_{5678} e^{\dagger}_{12,56}\, R^{\mathrm{eff}}_{56,78}(\omega) e_{78,34} + \sum_{56} B_{12,56} e_{56,34}. \tag{3.7}$$

One of the basic quantities, which determines the physical observables in this approach, is the nuclear polarizability $\Pi(\omega)$. More precisely, it determines the distribution of the transition strength caused by an external field $V^{0}(x, x')$. The function $\Pi(\omega)$ is defined as

$$\Pi(\omega) = -\frac{1}{2} \sum_{1234} (e\, V^{0})^{*}_{21}\, R^{\mathrm{eff}}_{12,34}(\omega) (e\, V^{0})_{43}, \tag{3.8}$$

where

$$(e\, V^{0})_{12} = \sum_{34} e_{21,43} V^{0}_{34}, \tag{3.9}$$

$$V^{0}_{12} = \int dy\, dy'\, \psi^{*}_{1}(y)\, \psi_{2}(y')\, \delta_{\chi,\chi'} [\delta_{\chi,+1}\, V^{0}(x, x') - \delta_{\chi,-1}\, V^{0}(x', x)] = -V^{0}_{\bar{2}\bar{1}}. \tag{3.10}$$

In particular, the strength function $S(E)$ which is frequently used for the description of nuclear excitations is expressed in terms of the polarizability as

$$S(E) = \frac{1}{2\pi} \,\mathrm{Im} \sum_{1234} V^{0*}_{21}\, R_{12,34}(E + i\,\Delta) V^{0}_{43} = -\frac{1}{\pi}\,\mathrm{Im}\,\Pi(E + i\,\Delta), \tag{3.11}$$

where Δ is a smearing parameter. The formulas (3.4)–(3.9), (3.11) are completely analogous to the ones for the normal Fermi system (see Ref. [3]), except for the factors $\frac{1}{2}$ in Eqs. (3.8) and (3.11) which arise due to definition (3.10) of the operator V^{0} in the extended space taken in the antisymmetric form.

B. Correlated propagator within the QTBA

Eq. (3.4) for the response function is still quite general. To formulate a model, we have to define the correlated propagator $A(\omega)$. In particular, if we neglect the dynamic contributions of complex configurations, i.e., if we put $\mathcal{U}^{e} = 0$ and $\Sigma^{e} = 0$, we come to the QRPA. In this case, we have $A(\omega) = \tilde{A}(\omega)$, where $\tilde{A}(\omega)$ is the uncorrelated QRPA propagator

$$\tilde{A}_{12,34}(\omega) = -\frac{\eta_1\, \delta_{\eta_1,-\eta_2}\, \delta_{13}\, \delta_{24}}{\omega - E_{12}}, \quad E_{12} = E_1 - E_2. \tag{3.12}$$

To go beyond the QRPA, we have to find reasonable approximations for the quantities $\mathcal{U}^{e}$ and Σ^{e}. In the present work, we will use a QRPA-based version of the quasiparticle-phonon coupling (QPC) model (see Ref. [25]). This model is discussed and used in a variety of papers; see, e.g., Refs. [2,3,8,13,20]. Within the QPC model, one can restrict oneself to the so-called g^2 approximation, where g is an amplitude of the quasiparticle-phonon interaction (see Ref. [3] for more details). Under some simplifying assumptions, this approximation can be obtained in the GF method (see Refs. [26–28]). Within the QPC model and g^2 approximation, we have the following formulas for the quantities $\mathcal{U}^{e}$ and Σ^{e}:

$$\mathcal{U}^{e}_{12,34}(\omega,\, \varepsilon,\, \varepsilon') = \sum_{\eta,m} \frac{\eta\, g^{m(\eta)*}_{31}\, g^{m(\eta)}_{42}}{\varepsilon - \varepsilon' + \eta\, (\omega_m - i\cdot 0)}, \tag{3.13}$$

$$\Sigma^{e}_{12}(\varepsilon) = \sum_{3,\eta,m} \frac{\delta_{\eta,\eta_3} g^{m(\eta)*}_{13}\, g^{m(\eta)}_{23}}{\varepsilon - E_3 - \eta\, (\omega_m - i\cdot 0)}, \tag{3.14}$$

where m is an index of the phonon, and ω_m is the phonon energy, $\eta = \pm 1$. Representation of the response function R^{e}, which determines the correlated propagator within this model according to Eqs. (2.58) and (3.5), in terms of Feynmann diagrams is shown in Fig. 1.

Figure 2 shows examples of diagrams that correspond to the intermediate 2q $\otimes$ 2phonon states and are blocked in the model.

Hereafter, it is assumed that the quasiparticle-phonon amplitudes $g^{m(\eta)}_{12}$ are related to the transition amplitudes $\rho^{m(\eta)}_{12}$ [see Eq. (2.73)] by means of QRPA equations, that is,

$$g^{m(\eta)}_{12} = \sum_{34} \tilde{\mathcal{F}}_{12,34}\, \rho^{m(\eta)}_{34}, \quad \rho^{m(\eta)}_{12} = \frac{\eta_1\, \delta_{\eta_1,-\eta_2}}{\eta\, \omega_m - E_{12}}\, g^{m(\eta)}_{12}, \tag{3.15}$$

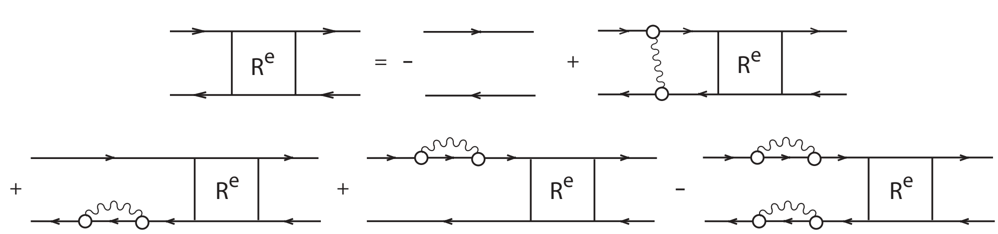

FIG. 1. Equation (2.58) for the response function R^{e} determining correlated QTBA propagator. Conventional notations are used for single-particle Green functions $\tilde{G}$ (solid lines with arrows), phonon propagators (wavy lines), and amplitudes of the quasiparticle-phonon interaction (small circles). First term on the right-hand side corresponds to the uncorrelated QRPA propagator. Diagrams are not ordered in time.

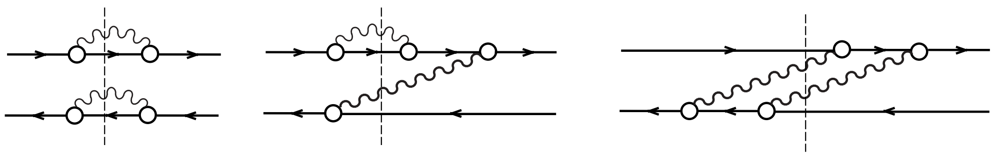

FIG. 2. Examples of intermediate 2q ⊗ 2 phonon states, which are blocked in the QTBA. Vertical dashed lines denote the time cut of the diagrams at fixed time. Diagrams are ordered in time.

where $\tilde{\mathcal{F}}$ is an amplitude of the effective interaction which generally differs from the amplitude $\mathcal{F}$ entering Eq. (3.4). Notice that the QRPA equations acquire very simple form in the representation of single-quasiparticle ψ functions. Equations (3.15) have to be supplemented by the normalization condition

$$\frac{1}{2}\sum_{12}\eta\,\eta_1\left|\rho^{m(\eta)}_{12}\right|^2 = 1 \tag{3.16}$$

and by the condition of the antisymmetry

$$\rho^{m(\eta)}_{12} = -\rho^{m(\eta)}_{\bar{2}\bar{1}}, \tag{3.17}$$

which is obviously fulfilled for the exact transition amplitudes defined by Eq. (2.73). Notice, however, that in contrast to the case considered in Refs. [3,11], the quasiparticle-phonon amplitudes $g^{m(\eta)}_{12}$ in Eqs. (3.13) and (3.14) determine the coupling with excitations in both the ph and pp channels [see Eqs. (3.15) and comments after Eq. (2.73)].

The QTBA in combination with Eqs. (3.13) and (3.14) leads to the following ansatz for the correlated propagator:

$$A_{12,34}(\omega) = \sum_{5678}[\delta_{15}\,\delta_{26} + Q^{(+-)}_{12,56}(\omega)]A^{(--)}_{56,78}(\omega) \times [\delta_{73}\,\delta_{84} + Q^{(-+)}_{78,34}(\omega)] + P^{(++)}_{12,34}(\omega), \tag{3.18}$$

where the upper indices denote products of the first and second pairs of lower η indices. In particular, for the component $A^{(--)}_{12,34}(\omega)$ of the propagator, we have $\eta_1\eta_2 = \eta_3\eta_4 = -1$. This component is determined by the equation

$$A^{(--)}_{12,34}(\omega) = \tilde{A}_{12,34}(\omega) - \sum_{5678}\tilde{A}_{12,56}(\omega)\,\Phi_{56,78}(\omega)A^{(--)}_{78,34}(\omega), \tag{3.19}$$

where $\tilde{A}(\omega)$ is the QRPA propagator defined by Eq. (3.12). For the remaining quantities in the Eqs. (3.18) and (3.19), we obtain

$$Q^{(+-)}_{12,34}(\omega) = Q^{(+-)\,\mathrm{res}}_{12,34}(\omega) + \delta_{\eta_1,\eta_2}\,\delta_{\eta_3,-\eta_4} \times \left(\frac{\Sigma^{\mathrm{GSC}}_{31}}{E_{31}}\,\delta_{24} - \delta_{31}\,\frac{\Sigma^{\mathrm{GSC}}_{24}}{E_{24}}\right), \tag{3.20}$$

$$Q^{(-+)}_{12,34}(\omega) = Q^{(-+)\,\mathrm{res}}_{12,34}(\omega) - \delta_{\eta_1,-\eta_2}\,\delta_{\eta_3,\eta_4} \times \left(\frac{\Sigma^{\mathrm{GSC}}_{31}}{E_{31}}\,\delta_{24} - \delta_{31}\,\frac{\Sigma^{\mathrm{GSC}}_{24}}{E_{24}}\right), \tag{3.21}$$

$$\Phi_{12,34}(\omega) = \Phi^{\mathrm{res}}_{12,34}(\omega) + \bar{\Phi}^{\mathrm{GSC}}_{12,34} + \Phi^{\mathrm{GSC\,s.e.}}_{12,34}(\omega). \tag{3.22}$$

In these formulas, a superscript "res" denotes the resonant parts of the amplitudes, the quantities $\bar{\Phi}^{\mathrm{GSC}}$ and $\Phi^{\mathrm{GSC\,s.e.}}(\omega)$ represent contributions of the GSC. They consist of the static part arising from the induced interaction ($\bar{\Phi}^{\mathrm{GSC}}$) and the part arising from the self-energy insertions ($\Phi^{\mathrm{GSC\,s.e.}}$),

$$\bar{\Phi}^{\mathrm{GSC}}_{12,34} = -\delta_{\eta_1,-\eta_2}\,\delta_{\eta_3,-\eta_4}\sum_{\eta,m}\big(\delta_{\eta,\eta_3}\,\rho^{m(\eta)}_{13}\,g^{m(\eta)*}_{24} + \delta_{\eta,\eta_4}g^{m(\eta)}_{13}\,\rho^{m(\eta)*}_{24}\big), \tag{3.23}$$

$$\Phi^{\mathrm{GSC\,s.e.}}_{12,34}(\omega) = \eta_1\,\delta_{\eta_1,-\eta_2}\,\delta_{\eta_3,-\eta_4} \times \big(\Sigma^{\mathrm{GSC}}_{31}\,(\delta_{24} + q_{24}) - (\delta_{31} + q_{31})\,\Sigma^{\mathrm{GSC}}_{24} - (q_{31}\,\delta_{24} + \delta_{31}\,q_{24} + q_{31}\,q_{24}) \times \big[\omega - \tfrac{1}{2}\,(E_{12} + E_{34})\big]\big), \tag{3.24}$$

where

$$\Sigma^{\mathrm{GSC}}_{12} = \tfrac{1}{2}\,\big(1 + \delta_{\eta_1,-\eta_2}\big)\sum_{3,\eta,m}\eta\,\delta_{\eta,\eta_3}\,\big(\rho^{m(\eta)*}_{13}\,g^{m(\eta)}_{23} + g^{m(\eta)*}_{13}\,\rho^{m(\eta)}_{23}\big), \tag{3.25}$$

$$q_{12} = \sum_{3,\eta,m}\delta_{\eta,\eta_3}\,\rho^{m(\eta)*}_{13}\,\rho^{m(\eta)}_{23}. \tag{3.26}$$

The component $P^{(++)}(\omega)$ of the correlated propagator and the resonant parts of the amplitudes entering Eqs. (3.20)–(3.22) are defined as

$$P^{(++)}_{12,34}(\omega) = \sum_{5678,\eta,m}\zeta^{\,m56(\eta)}_{12}\,\tilde{A}^{(\eta)}_{56,78}(\omega - \eta\,\omega_m)\,\zeta^{\,m78(\eta)*}_{34}, \tag{3.27}$$

$$Q^{(+-)\,\mathrm{res}}_{12,34}(\omega) = \sum_{5678,\eta,m}\zeta^{\,m56(\eta)}_{12}\,\tilde{A}^{(\eta)}_{56,78}(\omega - \eta\,\omega_m)\,\gamma^{\,m78(\eta)*}_{34}, \tag{3.28}$$

$$Q^{(-+)\,\mathrm{res}}_{12,34}(\omega) = \sum_{5678,\eta,m}\gamma^{\,m56(\eta)}_{12}\,\tilde{A}^{(\eta)}_{56,78}(\omega - \eta\,\omega_m)\,\zeta^{\,m78(\eta)*}_{34}, \tag{3.29}$$

$$\Phi^{\mathrm{res}}_{12,34}(\omega) = -\sum_{5678,\eta,m}\gamma^{\,m56(\eta)}_{12}\,\tilde{A}^{(\eta)}_{56,78}(\omega - \eta\,\omega_m)\,\gamma^{\,m78(\eta)*}_{34}, \tag{3.30}$$

where

$$\gamma^{\,m56(\eta)}_{12} = \delta_{\eta,\eta_5}\,\delta_{\eta_1,-\eta_2}\,\delta_{\eta_5,-\eta_6}\,\big(\delta_{15}\,g^{m(\eta)}_{62} - g^{m(\eta)}_{15}\delta_{62}\big), \tag{3.31}$$

$$\zeta^{\,m56(\eta)}_{12} = \delta_{\eta,\eta_5}\,\delta_{\eta_1,\,\eta_2}\,\delta_{\eta_5,-\eta_6}\,\big(\delta_{15}\,\rho^{m(\eta)}_{62} - \rho^{m(\eta)}_{15}\delta_{62}\big), \tag{3.32}$$

and $\tilde{A}^{(+)}(\omega)$ and $\tilde{A}^{(-)}(\omega)$ are the positive and negative frequency parts of the QRPA propagator defined by Eq. (3.12),

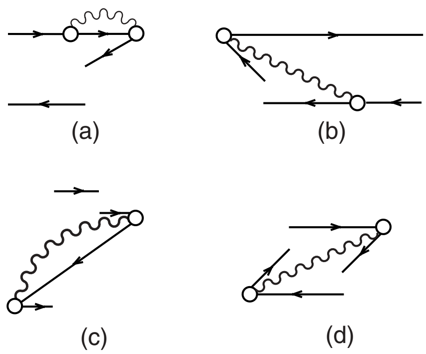

FIG. 3. Examples of the dynamic contributions of the ground state correlations of order g^2 into the correlated propagator. Diagrams a and b represent contributions of the amplitudes $Q^{(-+)}(\omega)$ and $Q^{(+-)}(\omega)$, correspondingly. Diagrams c and d represent contributions of the component $P^{(++)}(\omega)$. Diagrams are ordered in time.

i.e., $\tilde{A}(\omega) = \tilde{A}^{(+)}(\omega) + \tilde{A}^{(-)}(\omega)$,

$$\tilde{A}^{(\eta)}_{12,34}(\omega) = -\frac{\eta\,\delta_{\eta,\eta_1}\,\delta_{\eta_1,-\eta_2}\,\delta_{13}\,\delta_{24}}{\omega - \eta\,\eta_1 E_{12}}. \tag{3.33}$$

Correlated propagator $A(\omega)$ defined by Eq. (3.18) and subsequent equations includes contributions of three types: (i) pure 2q configurations associated with uncorrelated QRPA propagator $\tilde{A}(\omega)$, (ii) 2q $\otimes$ phonon+GSC2 configurations introduced by the quantities $\mathcal{U}^e$ and Σ^e, and (iii) uncontrollable more complicated configurations arising due to the GSC2 effects and their combinations with the above-mentioned configurations. The GSC2 effects are included both in the component $A^{(--)}(\omega)$ of the propagator through the amplitude $\Phi(\omega)$ in Eq. (3.19) and in the quantities $Q^{(-+)}(\omega)$, $Q^{(+-)}(\omega)$, and $P^{(++)}(\omega)$. The latter quantities include dynamic contributions of the GSC2. Diagram representation of some of these contributions is shown in Fig. 3.

C. Sum rule analysis and a refinement of the model

The formulas of the previous subsection completely determine the correlated propagator of the model within the g^2 approximation. By construction, this propagator contains all the g^2 contributions, including those from GSC. However, exact fulfillment of the sum rules in this approach is not guaranteed. Let us consider this question in more detail. Usually, the sum rule is meant in the sense of relation between the moment m_k of the strength function $S(E)$ and the ground state expectation value of certain operator (see, e.g., Ref. [29]). The moment m_k is defined as

$$m_k = \frac{1}{2}\int_{-\infty}^{\infty} S(E)\,E^k dE \tag{3.34}$$

at $\Delta \to +0$ in Eq. (3.11). Introducing asymptotic expansion of the exact response function,

$$R_{12,34}(\omega) \sim -\sum_{k=0}^{\infty} M^{(k)}_{12,34}\,\omega^{-k-1}, \tag{3.35}$$

and using Eqs. (2.71), (2.72), (3.10), (3.11), one can show that the moments m_k are expressed through the coefficient functions $M^{(k)}_{12,34}$ by the formula

$$m_k = \frac{1}{4}\sum_{1234} V^{0^*}_{21}\,M^{(k)}_{12,34}\,V^{0}_{43}. \tag{3.36}$$

In particular, by making use of the BSE (2.42) in the energy representation, one can obtain

$$M^{(0)}_{12,34} = \delta_{31}\,\rho_{24} - \rho_{31}\,\delta_{24}, \tag{3.37}$$

where $\rho_{12} = \langle 0|b^{\dagger}_2\,b_1|0\rangle$ is the extended density matrix (EDM). Substituting Eq. (3.37) into Eq. (3.36), we get the so-called non-energy-weighted sum rule (NEWSR):

$$m_0 = \tfrac{1}{4}\,\mathrm{Tr}\,(\rho\,[V^0, V^{0^\dagger}]). \tag{3.38}$$

Notice that the factor $\frac{1}{4}$ in this formula (instead of the usual factor $\frac{1}{2}$) arises from the definition (3.10) of the external field operator in the extended space taken in the antisymmetric form.

Thus, to ensure exact fulfillment of the NEWSR, the coefficient function $M^{(0)}_{12,34}$ of the model must have the form (3.37) with properly normalized EDM ρ. Using the formulas of the previous subsection and the definition of the quantity $M^{(0)}_{12,34}$ through the expansion (3.35) one can show that (i) the NEWSR is fulfilled exactly within the QRPA and (ii) Eq. (3.37) is not fulfilled rigorously in the considered version of the QTBA and the NEWSR is fulfilled only up to the terms of order g^2 within this model.

It is not difficult, however, to remedy this drawback within the above-described scheme based on the g^2 approximation. First of all, let us include energy-independent operator $\Sigma^{\,\mathrm{GSC}}$ defined by Eq. (3.25) into the mean-field part $\tilde{\Sigma}$ of the total mass operator $\Sigma(\varepsilon)$. It can be done because the only constraint on the operator $\tilde{\Sigma}$ was the condition of its energy independence. On the same grounds in the following we include the energy-independent amplitude $\bar{\Phi}^{\,\mathrm{GSC}}$ entering Eq. (3.22) into the amplitude $\tilde{\mathcal{U}}$. Thus, instead of Eq. (2.49), we now use the decompositions

$$\Sigma = \tilde{\Sigma}' + \bar{\Sigma}^{\,e}, \quad \mathcal{U} = \tilde{\mathcal{U}}' + \bar{\mathcal{U}}^{\,e}, \tag{3.39}$$

where

$$\tilde{\Sigma}' = \tilde{\Sigma} + \Sigma^{\,\mathrm{GSC}}, \quad \tilde{\mathcal{U}}' = \tilde{\mathcal{U}} + \bar{\Phi}^{\,\mathrm{GSC}}, \tag{3.40}$$

$$\bar{\Sigma}^{\,e}(\varepsilon) = \Sigma^{\,e}(\varepsilon) - \Sigma^{\,\mathrm{GSC}},$$
$$\bar{\mathcal{U}}^{\,e}(\omega,\,\varepsilon,\,\varepsilon') = \mathcal{U}^{\,e}(\omega,\,\varepsilon,\,\varepsilon') - \bar{\Phi}^{\,\mathrm{GSC}}, \tag{3.41}$$

with $\mathcal{U}^{\,e}(\omega,\,\varepsilon,\,\varepsilon')$ and $\Sigma^{\,e}(\varepsilon)$ defined by Eqs. (3.13) and (3.14).

These redefinitions mean that we have to use in all the equations the quantities $\bar{\Sigma}^{\,e}$ and $\bar{\mathcal{U}}^{e}$ instead of $\Sigma^{\,e}$ and $\mathcal{U}^{e}$. The replacement of $\mathcal{U}^{e}$ by $\bar{\mathcal{U}}^{\,e}$ leads to disappearance of the amplitude $\bar{\Phi}^{\,\mathrm{GSC}}$ from the right-hand side of Eq. (3.22). The replacement of $\Sigma^{\,e}$ by $\bar{\Sigma}^{\,e}$ leads to disappearance of all the terms containing $\Sigma^{\,\mathrm{GSC}}$ in Eqs. (3.20), (3.21), and (3.24). The remaining part of the amplitude $\Phi^{\,\mathrm{GSC\;s.e.}}(\omega)$ in Eq. (3.22) can be taken into account through the renormalization of the QRPA propagator $\tilde{A}(\omega)$ within the g^2 approximation.

To this aim, let us introduce matrix $\tilde{Z}_{12,34}$ defined by

$$\sum_{56}\tilde{Z}_{12,56}\,\tilde{Z}_{56,34} = \delta_{31}\,\delta_{24} - q_{31}\,\delta_{24} - \delta_{31}\,q_{24},$$
$$\tilde{Z}_{12,34} = \tilde{Z}^{*}_{34,12}, \tag{3.42}$$

where the matrix q_{12} is defined by Eq. (3.26). In addition, it is supposed that the matrix $\tilde{Z}_{12,34}$ is positive-definite, which can always be fulfilled if all the eigenvalues q_i of the matrix q_{12} satisfy the condition $q_i < \frac{1}{2}$ [notice that $q_i \geqslant 0$, as follows from Eq. (3.26)]. Because according to Eqs. (3.15) and (3.26) we have $q_{12} = O(g^2)$, the pointed condition is consistent with the previous model assumptions. Thus, from Eq. (3.42) it follows that

$$\tilde{Z}_{12,34} = \delta_{31}\,\delta_{24} - \tfrac{1}{2}\,(q_{31}\,\delta_{24} + \delta_{31}\,q_{24}) + O(g^4). \quad (3.43)$$

Further, using Eqs. (3.12), (3.24) (without terms containing operator $\Sigma^{\,\mathrm{GSC}}$), and (3.43), we obtain

$$\tilde{A}(\omega) - \tilde{A}(\omega)\,\Phi^{\,\mathrm{GSC\,s.e.}}(\omega)\,\tilde{A}(\omega) = \tilde{Z}\,\tilde{A}(\omega)\,\tilde{Z} + O(g^4). \quad (3.44)$$

It enables one to redefine the correlated propagator replacing Eq. (3.18) by the ansatz

$$A_{12,34}(\omega) = \sum_{5678} Z^{L}_{12,56}(\omega) A^{(--)}_{56,78}(\omega) Z^{R}_{78,34}(\omega) + P^{(++)}_{12,34}(\omega), \quad (3.45)$$

where

$$Z^{L}_{12,34}(\omega) = \sum_{56} \big[\delta_{15}\,\delta_{26} + Q^{(+-)\,\mathrm{res}}_{12,56}(\omega)\big]\,\tilde{Z}_{56,34}, \quad (3.46)$$

$$Z^{R}_{12,34}(\omega) = \sum_{56} \tilde{Z}_{12,56}\,\big[\delta_{53}\,\delta_{64} + Q^{(-+)\,\mathrm{res}}_{56,34}(\omega)\big]. \quad (3.47)$$

In Eq. (3.45), the propagator $A^{(--)}(\omega)$ is determined by Eq. (3.19), in which the amplitude $\Phi(\omega)$ is now defined as

$$\Phi_{12,34}(\omega) = \sum_{5678} \tilde{Z}_{12,56}\,\Phi^{\mathrm{res}}_{56,78}(\omega)\,\tilde{Z}_{78,34}, \quad (3.48)$$

instead of by Eq. (3.22).

It is easy to see that the propagator $A(\omega)$ defined by Eqs. (3.19), (3.42), and (3.45)–(3.48) coincides up to terms of order g^2 with the propagator defined in the previous subsection [see Eq. (3.18) and subsequent equations], if in addition we take into account Eqs. (3.39)–(3.41). On the other hand, assuming that the effective charge in Eq. (3.7) is equal to the unit operator and making use of the expansion (3.35), one can find that this new redefined propagator leads to the following result for the coefficient function $M^{(0)}_{12,34}$:

$$M^{(0)}_{12,34} = \eta_1\,\delta_{\eta_1,-\eta_2}\,(\delta_{31}\,\delta_{24} - q_{31}\,\delta_{24} - \delta_{31}\,q_{24}) + \eta_1\,\delta_{\eta_1,\eta_2} \times (\delta_{31}\,q_{24} - q_{31}\,\delta_{24}). \quad (3.49)$$

Here the terms containing $\delta_{\eta_1,-\eta_2}$ follow from Eq. (3.42). The terms containing δ_{η_1,η_2} arise from the contributions of the component $P^{(++)}(\omega)$ in Eq. (3.45). From Eq. (3.49) we obtain that in the modified version of the model, the coefficient function $M^{(0)}_{12,34}$ has the form (3.37) with the correlated EDM ρ defined as

$$\rho_{12} = \tilde{\rho}_{12} + \eta_1\,q_{12}, \quad (3.50)$$

where $\tilde{\rho}_{12} = \delta_{\eta_1,-1}\,\delta_{12}$ is the EDM of the HFB theory in the representation of ψ functions. Therefore, we conclude that if the EDM (3.50) is normalized by the usual condition

$$\int dy'\,\delta_{\chi',+1}\,\delta_{\tau',\tau} \sum_{12} \psi_1(y')\,\psi_2^{*}(y')\,\rho_{12} = N_\tau, \quad (3.51)$$

the NEWSR is fulfilled exactly within the QTBA.

The following remarks are in order. First, the EDM (3.50) arising in the QTBA coincides with the correlated EDM $\rho^{\,c}$, which can be obtained from the Dyson equation (2.54) and the Eqs. (3.1), (3.14), (3.25), (3.41) within the g^2 approximation:

$$\rho_{12} = \rho^{\,c}_{12} \equiv \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i}\, e^{i\varepsilon\tau}[\tilde{G}(\varepsilon) + \tilde{G}(\varepsilon)\,\bar{\Sigma}^{\,e}(\varepsilon)\,\tilde{G}(\varepsilon)]_{12}, \quad \tau \to +0. \quad (3.52)$$

Second, notice that the GSC effects included by means of renormalization of the QRPA propagator within the QTBA with the help of the matrix $\tilde{Z}$ are the same as the effects included in the renormalized QRPA (RQRPA, see, e.g., Ref. [7]). It is known (see Ref. [30]) that within the standard RQRPA, the Ikeda sum rule (being a particular case of the NEWSR) is violated. The above analysis allows us to understand the reason for this violation. It follows from Eq. (3.49) that to satisfy the NEWSR within the QTBA, it is necessary and sufficient to take into account contributions of all the terms in Eq. (3.45) including term $P^{(++)}(\omega)$. This term represents dynamic contributions of the GSC into the QTBA propagator (3.45), which cannot be reduced to the renormalization of the QRPA propagator $\tilde{A}(\omega)$ and which are absent in the RQRPA.

Let us consider in brief the question of the energy-weighted sum rule (EWSR). Usually, the EWSR is associated with the moment m_1. In contrast to the NEWSR, the model-independent formula for m_1 is not as simple as Eq. (3.38) (see Ref. [29]). So, in the general case, we are able to calculate and compare only the values of the EWSR obtained within different models. It is easy to find the moment m_1 within the QRPA using definitions (3.35), (3.36), and the equation for the QRPA response function $\tilde{R}$,

$$\tilde{R}(\omega) = \tilde{A}(\omega) - \tilde{A}(\omega)\,\tilde{\mathcal{F}}\,\tilde{R}(\omega), \quad (3.53)$$

where the QRPA propagator $\tilde{A}$ is defined by Eq. (3.12). The result reads

$$m_1^{\mathrm{QRPA}} = \tfrac{1}{4}\,\mathrm{Tr}(\tilde{\rho}[[V^{\,0},\mathcal{H}],V^{\,0\dagger}]) + \tfrac{1}{4}\sum_{1234}[V^{\,0\dagger},\tilde{\rho}]_{12} \times \tilde{\mathcal{F}}_{12,34}\,[\tilde{\rho},V^{\,0}]_{43}, \quad (3.54)$$

where the single-quasiparticle Hamiltonian $\mathcal{H}$ is defined by Eq. (2.62). The formula for the moment m_1 within the QTBA in the general case is much more complicated and is not drawn here. However, it is not difficult to find the value of m_1^{QTBA} when the GSC2 are not included. In this case, the correlated propagator $A(\omega)$ in Eq. (3.4) coincides with component $A^{(--)}(\omega)$ which is a solution of Eq. (3.19) with $\Phi(\omega) = \Phi^{\,\mathrm{res}}(\omega)$. Taking into account that the amplitude $\Phi^{\,\mathrm{res}}(\omega)$ goes down as $1/\omega$ when $\omega \to \infty$, we obtain the same result (3.54) in the QTBA as in the QRPA in which, however, the amplitude of the interaction $\tilde{\mathcal{F}}$ should be replaced by the amplitude $\mathcal{F}$. If, in addition, the QTBA amplitude $\mathcal{F}$ coincides with the QRPA amplitude $\tilde{\mathcal{F}}$, we arrive at the equality

$m_1^{\rm QTBA} = m_1^{\rm QRPA}$. Notice that analogous results are obtained for the EWSR in the RPA, the second RPA (SRPA), and the extended RPA (ERPA). Within the SRPA, the GSC2 are not included and that leads to the equality $m_1^{\rm SRPA} = m_1^{\rm RPA}$. On the other hand, within the ERPA, the GSC2 are included, and we have $m_1^{\rm ERPA} \neq m_1^{\rm RPA}$ (see Ref. [29] for more details).

D. Antisymmetrization of the equations and inclusion of the two-phonon configurations

As can be seen from the spectral expansion (2.72), the physical observables of the theory are completely determined by the antisymmetric response function $L(\omega)$. Within the QTBA, this exact function is approximated by the effective antisymmetric response function $L^{\rm eff}(\omega)$ defined as [cf. Eq. (2.71)] $L^{\rm eff}_{12,34}(\omega) = R^{\rm eff}_{12,34}(\omega) - R^{\rm eff}_{\bar{2}\bar{1},34}(\omega)$, where $R^{\rm eff}(\omega)$ is the solution of Eq. (3.4). It is easy to prove the following. First, the polarizability $\Pi(\omega)$ [see Eq. (3.8)] is actually determined by the function $L^{\rm eff}(\omega)$, while the symmetric part of the function $R^{\rm eff}(\omega)$ does not contribute to the Eq. (3.8). In other words, $\Pi(\omega)$ is invariant under the transformation $R^{\rm eff}(\omega) \to \frac{1}{2} L^{\rm eff}(\omega)$. Second, the function $L^{\rm eff}(\omega)$ is the doubled solution of the antisymmetrized QTBA equation obtained from Eq. (3.4) with the help of antisymmetrization of the correlated propagator $A(\omega)$. This antisymmetrization can be implemented by means of the following transformations in Eqs. (3.19), (3.27)–(3.30): $\tilde{A}(\omega) \to \frac{1}{2}\,\tilde{L}^0(\omega)$ and $\tilde{A}^{(\eta)}(\omega) \to \frac{1}{2}\,\tilde{L}^{0(\eta)}(\omega)$, where $\tilde{L}^0(\omega)$ is the antisymmetric (uncorrelated) QRPA propagator, and $\tilde{L}^{0(\eta)}(\omega)$ represents its positive and negative frequency parts [cf. Eqs. (3.12) and (3.33)], that is,

$$
\begin{aligned}
\tilde{L}^{0}_{12,34}(\omega) &= \sum_{\eta=\pm 1} \tilde{L}^{0(\eta)}_{12,34}(\omega),\\
\tilde{L}^{0(\eta)}_{12,34}(\omega) &= (\delta_{\bar{2}3}\,\delta_{\bar{1}4} - \delta_{13}\,\delta_{24})\frac{\eta\,\delta_{\eta,\eta_1}\,\delta_{\eta_1,-\eta_2}}{\omega - \eta\,\eta_1 E_{12}}.
\end{aligned}
\tag{3.55}
$$

We did not use the antisymmetric form of the QTBA equations from the very beginning to simplify their derivation and analysis. However, the antisymmetrization facilitates the numerical solution because of the reduction of the dimensions of matrices entering these equations.

The model described above allows for the following straightforward extension related to the definition of the resonant parts of the amplitudes entering Eqs. (3.19) and (3.45)–(3.48) for the correlated propagator of the QTBA. Contributions from these resonant parts [defined by Eqs. (3.27)–(3.30)] to the response function describe simultaneous propagation of the phonon and the uncorrelated quasiparticle pair. Natural generalization of this model is the inclusion of the correlations in the quasiparticle pair entering the 2q ⊗ phonon configuration, i.e., replacement of the uncorrelated pair by the phonon. For the ph-channel BSE in the normal Fermi system, a similar generalization, corresponding to the replacement of the 1p1h ⊗ phonon configurations by the two-phonon intermediate states, was discussed in Ref. [31]. For the pp-channel BSE, an analogous procedure was implemented in Ref. [23].

Within the QTBA, two-quasiparticle correlations in the 2q ⊗ phonon intermediate states (i.e., two-phonon configurations) can be included in the following way. The correlated counterpart of the above-defined quantity $\tilde{L}^{0(\eta)}(\omega)$ is $\tilde{L}^{(\eta)}(\omega)$ representing the positive and negative frequency parts of the antisymmetric QRPA response function $\tilde{L}(\omega)$:

$$
\begin{aligned}
\tilde{L}_{12,34}(\omega) &= \sum_{\eta=\pm 1} \tilde{L}^{(\eta)}_{12,34}(\omega),\\
\tilde{L}^{(\eta)}_{12,34}(\omega) &= -\sum_{n} \frac{\eta\,\rho^{n(\eta)}_{12}\,\rho^{n(\eta)*}_{34}}{\omega - \eta\,\omega_n}.
\end{aligned}
\tag{3.56}
$$

In Eq. (3.56), it is supposed that the QRPA energies ω_n and transition amplitudes $\rho^{n(\eta)}_{12}$ satisfy Eqs. (3.15)–(3.17). The above considerations imply that transition to the two-phonon configurations within the QTBA can be accomplished by means of the replacement $\tilde{A}^{(\eta)}(\omega) \to \frac{1}{2}\,\tilde{L}^{(\eta)}(\omega)$ in Eqs. (3.27)–(3.30), which leads to

$$
P^{(++)}_{12,34}(\omega) = -\frac{1}{2}\sum_{\eta,m,n} \frac{\eta\,\zeta^{mn(\eta)}_{12}\,\zeta^{mn(\eta)*}_{34}}{\omega - \eta\,\omega_{mn}}, \tag{3.57}
$$

$$
Q^{(+-)\,\rm res}_{12,34}(\omega) = -\frac{1}{2}\sum_{\eta,m,n} \frac{\eta\,\zeta^{mn(\eta)}_{12}\,\gamma^{mn(\eta)*}_{34}}{\omega - \eta\,\omega_{mn}}, \tag{3.58}
$$

$$
Q^{(-+)\,\rm res}_{12,34}(\omega) = -\frac{1}{2}\sum_{\eta,m,n} \frac{\eta\,\gamma^{mn(\eta)}_{12}\,\zeta^{mn(\eta)*}_{34}}{\omega - \eta\,\omega_{mn}}, \tag{3.59}
$$

$$
\Phi^{\rm res}_{12,34}(\omega) = \frac{1}{2}\sum_{\eta,m,n} \frac{\eta\,\gamma^{mn(\eta)}_{12}\,\gamma^{mn(\eta)*}_{34}}{\omega - \eta\,\omega_{mn}}, \tag{3.60}
$$

where $\omega_{mn} = \omega_m + \omega_n$, $\gamma^{mn(\eta)}_{12} = \sum_{56} \gamma^{m56(\eta)}_{12}\,\rho^{n(\eta)}_{56}$, and $\zeta^{mn(\eta)}_{12} = \sum_{56} \zeta^{m56(\eta)}_{12}\,\rho^{n(\eta)}_{56}$.

Physical arguments in favor of using Eqs. (3.57)–(3.60) instead of (3.27)–(3.30) are clear. Notice, however, that the derivation of Eqs. (3.57)–(3.60) has not been rigorous. It enables one only to assert that these formulas recover the original Eqs. (3.27)–(3.30) in the limit of vanishing quasiparticle interaction. One can also show, using the completeness of the set of QRPA transition amplitudes, that the NEWSR is fulfilled exactly within the two-phonon version of the QTBA. The rigorous derivation of Eqs. (3.57)–(3.60) is based on the inclusion of the additional (third order in the quasiparticle-quasiparticle interaction) contributions into the dynamic amplitude $\mathcal{U}^e$ defined by Eq. (3.13) and will not be considered here. It is worth noting that inclusion of the two-phonon configurations in Eqs. (3.57)–(3.60) brings the model closer to the QPM [2]. Comparing the QTBA and the QPM, one can infer that treatment of the GSC within the QTBA is more consistent. A more detailed comparison of these models is beyond the scope of the present paper.

E. Self-consistent scheme

Finally, we briefly outline the scheme that enables one to eliminate spurious states within the QTBA. These states, being a common problem of the microscopic theories, are associated with the existence of the nontrivial external field operators V^0 satisfying the condition: $[H, V^0] = [H^0, V^0]$, where H and H^0 are the total and the single-particle Hamiltonian, correspondingly [see Eq. (2.4)]. Elimination of the spurious states within a consistent theory implies that they must have zero excitation energy. In terms of the GF method, this means that the exact response function $R(\omega)$ must have a pole at $\omega = 0$ corresponding to the spurious states. In particular, it is well known that the QRPA response function $\tilde{R}(\omega)$ satisfying Eq. (3.53) has such a pole at $\omega = 0$ if the interaction amplitude $\tilde{\mathcal{F}}$ is related to the mean-field operator $\tilde{\Sigma}$ by the self-consistency condition

$$\tilde{\mathcal{F}} = \delta\,\tilde{\Sigma}\,/\,\delta\,\tilde{\rho}. \tag{3.61}$$

In the QTBA, the situation is more complicated since the correlated propagator $A(\omega)$ in Eq. (3.4) has no simple structure of the QRPA propagator $\tilde{A}(\omega)$. To avoid this difficulty, let us note that the exact solution of the Eq. (3.4) with the propagator $A(\omega)$ defined by Eqs. (3.45) and (3.19) can be represented in the form

$$\begin{aligned} R^{\,\mathrm{eff}}(\omega) = {} & [1 - P^{(++)}(\omega)\,\mathcal{F}^{\,P}(\omega)]Z^{L}(\omega)\,\tilde{R}^{\,\mathrm{eff}}(\omega)\,Z^{R}(\omega) \\ & \times [1 - \mathcal{F}^{\,P}(\omega)\,P^{(++)}(\omega)] + P^{(++)}(\omega) - P^{(++)}(\omega) \\ & \times \mathcal{F}^{\,P}(\omega)\,P^{(++)}(\omega), \end{aligned} \tag{3.62}$$

where the energy-dependent interaction amplitude $\mathcal{F}^{\,P}(\omega)$ and the renormalized response function $\tilde{R}^{\,\mathrm{eff}}(\omega)$ satisfy the equations

$$\mathcal{F}^{\,P}(\omega) = \mathcal{F} - \mathcal{F}\,P^{(++)}(\omega)\,\mathcal{F}^{\,P}(\omega), \tag{3.63}$$

$$\tilde{R}^{\,\mathrm{eff}}(\omega) = \tilde{A}(\omega) - \tilde{A}(\omega)\,\tilde{\mathcal{F}}(\omega)\,\tilde{R}^{\,\mathrm{eff}}(\omega), \tag{3.64}$$

with

$$\tilde{\mathcal{F}}(\omega) = Z^{R}(\omega)\,\mathcal{F}^{\,P}(\omega)\,Z^{L}(\omega) + \Phi(\omega). \tag{3.65}$$

If the energy-dependent amplitude $\tilde{\mathcal{F}}(\omega)$ in Eq. (3.64) coincides at $\omega = 0$ with the interaction amplitude $\tilde{\mathcal{F}}$ in Eq. (3.53), the renormalized response function $\tilde{R}^{\,\mathrm{eff}}(\omega)$ has the pole at $\omega = 0$ corresponding to the spurious states by the same reasons as the QRPA response function $\tilde{R}(\omega)$. To ensure the fulfillment of the relationship $\tilde{\mathcal{F}}(0) = \tilde{\mathcal{F}}$, we use the fact that the interaction amplitude $\mathcal{F}$ entering Eq. (3.4) has not been constrained so far by any conditions besides the property of its energy independence. Let us now assume that the amplitude $\mathcal{F}$ satisfies the equation

$$\mathcal{F} = \mathcal{F}^{\,P} + \mathcal{F}^{\,P}\,P^{(++)}(0)\,\mathcal{F}, \tag{3.66}$$

where

$$\mathcal{F}^{\,P} = [Z^{R}(0)]^{-1}[\tilde{\mathcal{F}} - \Phi(0)][Z^{L}(0)]^{-1}, \tag{3.67}$$

and the amplitudes $\Phi(0)$ and $\tilde{\mathcal{F}}$ are determined by Eqs. (3.48) and (3.61) correspondingly. If the Eqs. (3.66) and (3.67) are fulfilled, then it follows from Eqs. (3.63) and (3.65) that $\tilde{\mathcal{F}}(0) = \tilde{\mathcal{F}}$. Consequently, both functions $\tilde{R}^{\,\mathrm{eff}}(\omega)$ and $R^{\,\mathrm{eff}}(\omega)$ have the poles at $\omega = 0$ corresponding to the spurious states. It means that these states are eliminated, at least energetically, within the self-consistent version of the QTBA defined by the above equations.

Notice that in the case that the GSC2 are not included, Eqs. (3.66) and (3.67) are reduced to the ansatz $\mathcal{F} = \tilde{\mathcal{F}} - \Phi^{\,\mathrm{res}}(0)$. The difference $\tilde{\mathcal{F}} - \Phi(0)$ also enters Eq. (3.67). Thus, in addition to the elimination of the spurious states, the procedure described leads to subtraction of the static contributions of the quasiparticle-phonon coupling from both the effective interaction and the mass operator [because $\Phi(\omega)$ contains self-energy contributions also]. So, one can refer to this method as the subtraction procedure. A sense of this subtraction is to avoid double counting of the static QPC effects which usually are effectively included in both the interaction $\tilde{\mathcal{F}}$ and the mean-field operator $\tilde{\Sigma}$. For that reason, the subtraction procedure is applicable also in the non-self-consistent phenomenological schemes of the type described in Ref. [3].

IV. CONCLUSIONS

In this paper, the problem of the microscopic description of excited states of the even-even open-shell atomic nuclei is considered. The generalized Green function formalism (GGFF) has been presented and used to formulate the model including pairing, two-quasiparticle (2q), and the more complex quasiparticle-phonon correlations. The GGFF is a modification of the existing versions of Green function formalism and is more suitable for solving the problem considered here. Within the GGFF, the normal and anomalous Green functions in the Fermi systems with pairing are treated in a unified way in terms of the components of generalized Green functions in a space that is double the size of the usual single-particle space. This treatment is analogous to the method used in Ref. [18]. In the GGFF, this method is extended to Fermi systems interacting through two-, three-, and other many-particle effective forces, which is important to nuclear physics in which the many-particle forces play an essential role. Within the framework of this formalism, the generalization of the model of Ref. [11] including the pairing correlations has been developed. The physical content of the model is determined by the quasiparticle time blocking approximation (QTBA) which allows one to keep the contributions of the 2q and 2q $\otimes$ phonon configurations, while excluding (blocking) more complicated intermediate states. It has been shown that within the QTBA, the non-energy-weighted sum rule is fulfilled exactly. The model developed has been extended to include correlations in the quasiparticle pair entering a 2q $\otimes$ phonon configuration, i.e., to include two-phonon configurations. Finally, the method to eliminate the spurious states within the self-consistent QTBA and to avoid double counting of the complex configurations in general case has been considered.

ACKNOWLEDGMENTS

The author is very indebted to E. V. Litvinova for cooperation and useful discussions. The author acknowledges with gratitude financial support from the Deutsche Forschungsgemeinschaft under Grant No. 436 RUS 113/806/0-1 and from the Russian Foundation for Basic Research under Grant No. 05-02-04005-DFG_a.

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