Quasiparticle random-phase approximation (QRPA) is applied to two nuclei, and overlap of the QRPA excited states based on the different nuclei is calculated. The aim is to calculate the overlap of intermediate nuclear states of the double-beta decay. We use the like-particle QRPA after the closure approximation is applied to the nuclear matrix elements. The overlap is calculated rigorously by making use of the explicit equation of the QRPA ground state. The formulation of the overlap is shown, and a test calculation is performed. The effectiveness of the truncations used is shown.

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where $|i\rangle$ is the HFB ground state of the same nucleus as the one $|f\rangle$ describes, and $\hat{v}_I^{(K'\pi')}|i\rangle$ is a generator of the QRPA ground state. $N_I$ is the normalization factor. In this paper, for any equation only referring to the initial state denoted by $I$ or $i$, we have also provided the corresponding equation referring to $F$ or $f$. Latter equations are omitted. We have $[O^I_{m'},O^F_{m'}]=0$ in the QRPA, if $(K\pi) \neq (K_m',\pi m')$; hence, $\hat{v}_I^{(K'\pi')}\hat{v}_I^{(K'\pi')}$ with different $(K'\pi')$ are separately determined by

$$O^I_{m'} \exp \left[ i\hat{v}_I^{(K_m',\pi m')}\right] |i\rangle = 0.$$  

(3)

A general quasiparticle basis $\{\mu\}$ based on the initial state is introduced by $a^I_{\mu}|i\rangle = 0$, where the $a^I_{\mu}$ is an annihilation operator, $\mu = (q_\mu,\pi_\mu,j^z_\mu,i_\mu)$ being the label of a general quasiparticle state. $q_\mu$ denotes a proton or neutron, and $i_\mu$ is the label specifying a state in the subspace $(\mu_\pi,\pi_\mu,j^z_\mu)$. Notation $-\mu$ is used for expressing $(q_\mu,\pi_\mu,j^z_\mu,i_\mu)$. We use the canonical-quasiparticle basis $\{\mu\}$ for efficiency of the QRPA calculation $[26]$. $\hat{v}_I^{(K'\pi')}$ is expressed as

$$\hat{v}_I^{(K'\pi')} = \sum_{\mu_\nu'\mu''\nu''} C^{(K'\pi')}_{\mu_\nu'\mu''\nu''} a^I_{\mu_\nu'} a^I_{\mu''\nu''} a^{\dagger I}_{\mu_\nu'},$$  

(4)

$a^I_{\mu} a^{\dagger I}_{\mu}$ and $a^{\dagger I}_{\mu} a^I_{\mu}$ in Eq. (4) are the fermion image of the boson $[24]$: a condition is introduced that $C^{(K'\pi')}_{\mu_\nu'\mu''\nu''}$ does not vanish, only if $j^z_\mu + j^z_\mu' = K'$, $j^\nu_\mu + j^\nu_{\mu'} = -K'$, and $\pi_\mu \pi_{\mu'} = \pi_{\mu'} \pi_{\nu'} = \pi'$. We order the canonical-quasiparticle states and restrict $\mu < \nu$, $\mu' < \nu'$ in $C^{(K'\pi')}_{\mu_\nu'\mu''\nu''}$ without loss of generality.

The solution of the QRPA equation gives us

$$O^I_{m'} \sum_{\mu<\nu} \left( X^{I\mu_\nu}_{\mu_\nu'} a^I_{\mu_\nu'} a^{\dagger I}_{\mu_\nu'} - Y^{I\mu'\nu}_{-\mu'\nu} a^{\dagger I}_{-\mu'\nu} a^I_{-\mu'\nu} \right),$$  

(5)

where $j^z_\mu + j^z_\mu' = K_{m'}$ and $\pi_\mu \pi_{\nu'} = \pi_{m'}$. We define matrices

$$C^{(K'\pi')} = \begin{pmatrix} C^{(K'\pi')}_{11,-1,-1} & \cdots & C^{(K'\pi')}_{11,-n'-1} \\ \vdots & \ddots & \vdots \\ C^{(K'\pi')}_{n'-1,1,-1} & \cdots & C^{(K'\pi')}_{n'-1,1,-n'} \end{pmatrix},$$  

(6)

$$X^{(K'\pi')} = \begin{pmatrix} X^{I11}_{11} & \cdots & X^{IM}_{11} \\ \vdots & \ddots & \vdots \\ X^{I1M}_{n'-1,n'-1} & \cdots & X^{IM}_{n'-1,n'-1} \end{pmatrix},$$  

(7)

where the QRPA solutions having $(K'\pi')$ are used. The negative integers of the index correspond to $-\mu$. Matrices $Y^{(K'\pi')}F, X^{(K'\pi')}F, Y^{(K'\pi')}F$ are also introduced in the same way. $C^{(K'\pi')}I$ is obtained, by ignoring the exchange terms (the quasi-boson approximation), as follows:

$$C^{(K'\pi')} = \frac{1}{1 + \delta_{K0}} \left( Y^{(K'\pi')}F \frac{1}{X^{(K'\pi')}F} \right)^T,$$  

(8)

where suffix $T$ stands for transpose. Practically, $1/X^{(K'\pi')}F$ does not have a singularity.

The relation between the two HFB states can be written as $[17]$

$$|i\rangle = \frac{1}{N_I} \exp \left[ \sum_{\mu\nu} D_{\mu\nu} a^F_{\mu} a^{\dagger F}_{\nu} \right] |f\rangle,$$  

(9)

$$N_I = \frac{1}{\langle f|f\rangle} = \sqrt{\text{det}(I + D^T D)}.$$  

(10)

$I$ is the unit matrix of the size of matrix $D$, which is defined by

$$(D)_{ij} = D_{\mu_i-\mu_j}, i,j = 1, \ldots, n_T,$$  

(11)

$n_T$ is the dimension of the subspace $(q_\mu,\pi_\mu,j^z_\mu)$. $D_{\mu\nu}$ is not equal to 0 only for those $\mu$ and $\nu$ that satisfy $j^z_\mu + j^z_\mu' = 0$ and $\pi_\mu \pi_{\mu'} = \mp$. We restrict $j^z_\mu > 0$ in Eq. (10).

The unitary transformation from basis $\{a^F_{\mu}, a^{\dagger F}_{\mu}\}$ to basis $\{a^I_{\mu}, a^{\dagger I}_{\mu}\}$ is given by

$$a^I_{\mu} = \sum_{\mu'} \left( T^{I\mu}_{F\mu'} a^F_{\mu'} + T^{I\mu}_{F-\mu'} a^{\dagger F}_{-\mu'} \right),$$  

(12)

and its Hermite conjugate equation for $-\mu$ with $j^z_\mu = j^z_{\mu'}$ and $\pi_\mu = \pi_{\mu'}$. $T^{I\mu}_{F\mu'}$ and $T^{I\mu}_{F-\mu'}$ can be obtained from the volume integral of the product of the canonical-quasiparticle wave functions $[27]$ of the two bases. $D_{\mu-\nu}$ is given by

$$D = -\frac{1}{T^{I1F1}T^{I1F2}} \cdot$$  

(13)

$$T^{I1F1} = T^{I1F1}_{\mu_1\mu_2}, i,j = 1, \ldots, n_T.$$  

(14)

Matrix $T^{I1F2}$ is defined in the same way as matrix $D$. Practically, again, $1/T^{I1F1}$ does not have a singularity.

Now, we expand and truncate the overlap matrix element with respect to $\hat{v}_I^{(K'\pi')}$ and $\hat{v}_I^{(K'\pi')}$ as

$$\langle f|O^F_{m'} a^{\dagger I}_{m'}|i\rangle \approx \frac{1}{N_I N_F} \left( G^{F10}_{mm'} + G^{F11}_{mm'} + G^{F22}_{mm'} \right),$$  

(15)

$$G^{F10}_{mm'} = \langle f|O^F_{m'} O^I_{m'}|i\rangle,$$  

(16)

$$G^{F11}_{mm'} = \sum_{K_1\pi_1} \left( \langle f|\hat{v}_I^{(K_1\pi_1)}|O^I_{m'}|i\rangle \right),$$  

(17)

$$G^{F22}_{mm'} = \sum_{K_1\pi_1} \langle f|\hat{v}_I^{(K_1\pi_1)}|O^I_{m'}|i\rangle,$$  

(18)

$$N_I \approx \left[ \sum_{K_1\pi_1} \left\{ \langle i|\hat{v}_I^{(K_1\pi_1)}\hat{v}_I^{(K_1\pi_1)}|i\rangle \right\} + \frac{1}{4} |\langle i|\hat{v}_I^{(K_1\pi_1)}|i\rangle|^2 \right]^{1/2}.$$  

(19)
We test up to the second-order terms $G^{F12}_{mm}$, which use both $\tilde{v}^{F}_{F}(K\pi_1)$ and $\tilde{v}^{F}_{I}(K\pi_2)$ but only with $(K_1\pi_1) = (K_2\pi_2)$ in Eq. (15) (actually $G^{F12}_{mm}$ is negligible in most of the overlap matrix elements, as shown later). Up to the fourth-order terms are included in normalization factors $N_I$ and $N_F$, because its convergence of the $\tilde{v}$-expansion is slow as compared to the un-normalized overlap matrix elements (which are the result of the numerical test). Equations (16)–(18) can be calculated using $X_{\mu\nu}^{\mu\nu}$, $Y_{\mu\nu}^{\mu\nu}$, $C_{\mu\nu\mu'\nu'}^{K'\pi'}$, those of $F$, $T_{\mu\nu}^{IF}$, $T_{\mu\nu}^{IF^2}$, and $D_{\mu\nu}$. The concrete equations will be given in the forthcoming full paper.

We use the code of the HFB approximation [28] and that of the QRPA developed by us [26]. The wave functions are treated, in both the codes, on a mesh within the cylindrical box and are discretized by the vanishing boundary condition at the edge of the box. The HFB equation is solved using a cutoff of the quasiparticle energy at 20 MeV for convenience in performing the tests. We transform the wave functions of the quasiparticle states associated with $\beta_p$, $\Delta_p$, $\beta_n$, and $\Delta_n$ denote, respectively, the quadrupole deformation and the averaged pairing gap of the protons. $\beta_n$ and $\Delta_n$ denote the same for the neutrons.

| nucleus | $\beta_p$ (MeV) | $\Delta_p$ (MeV) | $\beta_n$ (MeV) | $\Delta_n$ (MeV) |
|---------|-----------------|-----------------|-----------------|-----------------|
| $^{26}$Mg | −0.199          | 0.794           | −0.195          | 1.510           |
| $^{26}$Si | −0.224          | 0.865           | −0.206          | 1.402           |

We show the results of the calculation of $(K\pi) = (0+)$ below. Let $N_F$ and $N_I$ be the number of the two-canonical-quasiparticle states associated with $|F\rangle$ and $|I\rangle$, truncated by the cutoff occupation probability for calculating Eqs. (17) and (18) (those with larger occupation probabilities than the cutoff are used). This is another truncation after the 20-MeV cutoff. The convergence of the overlap matrix elements is shown with respect to $N_F + N_I$ in Fig. 1. The same value of the cutoff is applied for the two bases, and we have $N_F \approx N_I$. It is seen that $N_F + N_I = 350$ is sufficient for the convergence. The total number without the truncation is $\geq3300$; thus, this truncation is rather efficient. $|I\rangle$ and $|F\rangle$ have different configurations at the Fermi surface; therefore, the high-energy components of $O^I_{mm}$ and $O^F_{mm}$ leaving the configuration around the Fermi surface intact do not contribute to the overlap matrix elements. On the other hand, it is necessary to calculate $N_I$ and $N_F$ without this truncation.

The major diagonal overlap matrix elements are shown in Fig. 2 obtained with $N_F + N_I = 134$. It is observed that the contribution of $G^{F11}_{mm}$ is negligible and that of $G^{F10}_{mm}$ is not significant for the small matrix elements. $G^{F10}_{mm}$ is sufficient in most of the matrix elements omitted in that figure.

The contribution of $(K_1\pi_1) \neq (0+)$ to the major overlap matrix elements through $G^{F11}$ is shown in Fig. 3 calculated with $N_F + N_I = 350$ and max $|K| = 4$. We also calculated the contribution of $(K_1\pi_1) = (0-) and (1-)$ and found that it was smaller than that of the positive parity by at least an order of magnitude: thus,
only the positive parity is used. The contribution of \((K_1 \pi_1) \neq (0+)\) is very small to all of \(G_F^{IJ}\) except for \(m = 1\), which is one of the spurious states. Actually, our method should be applied only to the cases that do not have large fluctuations of the particle number so that the spurious states are not crucial to the nuclear matrix elements [1]. \(N_F\) and \(N_I\) require \(|K|\) of up to 3 with both parities.

In summary, the overlap matrix elements of the QRPA states based on the ground states of different nuclei have been calculated using the QRPA ground states explicitly for relatively light nuclei with the Skyrme and the contact volume pairing energy functionals. The most important finding of this study is that the bold truncations are allowed in the calculation of the un-normalized overlap matrix elements. The normalization factors need a less-truncated calculation; however, the amount of this calculation is reduced tremendously by identifying \(|f\rangle\) and \(|i\rangle\) in each factor. Considering this advantage and the performance of the modern parallel computers, we believe that there is no reason to avoid the explicit wave function of the QRPA ground states.

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