Linear response calculation using the canonical-basis TDHFB with a schematic pairing functional

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Abstract. A canonical-basis formulation of the time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory is obtained with an approximation that the pair potential is assumed to be diagonal in the time-dependent canonical basis. The canonical-basis formulation significantly reduces the computational cost. We apply the method to linear-response calculations for even-even nuclei. $E1$ strength distributions for proton-rich Mg isotopes are systematically calculated. The calculation suggests strong Landau damping of giant dipole resonance for drip-line nuclei.

1. Introduction

The time-dependent Hartree-Fock (TDHF) theory has been extensively utilized to study nuclear many-body dynamics [1]. Recently, it has been revisited with modern energy density functionals and more accurate description of nuclear properties has been achieved [2, 3, 4, 5, 6, 7]. The TDHF theory uses only occupied orbitals, number of which is equal to the number of particles (N). However, it neglects the residual interactions in particle-particle and hole-hole channels, which are important for properties of open-shell heavy nuclei. It is well-known that the time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory [8] properly takes into account the pairing correlations. The TDHFB equation is formulated in a similar manner to the TDHF, however it requires us to calculate the time evolution of quasi-particle orbitals, number of which is, in principle, infinite. Therefore, the practical calculations with the TDHFB are very limited [9, 10].

Very recently, we have proposed a possible approximation for the TDHFB theory [11]. This is a time-dependent version of the BCS approximation [12] for the Hartree-Fock-Bogoliubov theory. Namely, we neglect off-diagonal elements of the pair potential in the time-dependent canonical basis. We show that this approximation results in significant reduction of the computational task. We call the equations obtained with this approximation, "Canonical-basis TDHFB" (Cb-TDHFB) equations. We apply the method to the linear-response calculations using the full Skyrme functionals of the parameter set of SkM*, and discuss properties of the $E1$ strength distribution in even-even Mg isotopes.

The paper is organized as follows. In Sec. 2, we present the basic equations of the present method and their derivation. It is emphasized that the basic equations possess a gauge invariance. A schematic choice of the pairing functional leads to violation of the gauge invariance, which requires us to choose a specific gauge to minimize the violation. In Sec. 3, we present numerical results of the real-time calculations of the linear response for Mg isotopes. Finally, the conclusion is given in Sec. 4.

2. Formalism of the Cb-TDHFB theory

In this section, we show the basic equations of the Cb-TDHFB and recapitulate their derivation. See Ref. [11] for more details.

2.1. Basic equations

Let us first show the Cb-TDHFB equations we derive in the followings.

$$i\frac{\partial}{\partial t}|\phi_k(t)\rangle = (h(t) - \eta_k(t))|\phi_k(t)\rangle, \qquad i\frac{\partial}{\partial t}|\phi_{\bar{k}}(t)\rangle = (h(t) - \eta_{\bar{k}}(t))|\phi_{\bar{k}}(t)\rangle, \qquad (1a)$$

$$i\frac{d}{dt}\rho_k(t) = \kappa_k(t)\Delta_k^*(t) - \kappa_k^*(t)\Delta_k(t), \qquad (1b)$$

$$i\frac{d}{dt}\kappa_k(t) = (\eta_k(t) + \eta_{\bar{k}}(t))\,\kappa_k(t) + \Delta_k(t)\,(2\rho_k(t) - 1)\,. \qquad (1c)$$

These basic equations determine the time evolution of the canonical states, $|\phi_k(t)\rangle$ and $|\phi_{\bar{k}}(t)\rangle$, their occupation, $\rho_k(t)$, and pair probabilities, $\kappa_k(t)$. The real functions of time, $\eta_k(t)$ and $\eta_{\bar{k}}(t)$, are arbitrary and associated with the gauge degrees of freedom. The time-dependent pairing gaps, $\Delta_k(t)$, which are given in Eq. (12), are similar to the BCS pairing gap [12] except for the fact that the canonical pair of states are no longer related to each other by time reversal. Although we use the same symbols, (ρ, κ, Δ), for matrixes in Eqs. (3a) and (3b), the quantities in the Cb-TDHFB equations are only their diagonal elements with a single index for the canonical states k. It should be noted that similar equations can be found in Ref. [13] for a simple pairing energy functional.

2.2. Derivation of the basic equations

We now derive the Cb-TDHFB equations starting from the generalized density-matrix formalism. The TDHFB equation can be written in terms of the generalized density matrix $R(t)$ as [8]

$$i\frac{\partial}{\partial t}R(t) = [\mathcal{H}(t), R(t)]\,. \qquad (2)$$

This is equivalent to the following equations for one-body density matrix, $\rho(t)$, and the pairing-tensor matrix, $\kappa(t)$.

$$i\frac{\partial}{\partial t}\rho(t) = [h(t), \rho(t)] + \kappa(t)\Delta^*(t) - \Delta(t)\kappa^*(t), \qquad (3a)$$

$$i\frac{\partial}{\partial t}\kappa(t) = h(t)\kappa(t) + \kappa(t)h^*(t) + \Delta(t)(1 - \rho^*(t)) - \rho(t)\Delta(t)\,. \qquad (3b)$$

Here, $h(t)$ and $\Delta(t)$ are single-particle Hamiltonian and pair potential, respectively.

At each instant of time, we may diagonalize the density operator $\hat{\rho}$ in the orthonormal canonical basis, $\{\phi_k(t), \phi_{\bar{k}}(t)\}$ with the occupation probabilities ρ_k. Then, the TDHFB state is expressed in the canonical (BCS) form as

$$|\Psi(t)\rangle = \prod_{k>0}\left\{u_k(t) + v_k(t)c_k^\dagger(t)c_{\bar{k}}^\dagger(t)\right\}|0\rangle. \qquad (4)$$

For the canonical states, we use the alphabetic indexes such as k for half of the total space indicated by $k > 0$. For each state with $k > 0$, there exists a "paired" state $\bar{k} < 0$ which is orthogonal to all the states with $k > 0$. The set of states $\{\phi_k, \phi_{\bar{k}}\}$ generate the whole

single-particle space. We use the Greek letters $\mu, \nu, \cdots$ for indexes of an adopted representation (complete set) for the single-particle states. Using the following notations,

$$\langle\langle\mu\nu|\phi_k(t)\phi_{\bar{k}}(t)\rangle\rangle \equiv \langle\mu|\phi_k(t)\rangle\langle\nu|\phi_{\bar{k}}(t)\rangle - \langle\mu|\phi_{\bar{k}}(t)\rangle\langle\nu|\phi_k(t)\rangle, \tag{5}$$

$$\hat{\pi}_k(t) \equiv |\phi_k(t)\rangle\langle\phi_k(t)| + |\phi_{\bar{k}}(t)\rangle\langle\phi_{\bar{k}}(t)|, \tag{6}$$

the density and the pairing-tensor matrixes are expressed as

$$\rho_{\mu\nu}(t) = \sum_{k>0}\rho_k(t)\langle\mu|\hat{\pi}_k(t)|\nu\rangle, \tag{7}$$

$$\kappa_{\mu\nu}(t) = \sum_{k>0}\kappa_k(t)\langle\langle\mu\nu|\phi_k(t)\phi_{\bar{k}}(t)\rangle\rangle, \tag{8}$$

where $\rho_k(t) = |v_k(t)|^2$ and $\kappa_k(t) = u_k^*(t)v_k(t)$. It should be noted that the canonical pair of states, $|\phi_k(t)\rangle$ and $|\phi_{\bar{k}}(t)\rangle$, are assumed to be orthonormal but not necessarily related with each other by the time reversal, $|\phi_{\bar{k}}\rangle \neq T|\phi_k\rangle$.

We can invert Eqs. (7) and (8) for ρ_k and κ_k,

$$\rho_k(t) = \sum_{\mu\nu}\langle\phi_k(t)|\mu\rangle\rho_{\mu\nu}(t)\langle\nu|\phi_k(t)\rangle = \sum_{\mu\nu}\langle\phi_{\bar{k}}(t)|\mu\rangle\rho_{\mu\nu}(t)\langle\nu|\phi_{\bar{k}}(t)\rangle, \tag{9}$$

$$\kappa_k(t) = \frac{1}{2}\sum_{\mu\nu}\langle\langle\phi_k(t)\phi_{\bar{k}}(t)|\mu\nu\rangle\rangle\kappa_{\mu\nu}(t). \tag{10}$$

The derivative of $\rho_k(t)$ with respect to time t leads to

$$
\begin{aligned}
i\frac{d}{dt}\rho_k(t) &= \sum_{\mu\nu}\langle\phi_k(t)|\mu\rangle i\frac{d\rho_{\mu\nu}}{dt}\langle\nu|\phi_k(t)\rangle + i\rho_k(t)\frac{d}{dt}\langle\phi_k(t)|\phi_k(t)\rangle \\
&= \frac{1}{2}\sum_{\mu\nu}\left\{\kappa_k(t)\Delta_{\mu\nu}^*(t)\langle\langle\nu\mu|\phi_k(t)\phi_{\bar{k}}(t)\rangle\rangle + \kappa_k^*(t)\Delta_{\mu\nu}(t)\langle\langle\phi_k(t)\phi_{\bar{k}}(t)|\mu\nu\rangle\rangle\right\}. \tag{11}
\end{aligned}
$$

We used the assumption of norm conservation and the TDHFB equation (3a). This can be rewritten in the simple form of Eq. (1b) with the definition of the pairing gap,

$$\Delta_k(t) \equiv -\frac{1}{2}\sum_{\mu\nu}\Delta_{\mu\nu}(t)\langle\langle\phi_k(t)\phi_{\bar{k}}(t)|\mu\nu\rangle\rangle. \tag{12}$$

In the same way, we evaluate the time derivative of $\kappa_k(t)$ as

$$i\frac{d}{dt}\kappa_k(t) = \frac{1}{2}\sum_{\mu\nu}\langle\langle\phi_k(t)\phi_{\bar{k}}(t)|\mu\nu\rangle\rangle i\frac{d\kappa_{\mu\nu}}{dt} + i\kappa_k(t)\left(\langle\frac{d\phi_k}{dt}|\phi_k(t)\rangle + \langle\frac{d\phi_{\bar{k}}}{dt}|\phi_{\bar{k}}(t)\rangle\right). \tag{13}$$

Then, using the TDHFB equation (3b), we obtain Eq. (1c) with the real gauge functions

$$\eta_k(t) \equiv \langle\phi_k(t)|h(t)|\phi_k(t)\rangle + i\langle\frac{\partial\phi_k}{\partial t}|\phi_k(t)\rangle. \tag{14}$$

These functions control time dependence of phase for the canonical states, which are basically arbitrary.

So far, the derivation is based on the TDHFB equations, and no approximation beyond the TDHFB is introduced. However, to obtain simple equations for time evolution of the canonical basis, we need to introduce an assumption (approximation) that the pair potential is written as

$$\Delta_{\mu\nu}(t) = -\sum_{k>0} \Delta_k(t)\langle\langle \mu\nu|\phi_k(t)\phi_{\bar{k}}(t)\rangle\rangle. \tag{15}$$

This satisfies Eq. (12), but in general, Eq. (12) can not be inverted because the two-particle states $|\phi_k\phi_{\bar{k}}\rangle$ do not span the whole space. In other words, we only take into account the pair potential of the "diagonal" parts in the canonical basis, $\Delta_{k\bar{l}} = -\Delta_k\delta_{kl}$. In the stationary limit ($|\phi_{\bar{k}}\rangle = T|\phi_k\rangle$), this is equivalent to the ordinary BCS approximation [12]. With the approximation of Eq. (15), it is easy to see that the TDHFB equations, (3a) and (3b), are consistent with Eqs. (1).

2.3. Properties of the Cb-TDHFB equations

The Cb-TDHFB equations, (1), are invariant with respect to the gauge transformation with arbitrary real functions, $\theta_k(t)$ and $\theta_{\bar{k}}(t)$.

$$|\phi_k\rangle \to e^{i\theta_k(t)}|\phi_k\rangle \quad \text{and} \quad |\phi_{\bar{k}}\rangle \to e^{i\theta_{\bar{k}}(t)}|\phi_{\bar{k}}\rangle \tag{16}$$

$$\kappa_k \to e^{-i(\theta_k(t)+\theta_{\bar{k}}(t))}\kappa_k \quad \text{and} \quad \Delta_k \to e^{-i(\theta_k(t)+\theta_{\bar{k}}(t))}\Delta_k \tag{17}$$

simultaneously with

$$\eta_k(t) \to \eta_k(t) + \frac{d\theta_k}{dt} \quad \text{and} \quad \eta_{\bar{k}}(t) \to \eta_{\bar{k}}(t) + \frac{d\theta_{\bar{k}}}{dt}.$$

The phase relations of Eq. (17) are obtained from Eqs. (10) and (12). It is now clear that the arbitrary real functions, $\eta_k(t)$ and $\eta_{\bar{k}}(t)$, control time evolution of the phases of $|\phi_k(t)\rangle$, $|\phi_{\bar{k}}(t)\rangle$, $\kappa_k(t)$, and $\Delta_k(t)$.

In addition to the gauge invariance, the Cb-TDHFB equations possess the following properties.

 (i) Conservation law
    (a) Conservation of orthonormal property of the canonical states
    (b) Conservation of average particle number
    (c) Conservation of average total energy
 (ii) The stationary solution corresponds to the HF+BCS solution.
(iii) Small-amplitude limit
    (a) The Nambu-Goldstone modes are zero-energy normal-mode solutions.
    (b) If the ground state is in the normal phase, the equations are identical to the particle-hole, particle-particle, and hole-hole RPA with the BCS approximation.

2.4. Energy functionals and numerical procedure

We adopt a Skyrme functional with the SkM* parameter set for the particle-hole channels. For the pairing energy functional, we adopt a simple functional of a form

$$E_g(t) = -\sum_{k,l>0} G_{kl}\kappa_k^*(t)\kappa_l(t), = -\sum_{k>0}\kappa_k^*(t)\Delta_k(t), \quad \Delta_k(t) = \sum_{l>0} G_{kl}\kappa_l(t), \tag{18}$$

where $G_{kl} = Gf(\epsilon_k^0)f(\epsilon_l^0)$ with $G = 0.6$ MeV. The smooth cut-off function $f(\epsilon_k^0)$, whose explicit form can be found in Ref. [11], depends on the single-particle energy of the canonical state k at

Table 1. Ground-state properties of Mg isotopes calculated with the SkM* functional; quadrupole deformation parameters (β, γ), pairing gaps for neutrons and protons (Δ_n, Δ_p), chemical potentials for neutrons and protons (λ_n, λ_p). In the case of normal phase $(\Delta = 0)$, we define the chemical potential as the single-particle energy of the highest occupied orbital. The pairing gaps and chemical potentials are given in units of MeV.

	β	γ	Δ_n	Δ_p	$-\lambda_n$	$-\lambda_p$
^{18}Mg	0.31	0°	0.0	0.0	25.59	0.20
^{20}Mg	0.0	–	0.0	1.13	20.53	2.83
^{22}Mg	0.38	0°	0.0	0.0	16.31	6.42
^{24}Mg	0.39	0°	0.0	0.0	14.12	9.51
^{26}Mg	0.20	54°	0.0	0.86	13.08	11.23
^{28}Mg	0.0	–	0.0	1.03	9.21	13.30

the HF+BCS ground state. A drawback of the simple functional (18) is that it violates the gauge invariance, which results in breakdown of some of nice properties shown in Sec. 2.3. However, it is shown that all these properties can be recovered by choosing a special gauge condition [11]

$$\eta_k(t) = \epsilon_k(t) = \langle \phi_k(t)|h(t)|\phi_k(t)\rangle, \quad \eta_{\bar{k}}(t) = \epsilon_{\bar{k}}(t) = \langle \phi_{\bar{k}}(t)|h(t)|\phi_{\bar{k}}(t)\rangle. \tag{19}$$

For numerical calculations, we extended the computer program of the TDHF in the three-dimensional coordinate-space representation [2] to include the pairing correlations. The ground state is first constructed by the HF+BCS calculation. Then, we solve the Cb-TDHFB equations in real time, under a weak impulse isovector dipole field, yielding a time-dependent E1 moment, $D_{E1}(t)$. To obtain the $E1$ strength distribution, we perform the spectral analysis with an exponential smoothing with $\Gamma = 1$ MeV: $D_{E1}(t) \to D_{E1}(t)e^{-\Gamma t/2}$. The readers should refer to Ref. [11] for more details.

3. Electric dipole strength distribution in proton-rich Mg isotopes

In Table 1, the ground-state deformations, pairing gaps, and chemical potentials are listed for stable to proton-rich Mg isotopes. In the present calculation with SkM*, ^{18}Mg turns out to be bound with a small binding energy of 200 keV. Thus, we include this nucleus in our calculation as a "fictitious" proton halo nucleus. The neutron pairing gap is absent for all these nuclei. The proton gap also vanishes for nuclei with prolate shapes, $\beta = 0.3 \sim 0.4$.

Calculated $E1$ strength distributions are shown in Fig. 1. The double-peak structure of the giant dipole resonance (GDR) due to the deformation splitting can be seen in ^{22,24}Mg. The $K = 0$ peak is located around 15 MeV and the $K = 1$ is near 22 MeV. In contrast, for ^{18}Mg, although the ground state is deformed in a prolate shape with $\beta \approx 0.3$, the double-peak structure is not clearly seen. In this nucleus, the $E1$ strength of both the $K = 0$ and $K = 1$ components are fragmented into a wide range of energy. Previously, we calculated the $E1$ strength distribution in neutron-rich Mg isotopes [11], and found the similar damping effects near the drip line. This strong Landau damping near the drip lines may be understood by the high level density of one-particle-one-hole (1p1h) states near the GDR energy.

The low-energy $E1$ strength in $E < 10$ MeV is negligible for stable nuclei (^{24,26}Mg). For the neutron-rich side, we see a small low-energy peak in ^{28}Mg. Since the neutron separation energy is still sizable (about 9 MeV), we assume that this is due to the occupation of the neutron $s_{1/2}$ orbital which is spatially extended. For the proton-rich (neutron-deficient) side, the low-energy
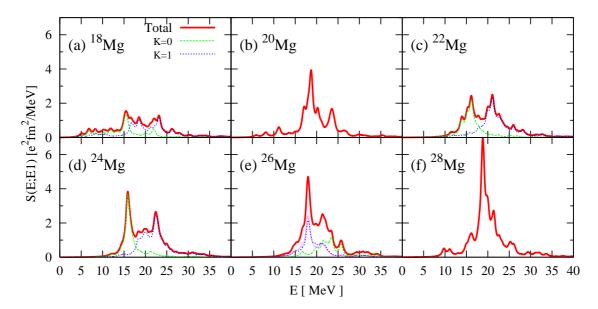
Figure 1. Calculated $E1$ strength distribution for even-even Mg isotopes ($N = 8 \sim 16$). For deformed nuclei, the total strength is decomposed into $K = 0$ (green dashed line) and $K = 1$ (blue dotted line) components. The z-axis is chosen as the symmetry axis for axially deformed cases. The smoothing parameter of $\Gamma = 1$ MeV is used.

strength is seen in ^{18,20}Mg. This should be due to the weak binding of the last-occupied proton $d_{5/2}$ orbitals, since the calculated proton separation energies are less than 3 MeV for these nuclei.

4. Summary

We presented an approximate and feasible approach to the TDHFB; canonical-basis TDHFB method. Since the number of the canonical states we need to calculate is the same order as the particle number, this method significantly reduces the computational task of the TDHFB. We calculated the $E1$ strength distribution in proton-rich Mg isotopes, using the real-time real-space method. We found a strong Landau damping effect in the drip-line nuclei, that may be related to high level density of the background 1p1h states with negative parity. The calculation also indicates an increase of the low-energy $E1$ strength as the nucleus approaches the proton drip line.

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