I. INTRODUCTION

The structure and dynamics of exotic nuclei have been the main subject of investigation both in the theoretical and the experimental nuclear physics. The peculiar feature of the exotic nuclei is that the Fermi level is located near the continuum levels. In this situation, the nucleons near the Fermi level are easily brought to the continuum states by pairing correlations. The low-energy excitation modes are often in the continuum energy region.

The general mean-field method to treat the pairing correlations as well as the mean-field is the Hartree-Fock Bogoliubov (HFB) method, which has played a central role in the investigation of the static ground state properties of the nuclei in a wide area of the nuclear chart. The typical method to study the excited collective states of nuclei on top of the mean-field ground state with the pairing correlations is the quasiparticle random phase approximation (QRPA) as a small amplitude quadrupole oscillations are shown.

In the practical QRPA calculations, two major methods so far developed are the Green’s function method through the response function formalism and the diagonalization method of the QRPA matrix. From the theoretical point of view, the QRPA is a small amplitude approximation of the time-dependent Hartree-Fock Bogoliubov (TDHFB) equation. Considering the rich results of the time-dependent Hartree-Fock (TDHF) and the random phase approximation (RPA) as a small amplitude approximation of the TDHF, it is worthwhile establishing a self-consistent TDHFB framework together with the practical method of solving the TDHFB equation.

The widely used effective interactions both in the mean-field and the QRPA calculations are the Skyrme interactions with zero-range pairing part or the Gogny interaction which consists of both the finite-range parts and the zero-range ones.

In the case of the HFB calculations with the Skyrme interactions (Skyrme HFB), the Skyrme interaction is used for the particle-hole channel, while the pairing interaction is introduced only for the particle-particle channel. Since the zero-range interaction is assumed in the Skyrme HFB, it is necessary to set the appropriate cut-off energy and choose the optimum parameter set in the pairing part.

In contrast with the Skyrme HFB, in the HFB calculations with the Gogny interaction (Gogny HFB), the particle-hole channel and the particle-particle channel are treated on an equal footing. Therefore, the Gogny interaction is suitable for the formulation of the self-consistent TDHFB together with a practical numerical method of integrating the TDHFB equation.

In this paper, we report the formulation of the self-consistent TDHFB with the Gogny interaction and a numerical method to integrate the TDHFB equations. With the aim at illustrating the feasibility of the method, we apply the method to the case of oxygen isotope $^{20}\text{O}$, carrying out the numerical integration of the TDHFB equations.

This paper consists of the following sections: In Sec. II, a derivation of the self-consistent TDHFB equation is given together with a numerical method of solving the TDHFB equation. In Sec. III, the results of applying the TDHFB equation to the oxygen isotope $^{20}\text{O}$ are shown. Section IV is for summary and concluding remarks.

II. TDHFB EQUATION AND NUMERICAL SOLUTION

1. TDHFB equation

Let us assume that the Hamiltonian is written as a sum of the kinetic energy and the two-particle interactions with particle creation (annihilation) operator $C_\alpha^\dagger$ ($C_\alpha$),

$$H = \sum_{\alpha\beta} T_{\alpha\beta} C_\alpha^\dagger C_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \nu_{\alpha\beta\gamma\delta} C_\alpha^\dagger C_\beta^\dagger C_\gamma C_\delta,$$

(1)

where $T_{\alpha\beta}$ is the kinetic energy matrix element and $\nu_{\alpha\beta\gamma\delta}$ is an antisymmetrized two-body matrix element.

In the formal presentation of the TDHFB equation, it is convenient to start with the generalized density matrix $\mathcal{R}$

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix},$$

(2)
where $\rho$ and $\kappa$ are normal density and pairing tensor, respectively,

$$
\rho_{\alpha\beta} = (V^* V)_{\alpha\beta}, \quad (3)
$$

$$
\kappa_{\alpha\beta} = (V^* U)_{\alpha\beta}. \quad (4)
$$

The matrices $U_{\alpha k}$ and $V_{\alpha k}$ are introduced to connect the particle operators $\{C_{\alpha}, C_{\alpha}^\dagger\}$ with the quasiparticle operators $\{\beta_k, \beta_k^\dagger\}$ as follows:

$$
\beta_k = \sum_{\alpha} \left( U_{\alpha k} C_{\alpha} + V_{\alpha k} C_{\alpha}^\dagger \right), \quad (5)
$$

$$
\beta_k^\dagger = \sum_{\alpha} \left( U_{\alpha k}^* C_{\alpha}^\dagger + V_{\alpha k}^* C_{\alpha} \right). \quad (6)
$$

The equation of motion of the generalized density matrix $\mathcal{R}$ in Eq. (2) is given by

$$
i \hbar \frac{\partial}{\partial t} \mathcal{R} = [\mathcal{H}, \mathcal{R}], \quad (7)
$$

with the HFB Hamiltonian $\mathcal{H}$ given by

$$
\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \quad (8)
$$

Here, mean field Hamiltonian $h$ and pairing mean field $\Delta$ are introduced through the following relations:

$$
h_{\alpha\beta} = T_{\alpha\beta} + \Gamma_{\alpha\beta}, \quad \Gamma_{\alpha\beta} = \sum_{\gamma\delta} V_{\alpha\gamma\beta\delta} \rho_{\delta\gamma}, \quad (9)
$$

$$
\Delta_{\alpha\beta} = \frac{1}{2} \sum_{\gamma\delta} V_{\alpha\gamma\beta\delta} \kappa_{\gamma\delta}. \quad (10)
$$

From the definitions in Eqs. (3) and (4), the generalized density matrix $\mathcal{R}$ in Eq. (2) is rewritten as

$$
\mathcal{R} = \begin{pmatrix} V^T \\ U^* \end{pmatrix} \begin{pmatrix} V^T, U^T \end{pmatrix}, \quad (11)
$$

where $T$ stands for transposed matrix. Combining the formal solution $\mathcal{R}(t)$ of the equation of motion in Eq. (12) given as

$$
\mathcal{R}(t) = e^{-\frac{i}{\hbar} \int^t \text{d}\tau \mathcal{H}(\tau)} \mathcal{R}(0) e^{\frac{i}{\hbar} \int^t \text{d}\tau \mathcal{H}(\tau)}, \quad (12)
$$

with the rewritten form of the generalized density matrix $\mathcal{R}$ in Eq. (11), we have a formal solution of the matrices $U$ and $V$ as follows:

$$
\begin{pmatrix} V^*(t) \\ U^*(t) \end{pmatrix} = e^{-\frac{i}{\hbar} \int^t \text{d}\tau \mathcal{H}(\tau)} \begin{pmatrix} V^*(0) \\ U^*(0) \end{pmatrix}. \quad (13)
$$

The formal solution Eq. (13) of the matrices $U$ and $V$ is equivalent to the equation of motion of the matrices $U$ and $V$ given as

$$
i \hbar \frac{\partial}{\partial t} \begin{pmatrix} V^*(t) \\ U^*(t) \end{pmatrix} = \mathcal{H} \begin{pmatrix} V^*(t) \\ U^*(t) \end{pmatrix}, \quad (14)
$$

where the definition of the HFB Hamiltonian $\mathcal{H}$ in Eq. (8) is used. This form of the TDHFB equation was used by Bulgac in relation with Berry’s phase [14].

### 2. Numerical method of solution

The TDHF equation (14) takes a simple form, being similar to the TDHF equation with a TDHF Hamiltonian $h_{TDHF}$,

$$
i \hbar \frac{\partial}{\partial t} \psi_j(x, t) = h_{TDHF} \psi_j(x, t), \quad (15)
$$

for the wave functions $\psi_j(x, t)(j = 1, 2, \cdots, N)$ of $N$ orbitals. The solution of the TDHF equation is calculated by making use of the relation,

$$
\psi_j(x, t_{n+1}) = e^{-\frac{i}{\hbar} \Delta h^{(n+1/2)}} \psi_j(x, t_n), \quad (16)
$$

at every time step from $t_n$ to $t_{n+1} = t_n + \Delta t$ with an adequate Hamiltonian $h^{(n+1/2)}$ to conserve the total energy [15]. Applying the method in [16] to the TDHFB equation (14), we get the solution of the TDHFB equation (14) in the form given as

$$
\begin{pmatrix} U \\ V \end{pmatrix}^{(n+1)} = \exp \left(-\frac{i}{\hbar} \Delta \mathcal{H}^{(n+1/2)} \right) \begin{pmatrix} U \\ V \end{pmatrix}^{(n)}, \quad (17)
$$

with an adequate TDHFB Hamiltonian $\mathcal{H}^{(n+1/2)}$ at every time step from $t_n$ to $t_{n+1} = t_n + \Delta t$.

In the present case with the Hamiltonian (1), the expectation value of the Hamiltonian (1) with respect to HFB state $|\Phi\rangle$ is given as

$$
E = \langle \Phi | H | \Phi \rangle = \sum_{\alpha\beta} T_{\alpha\beta} \rho_{\beta\alpha} + \frac{1}{2} \kappa_{\alpha\beta} \Delta_{\alpha\beta} \rho_{\beta\alpha} + \frac{1}{2} \kappa_{\alpha\beta} \Delta_{\alpha\beta}, \quad (18)
$$

where the mean potential $\Gamma$ and mean pairing potential $\Delta$ are defined in Eqs. (9) and (10). Since in the TDHFB calculation the energy conservation is one of the most important conditions to be fulfilled, let us see how the energy in (18) is conserved with respect to a small variation in the matrices $U$ and $V$. Within the first order of the parameter $\lambda = \frac{\Delta}{h}$, the matrices $U$ and $V$ at a time $t$ is changed into the new matrices $U'$ and $V'$ according to the following relation,

$$
\begin{pmatrix} U' \\ V' \end{pmatrix} = \begin{pmatrix} U \\ V \end{pmatrix} - i\lambda \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} U - i\lambda (h U + \Delta V) \\ V + i\lambda (h^* V + \Delta^* U) \end{pmatrix}. \quad (19)
$$

Here, for the case of the discussion, let us assume that the time increment $\Delta t$ is small enough so that we can identify the mean field Hamiltonian $h^{(n+1/2)}$ and mean pairing potential $\Delta^{(n+1/2)}$ in the TDHFB Hamiltonian $\mathcal{H}^{(n+1/2)}$ with $h$ and $\Delta$, respectively, at the time $t$. Using the relations in Eq. (19), the variations in the density $\rho$ in Eq. (6) and pairing tensor $\kappa$ in Eq. (4) are represented, respectively, as
\[
\rho' = V^* V/T
\]
\[
= (V^* - i \lambda (\Delta U^* + hV^*)) (V^T + i \lambda (U^T\Delta^T + V^T h^T))
\]
\[
= \rho - i \lambda [h, \rho] - i \lambda (-\Delta \kappa^* + \kappa \Delta^*),
\]
(20)

\[
\kappa' = V'' U^T
\]
\[
= (V^* - i \lambda (\Delta U^* + hV^*)) (U^T - i \lambda (U^T h^T + V^T \Delta T))
\]
\[
= \kappa - i \lambda (\Delta U^* U^T + h\kappa + \kappa h^* - \rho \Delta).
\]
(21)

Putting these expressions of the density and pairing tensor up to the first order in the parameter \( \lambda \) into the expression of the energy in Eq. (18), we have the variation of the energy as follows:

\[
\delta E = \text{Tr} \{-i \lambda h [h, \rho] - i \lambda h (-\Delta \kappa^* + \kappa \Delta^*)\}
\]
\[
- \frac{i \lambda}{2} \text{Tr} \{-\Delta^* \Delta - \Delta^* h \kappa - \Delta^* \kappa h^* + \Delta^* \Delta \rho^* + \Delta \rho \Delta\}
\]
\[
- \frac{i \lambda}{2} \text{Tr} \{\Delta^* \Delta + h^* \kappa^* \Delta + \kappa^* h \Delta - \Delta^* \rho \Delta - \rho \Delta^* \Delta\}
\]
\[
= 0,
\]
(22)

where the relations \( h^* = h^T, \kappa^T = -\kappa, \) and \( \Delta^T = -\Delta \) are used. The notation \( \text{Tr} \) stands for taking the trace of the matrices. From Eq. (22), we see that we can integrate the TDHFB equation (14) with a conserved energy expressed as in Eq. (18), setting the time increment \( \Delta t \) and intermediate TDHFB Hamiltonian \( H(n+1/2) \) adequately.

When the Gogny interaction is used, there is a part in the mean potential \( \Gamma \) which comes from the density-dependent term through the variation of the density matrix \( \rho \), just as in Eq. (20). Owing to the parameter set of the Gogny interaction, there is no contribution of the density-dependent term to the pairing energy. The contribution of the density-dependent term is included only in the mean-field Hamiltonian \( h \) in the HFB Hamiltonian \( \mathcal{H} \). Then, the energy conservation relation (22) holds when the Gogny interaction is adopted in the Hamiltonian \( \mathcal{H} \).

In the numerical calculation, we expand the exponential function in Eq. (17) in terms of the power series up to the tenth order in the time increment \( \Delta t \). The intermediate TDHFB Hamiltonian \( \mathcal{H}(n+1/2) \) is made by using the predictor-corrector method at each time step: In the predictor-corrector method, the predictor solutions \( U' \) and \( V' \) are calculated according to the method in Eq. (17) by using the TDHFB Hamiltonian \( \mathcal{H}(n) \) with the quantities \( h \) and \( \Delta \), which are made by using density \( \rho^{(n)} \) and pairing tensor \( \kappa^{(n)} \) at the time \( t_n \), respectively. Then, using the predictor density \( \rho' = V'^* V'/T \) and pairing tensor \( \kappa' = V'' U'/T \), the intermediate density \( \rho^{(n+1/2)} = (\rho^{(n)} + \rho') / 2 \) and the pairing tensor \( \kappa^{(n+1/2)} = (\kappa^{(n)} + \kappa') / 2 \) are made, which enter the intermediate TDHFB Hamiltonian \( \mathcal{H}(n+1/2) \). The corrector solutions \( U'' \) and \( V'' \) are calculated according to the method in Eq. (17) with the intermediate TDHFB Hamiltonian \( \mathcal{H}(n+1/2) \). From the ideal point of view, this process is repeated until the energy is conserved within a desired order. In the practical calculations, however, we stop the predictor-corrector iterations after the first two iterations to save the cpu time.

The initial condition we adopt in the present calculation is of the impulse type: The static HFB solution \( U_0 \) and \( V_0 \) are changed into the initial matrices \( U^{(0)} \) and \( V^{(0)} \) by the relations given by

\[
V^{(0)} = \exp (i \varepsilon Q) V_0 = \sum_{\nu=1}^{N_{\text{max}}} \frac{i^{\nu} \varepsilon^\nu Q^\nu}{\nu!} V_0,
\]
(23)

\[
U^{(0)} = \exp (-i \varepsilon Q^*) U_0 = \sum_{\nu=1}^{N_{\text{max}}} \frac{i^{\nu} (-\varepsilon)^\nu Q^{\nu*}}{\nu!} U_0,
\]
(24)

where the expression \( Q \) stands for matrix representation of a multipole operator with respect to the numerical basis states. In the expression of the initial conditions (23) and (24), the exponential function is expanded into the power series with respect to the parameter \( \varepsilon \) up to the \( N_{\text{max}} \)-th order.
FIG. 1: Time dependence of expectation value of quadrupole moment.

FIG. 2: Total energy vs time in quadrupole oscillation in Fig. 1. Line labelled with "ground state" stands for the energy of the HFB ground state. Curve labelled with "TDHFB" is for the energy expectation value in the course of quadrupole oscillation.

FIG. 3: Deviation of neutron (proton) number expectation value from accurate number 12 (8) in quadrupole oscillation in Fig. 1.

FIG. 4: Quadrupole strength distribution of quadrupole oscillation in Fig. 1. Artificial width of 0.6 MeV is used.

III. APPLICATIONS

With the purpose of studying the feasibility of the TD-HFB equation and the method of solution proposed in the previous section, we apply the method to the oxygen isotope $^{20}\text{O}$. We adopt the Gogny force [16, 17] with D1 parameter set in the two-particle interaction part in the Hamiltonian (1).

As the numerical basis, we make use of the three-dimensional harmonic oscillator eigenstates. The two-particle matrix elements $V_{\alpha\beta\gamma\delta}$ in the Hamiltonian (1) are calculated after the method which was used by Girod and Grammaticos [18]. In the present calculations, we set the space of basis states so that the relation $n_x + n_y + n_z \leq N_{\text{shell}} = 4$ is satisfied, where $n_x$ ($n_y$, $n_z$) is the number of quanta of the harmonic oscillator basis states in the x (y, z) direction, respectively. The angular frequency parameters $\omega_x, \omega_y$, and $\omega_z$ of the harmonic oscillator basis states are optimized under the sphericity condition $\omega_x = \omega_y = \omega_z = \omega_0$ so that the HFB energy should be minimum. We have set $\hbar \omega_0 = 16.0 \text{ MeV}$.

In the initial conditions (23) and (24), we take the multipole operator $Q$ to be a quadrupole operator $Q_{\alpha\beta} = (2z^2 - x^2 - y^2)_{\alpha\beta}$, expressed as a matrix with respect to the basis states labelled by $\alpha$ and $\beta$. The parameter $\varepsilon$ is put to be $1.0 \times 10^{-3}$, which is small enough so that the linearity of the oscillation with respect to $\varepsilon$ is satisfied. The power series expansions of the exponential functions in Eqs. (23) and (24) are calculated up to the $N_{\text{max}}$-th order with $N_{\text{max}}$ put to be ten.

In the present calculations, we have omitted the Coulomb part in the two-body interactions, which leads to shorter cpu time. For the moment, it might not be a draw-back to neglect the Coulomb part with the aim at studying the feasibility of the method under consideration.

In Fig. 1 we display the time variation of the mass quadrupole moment $\langle 2z^2 - x^2 - y^2 \rangle$ of $^{20}\text{O}$. The time increment $c\Delta t$ used in the calculation is 0.2 fm, and total time step is 19000. After the initial impulse, we can see regular small-amplitude oscillations take place.

In Fig. 2 the total energy in the course of the oscillation is shown together with the ground state energy of
the static HFB calculation. The excitation energy 0.2 MeV is kept to a good extent in the integration process.

In Fig. 3 the deviation of the expectation values of the nucleon number from the accurate values (8 protons and 12 neutrons) is displayed with respect to time. In $^{20}$O, the protons are in the normal state, whereas the neutrons are in the superconducting state. Therefore, the integration of the equations of motion of the proton orbitals is equivalent to the TDHF case, where the occupation probability of each one of the orbitals is exactly 1 or 0. Then, the total number of protons are conserved within $10^{-11}$. The neutron number in Fig. 3 is kept up to around $10^{-5}$ in the present integration process. This result illustrates that we can keep the unitarity of the time development operator in Eq. (14) within a practically satisfying order with the following set of parameters such as $N_{shell} = 4$ and $c\Delta t = 0.2$ fm in the case of the excitation energy 0.2 MeV.

In Fig. 4 we display the strength function which is calculated by the Fourier transformation from the time series of the expectation value of the quadrupole operator in Fig. 1. The locations of the main peaks in Fig. 4 are similar to the results in Ref. 6. The low-energy $2^+$ levels of $^{20}$O are located at 1.7 MeV, 4 MeV, 5 MeV, and 10 MeV [19]. The three low-energy peaks in Fig. 4 are expected to correspond to these levels. Since the space of the basis states is not large enough, the energies corresponding to the peaks in Fig. 4 are somewhat higher than those of the observed levels.

On the other hand, the ratio of the lowest energy peak around 3 MeV to the high energy one around 24 MeV is quite different from the result in Ref. 6. Considering that the effect of the continuum is included in the RPA calculations in Ref. 6, and our space in the present calculations is limited within the major quantum number $N_{shell} = 4$, the differences of the low-energy peaks might come from the space of states taken in the calculations.

**IV. SUMMARY AND CONCLUDING REMARKS**

In this article, we have proposed a method to integrate the self-consistent TDHFB equation. We made use of an integration method which is widely used in the TDHF, i.e., a power series expansion of the time displacement operator at each time step. Adopting the Gogny interaction in the two-particle interaction parts in the Hamiltonian, we carried out the numerical calculations of the TDHFB equation in the case of oxygen isotope $^{20}$O.

The accuracy of conservation of the excitation energy and the particle numbers is illustrated in the calculation of small-amplitude quadrupole oscillation, which is started from an impulse-type initial condition.

The strength function of the quadrupole oscillation is calculated. The energies of the peaks of the strength function are similar to and somewhat higher than the experimental results of the low-energy $2^+$ levels.

The relative ratios of the peak heights, on the other hand, seem not to be enough to discuss their physical contents, in comparison with the results given by the QRPA with continuum space included [6]. One major reason of the situation might be the space of basis states in the present calculations, which is not large enough with the maximum major shell quantum number $N_{shell} = 4$. It is the foremost task to check the convergence of the results with respect to the cut-off $N_{shell}$ of the space of basis states.

Since the basis states in the present calculations are the three-dimensional harmonic oscillator states, the method proposed in this article seems to be useful in describing the excitational modes in deformed nuclei. The calculations in some deformed nuclei are now in progress.

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