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Particle-number conservation within self-consistent random-phase approximation

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The self-consistent random-phase approximation (SCRPA) is reexamined within a multilevel-pairing model with double degeneracy. It is shown that the expressions for occupation numbers used in the original version of the SCRPA violate the particle number for nonsymmetric particle-hole (ph) spectra. A renormalization is introduced to restore the particle number, which leads to the expressions of occupation numbers similar to those derived by Hara *et al*. for the ph case. The results of calculations within the ph symmetric case show that this number-conserving SCRPA yields the energies of the ground state and the first excited state of the system with $\Omega + 2$ particles relative to the ground state of the system with Ω particles in close agreement with those obtained within the original SCRPA. However, it gives a slightly larger correlation energy.

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I. INTRODUCTION

The random-phase approximation (RPA) has been a powerful tool in the theoretical study of many-body systems such as atomic nuclei. An essential ingredient of the RPA is the use of the quasiboson approximation (QBA), which considers fermion pairs as boson operators and just neglects the Pauli principle between them. Within the QBA, a set of linear equations, which is usually called the RPA equation, is derived, which makes computationally demanding problems become tractable. However, because of the violation of the Pauli principle within the QBA, the RPA equation breaks down at a certain critical value of the interaction's parameter, where the RPA yields imaginary solutions.

Several approaches were developed to remove this inconsistency of the RPA. One of the popular ones is the renormalized RPA (RRPA) [1–4]. The RRPA includes in the expectation value over the ground state the contribution of the diagonal elements of the commutator between two fermion-pair operators. In this way it takes the Pauli principle into account approximately. This includes the so-called ground-state correlations beyond the RPA, which eventually renormalize the interaction in such a way that the collapse of the RPA is avoided. However, the tests carried out within exactly solvable models also showed that there is still a large discrepancy between the solution obtained within the RRPA and the exact one that occurs beyond the RPA collapsing point (see, e.g., Ref. [4]).

Recently, the situation has been significantly improved within the self-consistent RPA (SCRPA) [5–7] because of the inclusion of screening corrections in the SCRPA equation. These screening corrections are in fact the expectation values of the products of two fermion pairs in the correlated ground state. As a result, the sign of the interaction is reversed so that within a particle-hole (ph) symmetric multilevel-pairing model with double degeneracy (the so-called picket-fence model), the SCRPA yields the solutions very close to the exact ones for the correlation energy of the system with Ω particles, as well as the energy of the first excited state of the system with $\Omega + 2$ particles [6,7].

Realistic nuclear single-particle spectra are in general ph nonsymmetric, which means that the particle-particle (pp) submatrix A and hole-hole (hh) submatrix C of the pp-RPA equation do not have the same dimension. The asymmetry is particularly strong, e.g., in light neutron-rich nuclei [8], for which the effect due to the Pauli principle cannot be neglected. It is therefore worthwhile to reexamine carefully the SCRPA before applying it to realistic nuclei.

The present paper employs the same picket-fence model that was used to test the validity of the SCRPA in Refs. [6,7]. It will be shown that in the general ph nonsymmetric case, using its original expressions of ground-state correlation factors, the SCRPA violates the particle number. A simple and consistent way to restore the particle number will be introduced and the consequences will be discussed.

The paper is organized as follows. The outline of the SCRPA for the picket-fence model is presented in Sec. II. The violation of particle number within the SCRPA for the ph nonsymmetric case and the construction of a number-conserving SCRPA are discussed in Sec. III. The results of numerical calculations are analyzed in Sec. IV. The paper is summarized in the last section, where conclusions are drawn.

II. SCRPA EQUATION FOR THE PICKET-FENCE MODEL

The detailed derivation of the self-consistent pp-RPA equation, which is simply called the SCRPA equation hereafter, has been described in Refs. [5–7]. The present section gives only a brief outline of the SCRPA for the picket-fence model, which is needed for the discussion in this paper.

A. Model Hamiltonian

The picket-fence model consists of Ω two-fold equidistant levels interacting via a pairing force with a constant parameter

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G. The model Hamiltonian is written as

$$H = \sum_{i=1}^{\Omega}(\epsilon_i - \lambda)N_i - G\sum_{i,j=1}^{\Omega} P_i^\dagger P_j, \qquad (1)$$

where the particle-number operator N_i and pairing operators $P_i^\dagger$, P_i are given as

$$N_i = c_i^\dagger c_i + c_{-i}^\dagger c_{-i}, \qquad P_i^\dagger = c_i^\dagger c_{-i}^\dagger, \qquad P_i = (P_i^\dagger)^\dagger. \qquad (2)$$

The exact commutation relations between the operators N_i, $P_i^\dagger$, and P_i are

$$[P_i, P_j^\dagger] = \delta_{ij}(1 - N_i), \qquad (3)$$

$$[N_i, P_j^\dagger] = 2\delta_{ij}P_j^\dagger, \qquad [N_i, P_j] = -2\delta_{ij}P_j. \qquad (4)$$

The single-particle energies take the values $\epsilon_i = i\epsilon$ with i running over all Ω levels. The original version of the SCRPA in Refs. [6,7] was applied only to a ph symmetric spectrum, where there are as many particles as levels (half filling). This means that in the absence of interaction ($G = 0$), the lowest $\Omega_h = \Omega/2$ levels are occupied with $N = \Omega$ particles (two particles in each level). However, in general, the number Ω_h of hole levels does not have to be the same as the number Ω_p of particle levels, i.e., $\Omega_h \neq \Omega_p \neq \Omega/2$. Numerating particle (p) and hole (h) levels from the levels closest to the Fermi surface, the particle and hole energies are equal to $\epsilon_p = \epsilon(\Omega_h + p)$ and $\epsilon_h = \epsilon(\Omega_h - h + 1)$, respectively, with h indices running from 1 to Ω_h, and p indices running from 1 to $\Omega_p = \Omega - \Omega_h$. The Fermi level λ is defined in the middle of the first h and the first p levels, i.e.,

$$\lambda = \epsilon\left(\Omega_h + \frac{1}{2}\right) - \frac{G}{2}. \qquad (5)$$

Therefore, in the ph symmetric case ($\Omega_p = \Omega_h = \Omega/2$), the Fermi level $\lambda = [\epsilon(\Omega + 1) - G]/2$ is located in the middle of the single-particle spectrum.

Using the notation of Ref. [7],

$$M_p = N_p, \qquad M_h = 2 - N_h, \qquad Q_p^\dagger = P_p^\dagger, \qquad Q_h = -P_h^\dagger, \qquad (6)$$

and also introducing the ground-state correlation operators D_p and D_h,

$$D_p = 1 - M_p = 1 - N_p, \qquad D_h = 1 - M_h = N_h - 1, \qquad (7)$$

the exact commutation relations (3) and (4) can be transformed into

$$[Q_p, Q_{p'}^\dagger] = \delta_{pp'}D_p, \qquad [Q_h, Q_{h'}^\dagger] = \delta_{hh'}D_h, \qquad (8)$$

$$[M_i, Q_j^\dagger] = 2\delta_{ij}Q_j^\dagger, \qquad [M_i, Q_j] = -2\delta_{ij}Q_j. \qquad (9)$$

Using the definition (5) of the Fermi energy λ together with notations (6) and (7), the Hamiltonian (1) is rewritten in the following form

$$H = -\epsilon\Omega_h^2 + \sum_{p=1}^{\Omega_p}\left[\epsilon\left(p - \frac{1}{2}\right) + \frac{G}{2}\right]M_p + \sum_{h=1}^{\Omega_h}\left[\epsilon\left(h - \frac{1}{2}\right) + \frac{G}{2}\right]M_h - G\sum_{pp'}Q_p^\dagger Q_{p'} - G\sum_{hh'}Q_h^\dagger Q_{h'} + G\sum_{ph}(Q_p^\dagger Q_h^\dagger + Q_p Q_h), \qquad (10)$$

which, in the ph symmetric case, coincides with Eq. (13) of Ref. [7].

B. SCRPA equation

The derivation of the SCRPA equation is based on the RRPA additional and removal operators, which have the form

$$A_\mu^\dagger = \sum_p^{\Omega_p} X_p^\mu \overline{Q}_p^\dagger - \sum_h^{\Omega_h} Y_h^\mu \overline{Q}_h \qquad (11)$$

and

$$R_\lambda^\dagger = \sum_h^{\Omega_h} X_h^\lambda \overline{Q}_h^\dagger - \sum_p^{\Omega_p} Y_p^\lambda \overline{Q}_p, \qquad (12)$$

respectively, with the abbreviation

$$\overline{\mathcal{O}}_i^\dagger = \frac{\mathcal{O}_i^\dagger}{\sqrt{\langle D_i\rangle}}, \qquad \overline{\mathcal{O}}_i = \frac{\mathcal{O}_i}{\sqrt{\langle D_i\rangle}}, \qquad (i = p, h), \qquad (13)$$

to denote the renormalized operator of an operator $\mathcal{O}_i^\dagger$. Operator $A_\mu^\dagger$ transfers the states in a system with Ω particles to those of a system with $\Omega + 2$ particles. Operator $R_\lambda^\dagger$ transfers the states of an Ω-particle system to those of a system with $\Omega - 2$ particles. The brackets $\langle \ldots \rangle \equiv \langle \Omega, 0| \ldots |\Omega, 0\rangle$ denote the average of any operator(s) over the correlated ground state $|\Omega, 0\rangle$ of the system with Ω particles, which is defined as the vacuum of operators A_μ and R_λ; i.e.,

$$A_\mu|\Omega, 0\rangle = R_\lambda|\Omega, 0\rangle = 0. \qquad (14)$$

Using the exact commutation relation (8) and the definition (14) of the RPA ground state $|\Omega, 0\rangle$, one can see that the additional and removal operators satisfy the boson commutation relations in the ground state $|\Omega, 0\rangle$

$$\langle[A_\mu, A_{\mu'}^\dagger]\rangle = \delta_{\mu\mu'}, \qquad \langle[R_\lambda, R_{\lambda'}^\dagger]\rangle = \delta_{\lambda\lambda'}, \qquad (15)$$

if the amplitudes X and Y satisfy the following normalization (orthogonality) conditions:

$$\sum_p X_p^\mu X_p^{\mu'} - \sum_h Y_h^\mu Y_h^{\mu'} = \delta_{\mu\mu'},$$
$$\sum_h X_h^\lambda X_h^{\lambda'} - \sum_p Y_p^\lambda Y_p^{\lambda'} = \delta_{\lambda\lambda'}, \qquad (16)$$
$$\sum_p X_p^\mu Y_p^\lambda - \sum_h X_h^\lambda Y_h^\mu = 0.$$

The closure relations

$$\sum_\mu X_p^\mu X_{p'}^\mu - \sum_\lambda Y_p^\lambda Y_{p'}^\lambda = \delta_{pp'},$$
$$\sum_\lambda X_h^\lambda X_{h'}^\lambda - \sum_\mu Y_h^\mu Y_{h'}^\mu = \delta_{hh'}, \qquad (17)$$
$$\sum_\lambda X_h^\lambda Y_p^\lambda - \sum_\mu X_p^\mu Y_h^\mu = 0$$

guarantee the following inverse transformation of Eqs. (11) and (12):

$$Q_p^\dagger = \sqrt{\langle D_p\rangle}\left[\sum_\mu X_p^\mu A_\mu^\dagger + \sum_\lambda Y_p^\lambda R_\lambda\right],$$
$$Q_h = \sqrt{\langle D_h\rangle}\left[\sum_\lambda X_h^\lambda R_\lambda + \sum_\mu Y_h^\mu A_\mu^\dagger\right]. \quad (18)$$

The SCRPA equation is obtained in a standard way by linearizing the equation of motion. The matrix form of the SCRPA equation for the additional mode is

$$\begin{pmatrix} A & B \\ -B & C\end{pmatrix}\begin{pmatrix} X^\mu \\ Y^\mu\end{pmatrix} = E_\mu \begin{pmatrix} X^\mu \\ Y^\mu\end{pmatrix}, \quad (19)$$

where the submatrices A, B, and C were derived in Ref. [7] using the definition (7) as well as the exact commutation relations (8) and (9) as

$$\begin{aligned} A_{\mathrm{pp'}} &= \langle[\overline{Q}_p,[H,\overline{Q}_{p'}^\dagger]]\rangle \\ &= 2\left\{\left[\epsilon\left(p-\frac{1}{2}\right)+\frac{G}{2}\right]+\frac{G}{\langle D_p\rangle}\left[\sum_{p''}\langle Q_{p''}^\dagger Q_p\rangle \right.\right.\\ &\quad \left.\left. - \sum_{h''}\langle Q_p Q_{h''}\rangle\right]\right\}\delta_{\mathrm{pp'}} - G\frac{\langle D_p D_{p'}\rangle}{\sqrt{\langle D_p\rangle\langle D_{p'}\rangle}}, \end{aligned} \quad (20)$$

$$B_{\mathrm{ph}} = -\langle[\overline{Q}_p,[H,\overline{Q}_h]]\rangle = G\frac{\langle D_p D_h\rangle}{\sqrt{\langle D_p\rangle\langle D_h\rangle}}, \quad (21)$$

$$\begin{aligned} C_{\mathrm{hh'}} &= -\langle[\overline{Q}_h,[H,\overline{Q}_{h'}^\dagger]]\rangle \\ &= -2\left\{\left[\epsilon\left(h-\frac{1}{2}\right)+\frac{G}{2}\right]+\frac{G}{\langle D_h\rangle}\left[\sum_{h''}\langle Q_h^\dagger Q_{h''}\rangle \right.\right.\\ &\quad \left.\left. - \sum_{p''}\langle Q_{p''}^\dagger Q_h^\dagger\rangle\right]\right\}\delta_{\mathrm{hh'}} + G\frac{\langle D_h D_{h'}\rangle}{\sqrt{\langle D_h\rangle\langle D_{h'}\rangle}}. \end{aligned} \quad (22)$$

The expectation values of the products of two pair operators at the right-hand side (rhs) of Eqs. (20) and (22) are

$$\langle Q_p^\dagger Q_{p'}\rangle = \langle P_p^\dagger P_{p'}\rangle = \sqrt{\langle D_p\rangle\langle D_{p'}\rangle}\sum_\lambda Y_p^\lambda Y_{p'}^\lambda, \quad (23)$$

$$\begin{aligned}\langle Q_p Q_h\rangle &= \langle Q_h^\dagger Q_p^\dagger\rangle = -\langle P_h^\dagger P_p\rangle = -\langle P_p^\dagger P_h\rangle \\ &= \sqrt{\langle D_p\rangle\langle D_h\rangle}\sum_\lambda X_h^\lambda Y_p^\lambda, \end{aligned}\quad (24)$$

$$\langle Q_h^\dagger Q_{h'}\rangle = \sqrt{\langle D_h\rangle\langle D_{h'}\rangle}\sum_\mu Y_h^\mu Y_{h'}^\mu = \langle P_{h'}^\dagger P_h\rangle - \delta_{\mathrm{hh'}}\langle D_h\rangle, \quad (25)$$

$$\text{with}\quad \langle P_{h'}^\dagger P_h\rangle = \sqrt{\langle D_h\rangle\langle D_{h'}\rangle}\sum_\lambda X_h^\lambda X_{h'}^\lambda.$$

They were derived using the inverse transformation (18) and the definition of the ground state (14). The RRPA equation was obtained from Eqs. (19)–(22) by using the factorization

$$\langle D_i D_j\rangle \simeq \langle D_i\rangle\langle D_j\rangle, \quad (26)$$

and neglecting all the expectation values $\langle Q_{p'}^\dagger Q_p\rangle$, $\langle Q_p Q_h\rangle$, and $\langle Q_h^\dagger Q_{h'}\rangle$. The RRPA submatrices have then the form

$$A_{\mathrm{pp'}}^{\mathrm{RRPA}} = 2\left[\epsilon\left(p-\frac{1}{2}\right)+\frac{G}{2}\right]\delta_{\mathrm{pp'}} - G\sqrt{\langle D_p\rangle\langle D_{p'}\rangle}, \quad (27)$$

$$B_{\mathrm{ph}}^{\mathrm{RRPA}} = G\sqrt{\langle D_p\rangle\langle D_h\rangle}, \quad (28)$$

$$C_{\mathrm{hh'}}^{\mathrm{RRPA}} = -2\left[\epsilon\left(h-\frac{1}{2}\right)+\frac{G}{2}\right]\delta_{\mathrm{hh'}} + G\sqrt{\langle D_h\rangle\langle D_{h'}\rangle}. \quad (29)$$

The RPA submatrices are obtained from the RRPA ones by putting $D_p = D_h = 1$, namely

$$A_{\mathrm{pp'}}^{\mathrm{RPA}} = 2\left[\epsilon\left(p-\frac{1}{2}\right)+\frac{G}{2}\right]\delta_{\mathrm{pp'}} - G, \quad (30)$$

$$B_{\mathrm{ph}}^{\mathrm{RPA}} = G, \quad (31)$$

$$C_{\mathrm{hh'}}^{\mathrm{RPA}} = -2\left[\epsilon\left(h-\frac{1}{2}\right)+\frac{G}{2}\right]\delta_{\mathrm{hh'}} + G. \quad (32)$$

By using definition (6), Eqs. (23)–(25), and recalling that

$$\epsilon_p - \lambda = \epsilon\left(p-\frac{1}{2}\right)+\frac{G}{2}, \quad (33)$$

$$\epsilon_h - \lambda = -\epsilon\left(h-\frac{1}{2}\right)+\frac{G}{2} = -\left[\epsilon\left(h-\frac{1}{2}\right)+\frac{G}{2}\right]+G, \quad (34)$$

one can rewrite Eqs. (20)–(22) in the notations of Ref. [6] as[1]

$$\begin{aligned} A_{\mathrm{pp'}} &= \langle[\overline{P}_p,[H,\overline{P}_{p'}^\dagger]]\rangle = 2\delta_{\mathrm{pp'}}(\epsilon_{p'}-\lambda) \\ &\quad + 2G\delta_{\mathrm{pp'}}\frac{\sum_{p''}\langle P_{p''}^\dagger P_p\rangle + \sum_{h''}\langle P_{h''}^\dagger P_p\rangle}{1-\langle N_p\rangle} \\ &\quad - G\frac{\langle(1-N_p)(1-N_{p'})\rangle}{\sqrt{(1-\langle N_p\rangle)(1-\langle N_{p'}\rangle)}}, \end{aligned} \quad (35)$$

$$B_{\mathrm{ph}} = \langle[\overline{P}_p,[H,\overline{P}_h^\dagger]]\rangle = G\frac{\langle(1-N_p)(N_h-1)\rangle}{\sqrt{(1-\langle N_p\rangle)(\langle N_h\rangle-1)}}, \quad (36)$$

$$\begin{aligned} C_{\mathrm{hh'}} &= -\langle[\overline{P}_h,[H,\overline{P}_{h'}^\dagger]]\rangle = 2\delta_{\mathrm{hh'}}(\epsilon_{h'}-\lambda) \\ &\quad - 2G\delta_{\mathrm{hh'}}\frac{\sum_{h''}\langle P_{h''}^\dagger P_h\rangle + \sum_{p''}\langle P_{p''}^\dagger P_h\rangle}{\langle N_h\rangle - 1} \\ &\quad + G\frac{\langle(N_h-1)(N_{h'}-1)\rangle}{\sqrt{(\langle N_h\rangle-1)(\langle N_{h'}\rangle-1)}}. \end{aligned} \quad (37)$$

[1] There are several misprints in Eq. (11) of Ref. [6]; namely, the factor 2 in front of all $\langle N_i N_j\rangle$ in the numerators of the last terms at the rhs of submatrices $\bar{A}$, $\bar{B}$, and $\bar{C}$ should be eliminated. Also, the factor $1-\langle N_{p'}\rangle$ in the denominator of the last term of $\bar{B}_{\mathrm{ph}}$ should be replaced with $\langle N_h\rangle - 1$, and the sign "–" in front of $2\delta_{\mathrm{hh'}}(\epsilon_{\mathrm{hh'}}-\lambda)$ in the expression of $\bar{C}_{\mathrm{hh'}}$ should be "+".

C. Correlation energy

The correlation energy $E_{\rm corr}^{\rm SCRPA}$ is defined as the difference between the energy $\mathcal{E}_0^{\Omega} \equiv \langle H\rangle$ in the ground state $|\Omega,0\rangle$ (14) and the Hartree-Fock (HF) energy $\mathcal{E}_{\rm HF}$. The former is easily obtained from Eq. (10) while the latter is $-\epsilon\Omega_h^2$. The final expression for the correlation energy is obtained as

$$E_{\rm corr}^{\rm SCRPA} \equiv \langle H\rangle - \mathcal{E}_{\rm HF} = \sum_p^{\Omega_p}\left[\epsilon\left(p-\frac{1}{2}\right)+\frac{G}{2}\right](1-\langle D_p\rangle) + \sum_h^{\Omega_h}\left[\epsilon\left(h-\frac{1}{2}\right)+\frac{G}{2}\right](1-\langle D_h\rangle) - G\left[\sum_{\rm pp'}\langle Q_p^\dagger Q_{p'}\rangle + \sum_{\rm hh'}\langle Q_h^\dagger Q_{h'}\rangle - 2\sum_{\rm ph}\langle Q_p^\dagger Q_h^\dagger\rangle\right], \tag{38}$$

where $\langle Q_i^\dagger Q_i\rangle$ and $\langle Q_p^\dagger Q_h^\dagger\rangle$ are given by Eqs. (23)–(25), and D_i by Eq. (47).

For comparison, the correlation energy within the RRPA is derived here by approximating the Hamiltonian (1) as

$$H \simeq H^{\rm RRPA} = \mathcal{E}_0^{(\Omega)}({\rm RRPA}) + \sum_\mu E_\mu^{\rm RRPA} A_\mu^\dagger A_\mu + \sum_\lambda E_\lambda^{\rm RRPA} R_\lambda^\dagger R_\lambda, \tag{39}$$

where $\mathcal{E}_0^{(\Omega)}$(RRPA) is the energy in the RRPA ground state, while the eigenvalues $E_\mu^{\rm RRPA}$ and $E_\lambda^{\rm RRPA}$ are the excitation energies (42) and (43) of the additional and removal modes, respectively, which are obtained by solving the RRPA equation, i.e., Eq. (19) with submatrices (27)–(29). The correlation energy $E_{\rm corr}^{\rm RRPA} = \mathcal{E}_0^{\Omega}({\rm RRPA}) - \mathcal{E}_{\rm HF}$ is obtained by calculating the expectation value of the Hamiltonian (39) in the HF ground state $|{\rm HF}\rangle$. By using Eqs. (11) and (12) as well as the definition of $|{\rm HF}\rangle$, for which $P_p|{\rm HF}\rangle = \langle{\rm HF}|P_p^\dagger = P_h^\dagger|{\rm HF}\rangle = \langle{\rm HF}|P_h = 0$, we finally obtain

$$E_{\rm corr}^{\rm RRPA} = \mathcal{E}_0^{\Omega}({\rm RRPA}) - \langle{\rm HF}|H|{\rm HF}\rangle = -\sum_\mu E_\mu^{\rm RRPA}\sum_h \frac{\left(Y_h^\mu\right)^2}{D_h} - \sum_\lambda E_\lambda^{\rm RRPA}\sum_p\frac{\left(Y_p^\lambda\right)^2}{D_p}. \tag{40}$$

The RPA correlation energy $E_{\rm corr}^{\rm RPA}$ is recovered from Eq. (40) setting $D_i = 1$, namely

$$E_{\rm corr}^{\rm RPA} = -\sum_\mu E_\mu^{\rm RPA}\sum_h\left(Y_h^\mu\right)^2 - \sum_\lambda E_\lambda^{\rm RPA}\sum_p\left(Y_p^\lambda\right)^2, \tag{41}$$

with $E_\mu^{\rm RPA}$ and $E_\lambda^{\rm RPA}$ denoting the RPA excitation energies of the additional and removal modes, respectively.

III. PARTICLE-NUMBER WITHIN SCRPA

The SCRPA equation [(19)–(22)] has Ω_p solutions for the additional mode with positive eigenvalues

$$E_\mu = \mathcal{E}_\mu^{\Omega+2} - \mathcal{E}_0^{\Omega} > 0, \qquad \mu = 1,\ldots,\Omega_p, \tag{42}$$

which are excitation energies of the $\Omega+2$ system relative to the ground state of the Ω system. Since the SCRPA equation for the removal mode has exactly the same form as that of Eqs. (19)–(22) with the only difference being that $(X_p^\mu, Y_h^\mu, E_\mu)$ should be replaced with $(Y_p^\lambda, X_h^\lambda, -E_\lambda)$, the Ω_h negative eigenvalues

$$E_\lambda = \mathcal{E}_\lambda^{\Omega-2} - \mathcal{E}_0^{\Omega} < 0, \qquad \lambda = 1,\ldots,\Omega_h, \tag{43}$$

of Eqs. (19)–(22) have physical meaning as excitation energies of the $\Omega-2$ system relative to the ground state of Ω system. This set of equations should be solved self-consistently with the normalization conditions (16) and the equations for the factor $\langle D_p\rangle$ and $\langle D_h\rangle$, which represent the ground-state correlations beyond the RPA. It is clear from Eq. (7) that, in the absence of ground-state correlations (beyond RPA), the ground state $|\Omega,0\rangle$ becomes the RPA ground state $|{\rm RPA}\rangle$, for which $\langle{\rm RPA}|D_i|{\rm RPA}\rangle = \langle{\rm HF}|D_i|{\rm HF}\rangle = 1$ $(i = p,h)$ because of the QBA. This means that $\langle{\rm RPA}|N_p|{\rm RPA}\rangle = 0$ and $\langle{\rm RPA}|N_h|{\rm RPA}\rangle = 2$. In this case, the SCRPA equation reaches its RPA limit with the RPA submatrices (30)–(32). In the general case, $0 < \langle D_i\rangle < 1$ $(i = p,h)$ since $0 < \langle N_p\rangle < 1$ and $1 < \langle N_h\rangle < 2$.

A. Violation of particle number within SCRPA

In order to derive the equations for the factors $\langle D_i\rangle$ $(i = p,h)$, Refs. [6,7] employed a procedure similar to the one used in Ref. [4] with the representation

$$N_i = 2P_i^\dagger P_i, \tag{44}$$

which becomes exact for the picket-fence model. Using Eqs. (7), (23), and (25), one finds immediately from Eq. (44) that

$$\langle N_p\rangle = 2\langle D_p\rangle\sum_\lambda\left(Y_p^\lambda\right)^2 = 2(1-\langle N_p\rangle)\sum_\lambda\left(Y_p^\lambda\right)^2,$$
$$\langle N_h\rangle = 2\langle D_h\rangle\left[1+\sum_\mu\left(Y_h^\mu\right)^2\right] = 2(\langle N_h\rangle - 1)\left[1+\sum_\mu\left(Y_h^\mu\right)^2\right]. \tag{45}$$

This yields

$$\langle N_p\rangle = 1-\langle D_p\rangle = 2\langle D_p\rangle\sum_\lambda\left(Y_p^\lambda\right)^2,$$
$$\langle N_h\rangle = 1+\langle D_h\rangle = 2\left[1-\langle D_h\rangle\sum_\mu\left(Y_h^\mu\right)^2\right], \tag{46}$$

with

$$\langle D_p\rangle = \frac{1}{1+2\sum_\lambda\left(Y_p^\lambda\right)^2}, \qquad \langle D_h\rangle = \frac{1}{1+2\sum_\mu (Y_h^\mu)^2}. \tag{47}$$

This result is a special (degenerate) case of the equations for the pp and hh ground-state correlation factors $\langle D_{\rm pp'}\rangle$ and $\langle D_{\rm hh'}\rangle$ in the general realistic spherical shell-model basis, which is derived here using the general expression of relation (44) in the form

$$N_j = \sum_m c^\dagger_{jm} c_{jm} \to \sum_{JMj'} P^\dagger_{jj'}(JM) P_{jj'}(JM), \qquad (48)$$

with

$$P^\dagger_{jj'}(JM) = \sum_{mm'} \langle jmj'm'|J'M'\rangle c^\dagger_{jm} c^\dagger_{j'm'},$$
$$P_{jj'}(JM) = [P^\dagger_{jj'}(JM)]^\dagger. \qquad (49)$$

Inserting in the rhs of Eq. (48) the general expression for $P^\dagger_{jj'}(JM)$,

$$P^\dagger_{\mathrm{pp}'}(JM) = \sqrt{\langle D_{\mathrm{pp}'}\rangle}\left(\sum_\mu X^{J\mu}_{\mathrm{pp}'} A^\dagger_{JM\mu} - \sum_\lambda Y^{J\lambda}_{\mathrm{pp}'} R_{JM\lambda}\right),$$
$$P^\dagger_{\mathrm{hh}'}(JM) = \sqrt{\langle D_{\mathrm{hh}'}\rangle}\left(\sum_\lambda X^{J\lambda}_{\mathrm{hh}'} R^\dagger_{JM\lambda} - \sum_\mu Y^{J\mu}_{\mathrm{hh}'} A_{JM\mu}\right), \qquad (50)$$

and using Eqs. (14) and (15), the final equations for $\langle D_{jj'}\rangle \equiv 1 - n_j - n_{j'}$ are obtained in the form

$$\langle D_{\mathrm{pp}'}\rangle = 1 - \sum_{J,\lambda}(2J+1)\sum_{p''}\left[\langle D_{\mathrm{pp}''}\rangle \frac{\left|Y^{J\lambda}_{\mathrm{pp}''}\right|^2}{(2j_p+1)} + \langle D_{p''p'}\rangle \frac{\left|Y^{J\lambda}_{p''p'}\right|^2}{(2j_{p'}+1)}\right],$$
$$\langle D_{\mathrm{hh}'}\rangle = 1 - \sum_{J,\mu}(2J+1)\sum_{h''}\left[\langle D_{\mathrm{hh}''}\rangle \frac{\left|Y^{J\mu}_{\mathrm{hh}''}\right|^2}{(2j_h+1)} + \langle D_{h''h'}\rangle \frac{\left|Y^{J\mu}_{h''h'}\right|^2}{(2j_{h'}+1)}\right], \qquad (51)$$

where j_p (j_h) denotes a p (h) orbital angular momentum, and J is the total angular momentum (multipolarity of the excitation). Obviously, Eq. (47) is recovered from Eq. (51) in the degenerate case, when $J = j_p = j_h = 0$, $p = p'$, and $h = h'$.

Equations (46) and (47) are the result given by Eq. (13) of Ref. [6][2] and Eq. (30) of Ref. [7]. This result for the pp case is similar to what was obtained previously in Ref. [4] for the ph case, according to which

$$\langle\langle N_p\rangle\rangle = 2\sum_{h\nu}\langle\langle D_{\mathrm{ph}}\rangle\rangle\left(Y^\nu_{\mathrm{ph}}\right)^2,$$
$$\langle\langle N_h\rangle\rangle = 2\left[1 - \sum_{p\nu}\langle\langle D_{\mathrm{ph}}\rangle\rangle\left(Y^\nu_{\mathrm{ph}}\right)^2\right], \qquad (52)$$

[2]The index λ in the sum at the rhs of the expression for $\langle N_p\rangle$ in Eq. (13) of Ref. [6] has been misprinted as μ, although this did not affect the results of calculations for the ph symmetric case, for which $\mu = \lambda$.

where

$$\langle\langle D_{\mathrm{ph}}\rangle\rangle = \frac{1}{1 + 2\sum_\nu\left(Y^\nu_{\mathrm{ph}}\right)^2}. \qquad (53)$$

Here, to avoid confusion with the notation for the pp case, the double brackets $\langle\langle\cdots\rangle\rangle$ are used to denote the average over the correlated ground state with respect to the ph renormalized RPA operators. Except for this formal similarity, the essential difference between the ph and pp cases is that Eq. (52) for the ph case always conserves the particle number, while Eq. (46) for the pp case, in general, does not. Indeed, in the ph case, Eq. (52) gives $\sum_p\langle\langle N_p\rangle\rangle \sum_p + \sum_h\langle\langle N_h\rangle\rangle = 2\sum_h^{\Omega/2} 1 = \Omega$ because the two sums at the rhs of Eq. (46) cancel each other exactly and, therefore, independently of how $\langle\langle D_{\mathrm{ph}}\rangle\rangle$ is estimated. Meanwhile, in the pp case, Eq. (46), in general, violates the particle number because it gives

$$\begin{aligned}\sum_p\langle N_p\rangle + \sum_h\langle N_h\rangle &= \Omega + 2\left[\sum_p\langle D_p\rangle\sum_\lambda\left(Y^\lambda_p\right)^2 - \sum_h\langle D_h\rangle\sum_\mu\left(Y^\mu_h\right)^2\right]\\ &= \Omega + 2\sum_\mu\left[\sum_p\langle D_p\rangle\left(X^\mu_p\right)^2 - \sum_h\langle D_h\rangle(Y^\mu_h)^2\right]\\ &\quad - 2\sum_p\langle D_p\rangle \neq \Omega,\end{aligned} \qquad (54)$$

as

$$\sum_\mu\left[\sum_p\langle D_p\rangle\left(X^\mu_p\right)^2 - \sum_h\langle D_h\rangle\left(Y^\mu_h\right)^2\right] \neq \sum_p\langle D_p\rangle, \qquad (55)$$

unless the condition $|Y^\lambda_p| = |Y^\mu_h|$ is assumed, which means $\langle D_p\rangle = \langle D_h\rangle$. This condition is satisfied only when the full ph symmetry holds; i.e., $\Omega_p = \Omega_h = \Omega/2$ for the equidistant spectrum. In the general ph nonsymmetric case, i.e., when $\Omega_p \neq \Omega_h \neq \Omega/2$ and/or the spectrum is not equidistant, there is no normalization condition such that (55) becomes an equality since this would be incompatible with the normalization condition (16) for the SCRPA X^μ_p and Y^μ_h amplitudes.

The measure $\delta\Omega$ of particle-number violation can be estimated by expanding $\langle D_i\rangle$ into the power series of $(Y^\nu_i)^2$. By using the normalization and closure relations (16) and (17), the lowest order of this expansion yields

$$\begin{aligned}|\delta\Omega| &\equiv \left|\sum_p\langle N_p\rangle + \sum_h\langle N_h\rangle - \Omega\right|\\ &= \left|2\sum_\mu\left[\sum_p\langle D_p\rangle\left(X^\mu_p\right)^2 - \sum_h\langle D_h\rangle\left(Y^\mu_h\right)^2\right] - 2\sum_p\langle D_p\rangle\right|\\ &\simeq \left|2\sum_\mu\left\{\sum_p\left[1 - 2\sum_\lambda\left(Y^\lambda_p\right)^2\right]\left(X^\mu_p\right)^2\right.\right.\\ &\qquad \left. - \sum_h\left[1 - 2\sum_{\mu'}\left(Y^{\mu'}_h\right)^2\right]\left(Y^\mu_h\right)^2\right\}\end{aligned}$$

$$-2\sum_p\left[1-2\sum_\lambda\left(Y_p^\lambda\right)^2\right]\Bigg|$$
$$=4\left|\sum_{\mu\mu'h}\left(Y_h^\mu\right)^2\left(Y_h^{\mu'}\right)^2-\sum_{\lambda\lambda'p}\left(Y_p^\lambda\right)^2\left(Y_p^{\lambda'}\right)^2\right|\sim\mathcal{O}(Y^4), \tag{56}$$

which means that the particle-number violation is expected to be small at least within the validity region of RPA, where $|Y_i^\nu|$ are small.

B. Restoration of particle-number conservation within SCRPA

Equations (46) have been derived making use of Eq. (44), which is compatible only with the exact ground state $|\Omega,0\rangle$ (14). However, as discussed in detail in Ref. [7], such exact ground state does not exist within the SCRPA, except for the case with $\Omega=2$, where the SCRPA and exact solutions coincide. Consequently, the SCRPA formalism still contains some violation of the Pauli principle, which leads to the particle-number violation in the ph nonsymmetric case.

In order to restore the particle number within the SCRPA, let us notice that the essential point of the SCRPA and RRPA is the renormalization of the operators $Q_i^\dagger$ and Q_i (6) in such a way that the renormalized operators incorporate the effect of the Pauli principle because of their fermion structure but behave at the same time like ideal boson operators with respect to the expectation value $\langle\ldots\rangle\equiv\langle\Omega,0|\ldots|\Omega,0\rangle$ [1,2]. The result of such renormalization yields the operators $\overline{Q}_i^\dagger\equiv Q_i^\dagger/\sqrt{\langle D_i\rangle}$ and $\overline{Q}_i\equiv Q_i/\sqrt{\langle D_i\rangle}$ in Eqs. (11) and (12), which satisfy the following exact relation:

$$\langle[\overline{Q}_i,\overline{Q}_j^\dagger]\rangle=\delta_{ij}. \tag{57}$$

This relation means that as far as the calculation of expectation values is concerned, the commutator $[\overline{Q}_i,\overline{Q}_j^\dagger]$ can be safely replaced with its ground-state expectation value $\langle[\overline{Q}_i,\overline{Q}_j^\dagger]\rangle$, namely,

$$[\overline{Q}_i,\overline{Q}_j^\dagger]=\langle[\overline{Q}_i,\overline{Q}_j^\dagger]\rangle=\delta_{ij}; \tag{58}$$

that is, $\overline{Q}_i^\dagger$ and $\overline{Q}_i$ are now considered as ideal boson operators (without fermion structure). From now on, the derivation proceeds only with expectation values using the replacement (58) under the condition

$$\langle A_\mu^\dagger A_{\mu'}\rangle=\langle R_\lambda^\dagger R_{\lambda'}\rangle=0 \tag{59}$$

instead of the vacuum condition (14).[3] Using Eq. (9), one can see that the renormalized operators $\overline{Q}_j^\dagger$ and $\overline{Q}_j$ satisfy the following exact commutation relations with operators M_i:

$$[M_i,\overline{Q}_j^\dagger]=2\delta_{ij}\overline{Q}_i^\dagger,\qquad [M_i,\overline{Q}_j]=-2\delta_{ij}\overline{Q}_i. \tag{60}$$

Since the standard derivation of RRPA equations is based on the algebra in (58) and (60) in terms of the boson operators $\overline{Q}_i^\dagger$ and $\overline{Q}_i$ [1,2,4], in order to derive the equations for the renormalization factor $\langle D_i\rangle$, the fermion operators M_i are also bosonized so that Eq. (60) still remains intact. Such boson representation exists and is equal to

$$M_i=2\overline{Q}_i^\dagger\overline{Q}_i, \tag{61}$$

which fulfills Eq. (60) exactly since

$$\begin{aligned}[M_i,\overline{Q}_j^\dagger]&=2\overline{Q}_i^\dagger[\overline{Q}_i,\overline{Q}_j^\dagger]=2\delta_{ij}\overline{Q}_i^\dagger,\\ [M_i,\overline{Q}_j]&=2[\overline{Q}_i^\dagger,\overline{Q}_j]\overline{Q}_i=-2\delta_{ij}\overline{Q}_i,\end{aligned} \tag{62}$$

as a result of Eq. (58). Representation (61) is apparently different from Eq. (44) since the latter is equivalent to

$$M_i=2Q_i^\dagger Q_i=2\langle D_i\rangle\overline{Q}_i^\dagger\overline{Q}_i \tag{63}$$

because of definition (6). The commutation relations between Eq. (63) and operators $\overline{Q}_i^\dagger$ and $\overline{Q}_i$ are different from the exact relations (60) by the factor $\langle D_i\rangle$, which causes the particle-number violation discussed in the preceding section.

Using the representation (61) instead of (63) together with Eqs. (23) and (25) immediately leads to

$$\begin{aligned}\langle N_p\rangle&=\langle M_p\rangle=2\sum_\lambda\left(Y_p^\lambda\right)^2,\\ \langle N_h\rangle&=2-\langle M_h\rangle=2\left[1-\sum_\mu\left(Y_h^\mu\right)^2\right],\end{aligned} \tag{64}$$

or

$$\langle D_p\rangle=1-2\sum_\lambda\left(Y_p^\lambda\right)^2,\qquad \langle D_h\rangle=1-2\sum_\mu\left(Y_h^\mu\right)^2, \tag{65}$$

instead of Eqs. (46) and (47). As mentioned previously, since $0\leqslant\langle N_p\rangle\leqslant 1$ and $1\leqslant\langle N_h\rangle\leqslant 2$, the values of ground-state factors given in Eq. (65) should also satisfy $0\leqslant D_i\leqslant 1$. These results are similar to those obtained by Hara [1] and later by Rowe [2] for the ph case. Therefore, the version of the SCRPA (RRPA) that uses Eqs. (64) and (65) instead of Eqs. (46) and (47) will be referred to as the Hara SCRPA (Hara RRPA) hereafter.[4] That Eq. (64) conserves the particle number is straightforward, making use of the normalization and closure relations (16) and (17). Indeed, using Eq. (64) instead of Eq. (46), one finds in the same way as it was done in proving the particle-number conservation within the pp RPA that

$$\sum_p\langle N_p\rangle+\sum_h\langle N_h\rangle=\Omega+2\left[\sum_p\sum_\lambda\left(Y_p^\lambda\right)^2-\sum_h\sum_\mu\left(Y_h^\mu\right)^2\right]$$

[3]This situation is somewhat similar to that of the statistical formalism, where a quantum mechanical ground state $|0(\beta)\rangle$ (β is the inverse temperature) so that $\langle 0(\beta)|\hat{\mathcal{O}}|0(\beta)\rangle=\mathrm{Tr}\{\mathcal{O}\mathcal{D}\}$ ($\mathcal{D}$ is the density operator) does not exist. The expectation value $\langle\hat{\mathcal{O}}\rangle$ is then replaced with the statistical average over the grand canonical ensemble with $\mathcal{D}=e^{-\beta(H-\lambda\hat{N})}/\mathrm{Tr}\{e^{-\beta(H-\lambda\hat{N})}\}$.

[4]The expressions for the factor $D_{\mathrm{pp}'}$ and $D_{\mathrm{hh}'}$ within the Hara SCRPA for the general shell-model spherical basis are obtained from Eqs. (51), setting $D_{jj'}$ at the rhs of Eqs. (51) equal to 1.

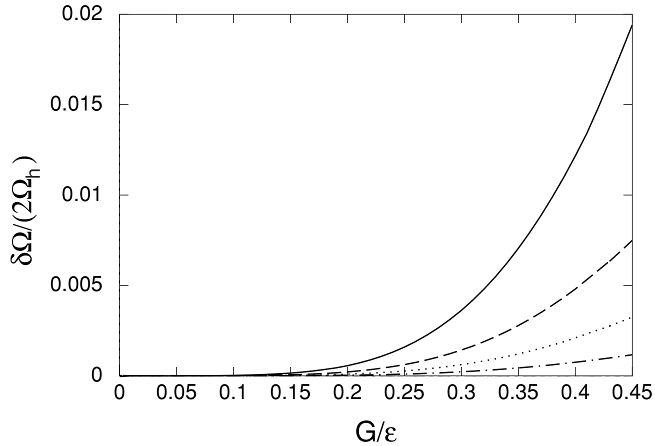

FIG. 1. Particle-number violations within the SCRPA for ph nonsymmetric cases with $\Omega = 10$ and $\Omega_h = 1$ (solid line), 2 (dashed line), 3 (dotted line), and 4 (dash-dotted line) as functions of interaction parameter G (in units of the level distance ϵ).

$$= \Omega + 2\left\{\sum_p\left[\sum_\mu \left(X_p^\mu\right)^2 - 1\right] - \sum_h\sum_\mu \left(Y_h^\mu\right)^2\right\}$$
$$= \Omega + \sum_\mu\left[\sum_p \left(X_p^\mu\right)^2 - \sum_h \left(Y_h^\mu\right)^2\right] - \Omega_p$$
$$= \Omega + \Omega_p - \Omega_p = \Omega. \quad (66)$$

Therefore, the Hara SCRPA and Hara RRPA always conserve the particle number exactly.

IV. NUMERICAL ANALYSIS

The calculations were carried out for several values of Ω and $\epsilon = 1$ MeV within the SCRPA and RRPA. The most representative case with $\Omega = 10$ is selected here for discussion. For simplicity, the factorization (26) was used, which has been verified in Ref. [7] to yield excellent results compared with those obtained when an involved set of nonlinear equations for the expectation values $\langle M_i M_j\rangle$ was solved instead. This factorization does not affect the discussion regarding the particle-number restoration in this work.

A. Degree of particle-number violation within SCRPA

Shown in Fig. 1 is the quantity $\delta\Omega/(2\Omega_h)$ as a function of the interaction parameter G (in units of level distance ϵ), which has been obtained within the SCRPA for ph nonsymmetric cases with the number of hole levels $\Omega_h = 1, 2, 3,$ and 4. The particle-number violation increases with G and with the asymmetry of the ph single-particle space. The strongest violation of about 2% is observed at the strongest asymmetry, i.e., with $\Omega_h = 1$ and $\Omega_p = 9$ (solid line), at the largest value of $G = 0.45$ MeV shown in the figure. In all other cases plotted on this figure, the particle-number violation is smaller than 1%. With increasing Ω_h, the symmetry is gradually restored, and the particle-number violation decreases to reach zero at $\Omega_h = 5$. Results of our calculations for larger Ω also show that the particle-number violation within the SCRPA decreases with increasing particle number.

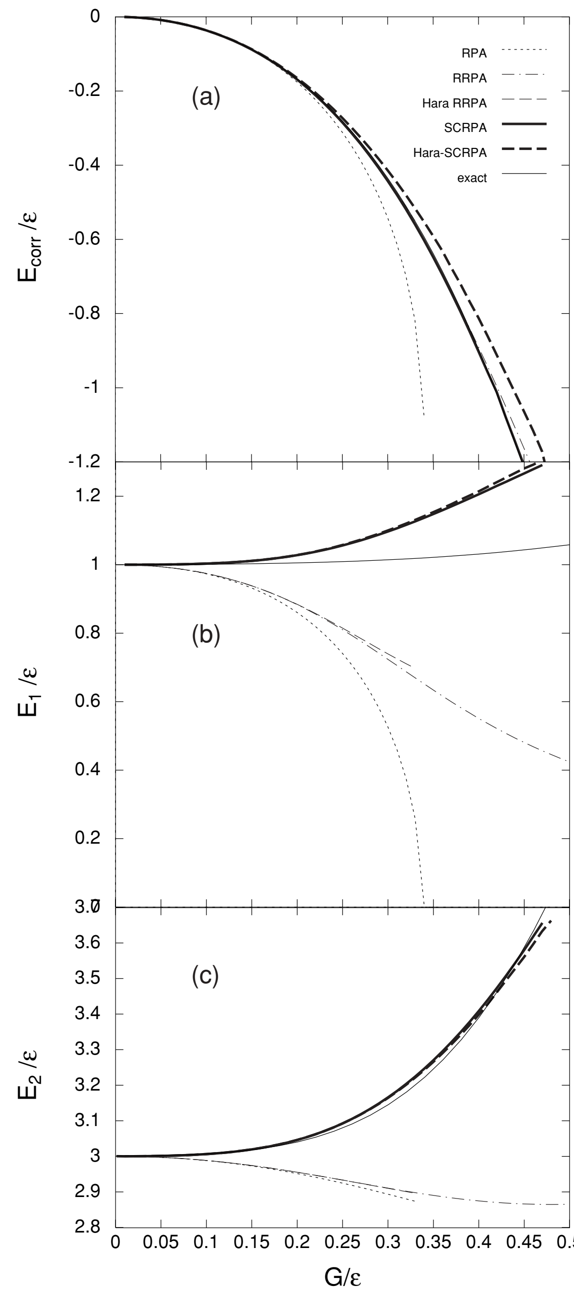

FIG. 2. Correlation energy $E_{\rm corr}$ in the system with $\Omega = 10$ particles (a), ground-state energy E_1 (b), and first-excited-state energy E_2 (c) of the system with $\Omega + 2 = 12$ particles relative to the ground state of the Ω-particle system as functions of interaction parameter G obtained within the RPA (dotted line), RRPA (dash-dotted line), Hara RRPA (thin dashed line), SCRPA (thick solid line), Hara SCRPA (thick dashed line), and exact (thin solid line) calculations.

B. Correlation, ground-state, and excited-state energies

Shown in Fig. 2 are the correlation energies of the system with $\Omega = 10$ particles, as well as the energies E_1 and E_2 of the ground state and first excited state, respectively, of the system

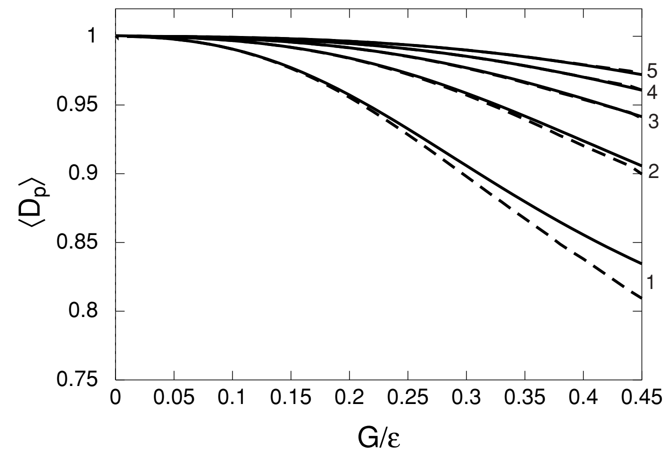

FIG. 3. Ground-state correlation factor $\langle D_p \rangle$ for particle levels as functions of interaction parameter G. The solid and dashed lines denote results obtained by using Eqs. (47) and (65), respectively. The numbers next to the lines numerate the particle level to which the lines correspond.

with $\Omega + 2 = 12$ particles relative to the ground state of the Ω-particle system as functions of the interaction parameter G (in units of ϵ). They were obtained within the RPA, RRPA, SCRPA, and are plotted in comparison with the exact results. The RRPA gives a quite good description of the correlation energy, which practically coincides with that given by the SCRPA and the exact result for $G \leqslant 0.45$ MeV. However, the RRPA fails badly in describing the the ground-state E_1 and first-excited-state E_2 energies of the $\Omega + 2$ system. Here, although the RRPA results do not collapse at $G_{\rm cr} \simeq 0.34$ MeV as the RPA results do, they decrease monotonously, while the exact results as well as those given by the SCRPA increase with increasing G (cf. Refs. [6,7]). The results obtained within the Hara SCRPA are close to those given by the RRPA, but they fail to converge in this model at $G > G_{\rm cr}$. The Hara SCRRPA, which conserves the particle number exactly in ph nonsymmetric cases, offers very close results to those given by the SCRPA for the E_1 and E_2 energies within the whole interval of values for G under consideration. However, the correlation energy $E_{\rm corr}$ obtained within this number-conserving version of the SCRPA is slightly larger than the exact result, and the discrepancy is already clearly visible starting from $G \geqslant 0.3$ MeV.

In general, the feature depicted in Fig. 2 is similar to that of the ph case considered in Ref. [4], where the solution obtained by using Eq. (53) approaches the exact solution at large G, while the one offered by the Hara approach fails to describe it, never approaching zero. This result comes from the overestimation of ground-state correlations beyond the RPA within the Hara approach, which can be clearly seen by examining the ground-state correlation factors $\langle D_i \rangle$ and/or the occupation number N_i. The factor $\langle D_p \rangle$, which is the same as $\langle D_h \rangle$ for the symmetric case of the picket-fence model, is shown in Fig. 3. This factor decreases from 1 with increasing G, approaching zero as $G \to \infty$. The deviation from 1 is stronger at the level closer to the Fermi one. The difference between the results obtained by using Eqs. (53) (the SCRPA) and (65) (the Hara SCRPA) is strongest for the lowest particle level, in which the Hara SCRPA gives stronger ground-state correlations beyond the RPA. It also increases with increasing G in line with the results obtained for the ph case in Ref. [4]. This also explains the larger discrepancy between the two approaches in the description of correlation energy $E_{\rm corr}$, while the differences in the energies E_1 of the ground states and E_2 of the first excited states are relatively smaller.

The behavior of $\langle D_i \rangle$ leads to the change of the occupation number $\langle N_p \rangle$ and $\langle N_h \rangle$ as shown in Fig. 4. At small G, the function N_i approaches the staircase with $\langle N_p \rangle \simeq 0$ and $\langle N_h \rangle \simeq 2$ for all ϵ_i. As G increases, the deviation from the staircase becomes more and more evident with the decrease of $\langle N_h \rangle$ from 2 and increase of $\langle N_p \rangle$ from 0. At $G/\epsilon = 0.4$, for example, $\langle N_h \rangle$ becomes 1.85 and $\langle N_p \rangle$ reaches 0.4 for levels closest to the Fermi one. The deviation caused by the Hara SCRPA is always stronger than that given by the

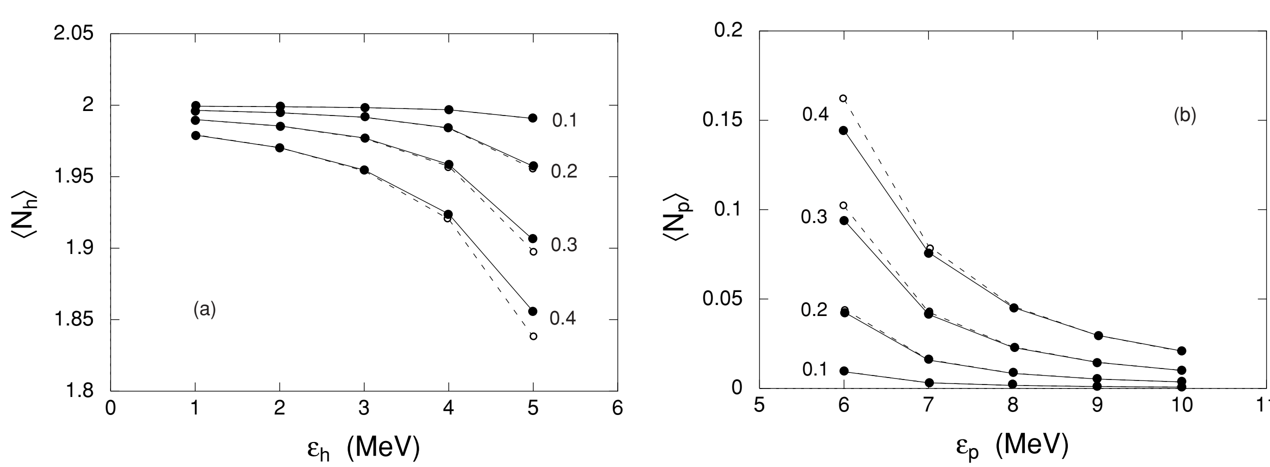

FIG. 4. Occupation number $\langle N_h \rangle$ for hole levels (a) and $\langle N_p \rangle$ for particle levels (b) as functions of single-particle energies ϵ_i at several values of G/ϵ indicated as the numbers next to the circles. The full and open circles denote results obtained by using Eqs. (47) and (65), respectively. The lines are drawn to guide the eye.

TABLE I. Correlation energy E_{corr}, ground-state energy E_1, and first-excited-state energy E_2 obtained within the "parametrized" Hara SCRPA using Eq. (67) with $\alpha = 1.9$ (a) in comparison with those given by the SCRPA (b) for $\Omega = 10$. All the values are given in MeV.

	E_{corr}		E_1		E_2	
G	a	b	a	b	a	b
0.01	-0.3265×10^{-3}	-0.3265×10^{-3}	1.0000	1.0000	3.0000	3.0000
0.05	-0.9018×10^{-2}	-0.8563×10^{-2}	1.0005	1.0005	3.0001	3.0001
0.10	-0.3850×10^{-1}	-0.3652×10^{-1}	1.0032	1.0033	3.0063	3.0063
0.15	-0.9263×10^{-1}	-0.8808×10^{-1}	1.0111	1.0112	3.0194	3.0194
0.20	−0.1760	−0.1686	1.0278	1.0279	3.0811	3.0460
0.25	−0.2930	−0.2846	1.0566	1.0563	3.0922	3.0926
0.30	−0.4470	−0.4424	1.0985	1.0970	3.1645	3.1657
0.35	−0.6401	−0.6475	1.1514	1.1481	3.2670	3.2703
0.40	−0.8823	−0.9023	1.2118	1.2058	3.4011	3.4087
0.45	−1.1608	−1.2094	1.2755	1.2667	3.5654	3.5804

SCRPA. Since $\langle D_i \rangle \to 0$ as $G \to \infty$ we have from Eq. (65) (the Hara SCRPA) the sum $\sum_\lambda (Y_p^\lambda)^2 = \sum_\mu (Y_h^\mu)^2 \to 1/2$, which makes $N_p = N_h \to 1$. For the SCRPA at the value $\sum_\lambda (Y_p^\lambda)^2 = \sum_\mu (Y_h^\mu)^2 = 1/2$, we obtain $\langle D_p \rangle = \langle D_h \rangle = 1/2$, which leads to $\langle N_p \rangle = 1/2$ and $\langle N_h \rangle = 3/2$. Again, this shows that ground-state correlations beyond the RPA are stronger within the Hara SCRPA than within the SCRPA.

The exaggeration of the ground-state correlations beyond RPA within the renormalization procedure, which leads to the number-conserving (Hara) type expressions (65), was pointed out before by Rowe [2], where, by using the number-operator method to insert the number operator twice at the center of $\langle N_i \rangle$, he found that the ph ground-state correlation factor $\langle\langle D_{\text{ph}} \rangle\rangle$ became $\sum_\nu |Y_{\text{ph}}^\nu|^2$ instead of $2\sum_\nu |Y_{\text{ph}}^\nu|^2$. The result of an infinite expansion by inserting repeatedly the number operator at the center of $\langle N_i \rangle$ is not available for pp RPA at this stage. However, the observation by Rowe suggests that the real $\langle D_p \rangle$ and $\langle D_h \rangle$ might be closer to 1 than those given by Eqs. (65). Therefore, a test was also carried out here by parametrizing $\langle D_p \rangle$ and $\langle D_h \rangle$ within the Hara SCRPA to see if it is possible to achieve results as good as those given by the SCRPA for all three quantities E_{corr}, E_1, and E_2. For this test, we used

$$\langle \widetilde{D}_p \rangle = 1 - \alpha \sum_\lambda \left(Y_p^\lambda\right)^2,$$
$$\langle \widetilde{D}_h \rangle = 1 - \alpha \sum_\mu \left(Y_h^\mu\right)^2, \qquad \alpha < 2, \tag{67}$$

instead of Eqs. (65) and repeated the calculations. The result of this test shows that the values E_{corr}, E_1, and E_2 obtained within the SCRPA can be fitted simultaneously rather well within such a "parametrized" Hara SCRPA with the parameter $\alpha \simeq 1.9$. These results are shown in Table I in comparison with the SCRPA ones. Such a parametrized Hara SCRPA also conserves exactly the particle number in the ph nonsymmetric case as does the Hara SCRPA.

V. CONCLUSIONS

The present work shows that the SCRPA violates the particle number in the ph nonsymmetric case if the occupation numbers are calculated according to Eq. (46) for the picket-fence model, which is a limit of Eq. (51) for the general shell-model spherical basis. Within the ph nonsymmetric picket-fence model, this particle-number violation increases with the asymmetry and interaction strength G, but it decreases with increasing particle number. However, within the interval of values for G under consideration ($G \leqslant 0.5$ MeV), we also found that the particle-number violation reaches at most around 0.2% for the most asymmetric case with the level number $\Omega = 10$, where the number of hole levels $\Omega_h = 1$ and number of particle levels $\Omega_p = 9$. In all other less asymmetric cases, this violation is smaller than 0.1%.

In order to maintain the exact particle-number conservation within the SCRPA, a renormalization was proposed, which represents the number operator in terms of the product of renormalized pairing operators. As a result, a number-conserving SCRPA was derived, which is called the Hara SCRPA as it has the equations for the occupation numbers similar to those obtained in the pioneering works by Hara *et al.* for the ph case [1]. The results of numerical calculations show that the Hara SCRPA yields values for the ground-state energy and energy of the first excited state of the $\Omega + 2$ system that are very close to the corresponding values obtained within the SCRPA. However, the correlation energy that the Hara SCRPA offers is slightly larger than that obtained within the SCRPA.

The results of this study also indicate that in realistic calculations using nonsymmetric single-particle spectra within RPA, in particular for light systems, one should carefully examine the violation of the Pauli principle to see if it is important to include the ground-state correlations beyond the RPA. As a matter of fact, the preliminary results of the RRPA calculations, which were carried out recently for ^{12,14}Be using the Gogny interaction [9], have shown that ground-state correlations beyond the RPA increased the correlation energy by 20–24% compared to the RPA results. This shifted up the ground-state energy by 13% for ^{12}Be and 48% for ^{14}Be. At the same time, the particle-number violation within the RRPA due to the use of Eq. (51) did not exceed 0.2%. In this case, the SCRPA can still be well justified and has the advantage over the Hara SCRPA, as the former offers a better description of the correlation energy.

In the cases where the particle-number violation cannot be neglected (e.g., $>1\%$) in calculations with realistic spectra and interactions, a number-conserving approach like the Hara SCRPA proposed in the present work might have to be used instead of the SCRPA. However, the improvement of the correlation energy in this case cannot be achieved by simply renormalizing RPA as has been done in the approaches under discussion. The test of parametrizing the Hara SCRPA to yield all three energies $E_{\rm corr}$, E_1, and E_2 close to the values given by the SCRPA suggests that higher-order correlations may have to be included in order to reproduce all three quantities within a number-conserving SCRPA. This indicates that coupling to configurations more complicated than the ph, pp, or hh ones should also be taken into account.

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