Solving RPA Eigenvalue Equation in Real-Space*)

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We present a computational method to solve RPA eigenvalue equation employing a uniform grid representation in the three-dimensional Cartesian coordinate. The conjugate gradient method, an iterative method for a generalized eigenvalue problem, is used for this purpose. We apply the present method to Hartree-Fock +RPA calculation with BKN-like interaction and Skyrme interaction.

我々は３次元正方メッシュ表現に於けるＲＰＡ方程式の解法を開発した。これまで主に限られた少数の原子核である球形の原子核を対象としたＲＰＡ計算が行われていたが、我々の計算により、一般的な原子核である変形核も扱えるようになった。我々は球形核の例として簡単な相互作用を用いて酸素１６を、変形核の例としてネオン２０を計算した。ＴＤＨＦ、メッシュ間隔依存性等を通じて解が正しく求まっている事を確認した。さらに現実的な核力であるスキルムＩＩＩを用いてテスト計算を行った。

In the present report, we show the method of calculating the 3D solution of RPA equation with BKN-like and Skyrme III interaction.
We summarize RPA eigenvalue equation expressed in the coordinate representation. [3)] We start with the time-dependent mean-field equation under an external potential $V_{\text{ext}}(\mathbf{r})$,

$$i\hbar\frac{\partial}{\partial t}\psi_i(\mathbf{r},t) = \{h[\rho(\mathbf{r},t)] + V_{\text{ext}}(\mathbf{r})\}\,\psi_i(\mathbf{r},t),$$
$$\rho(\mathbf{r},t) = \sum_{i\in occ} |\psi_i(\mathbf{r},t)|^2. \qquad (0\cdot1)$$

We assume that the mean-field Hamiltonian $h[\rho]$ depends on the wave functions ψ_i only through the density ρ. Spin and other internal coordinate are dropped for simplicity.

Static mean-field solution satisfies

$$h_0(\mathbf{r})\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r}), \qquad (0\cdot2)$$

where $h_0(\mathbf{r}) = h[\rho_0(\mathbf{r})]$ and $\rho_0(\mathbf{r}) = \sum_{i\in occ}|\phi_i(\mathbf{r})|^2$. To investigate small amplitude oscillation around the static mean-field solution, we put the wave function $\psi_i(\mathbf{r},t)$ as

$$\psi_i(\mathbf{r},t) = (\phi_i(\mathbf{r}) + \delta\psi_i(\mathbf{r},t))\,e^{-i\epsilon_i t/\hbar}. \qquad (0\cdot3)$$

*) Details of the present report will be shown in the paper[1)]

Putting it into Eq. (0·1), the zero-th order equation is nothing but the static mean-field equation (0·2). The first order equation reads

$$i\hbar\frac{\partial}{\partial t}\delta\psi_i(\mathbf{r},t) = \left(h_0(\mathbf{r}) - \epsilon_i\right)\delta\psi_i(\mathbf{r},t) + \left(\int d\mathbf{r}'\frac{\delta h(\mathbf{r})}{\delta\rho(\mathbf{r}')}\delta\rho(\mathbf{r}',t) + V_{\mathrm{ext}}(\mathbf{r})\right)\phi_i(\mathbf{r}). \tag{0·4}$$

The induced density $\delta\rho(\mathbf{r},t)$ is defined by $\rho(\mathbf{r},t) = \rho_0(\mathbf{r}) + \delta\rho(\mathbf{r},t)$ and is expressed in terms of $\delta\psi_i(\mathbf{r},t)$ as

$$\delta\rho(\mathbf{r},t) = \sum_{i\in occ}\phi_i^*(\mathbf{r})\delta\psi_i(\mathbf{r},t) + \phi_i(\mathbf{r})\delta\psi_i^*(\mathbf{r},t). \tag{0·5}$$

We use the Conjugate Gradient Method (CGM) to obtain the 3D solutions of RPA equation.

§1. Numerical Examples

1.1. *Light nuclei with simplified mean-field model*

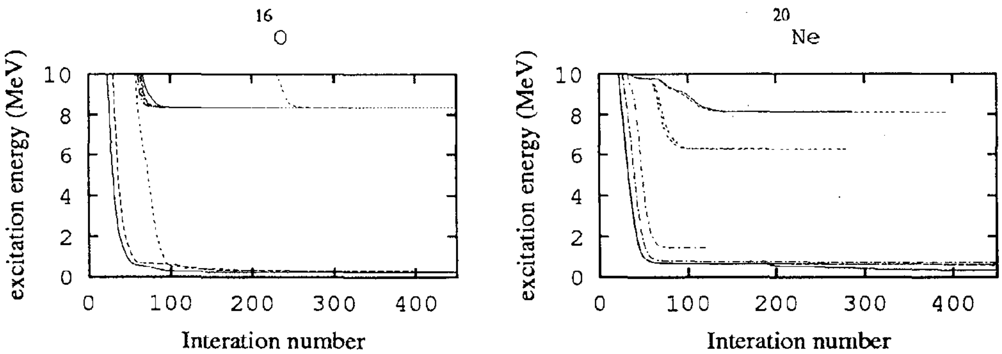

Fig. 1. Excitation energies of the nuclei ^{16}O and ^{20}Ne in the nuclear mean-field model with simplified interaction. Convergence of excitation energies is plotted against the iteration number in the conjugate gradient method.

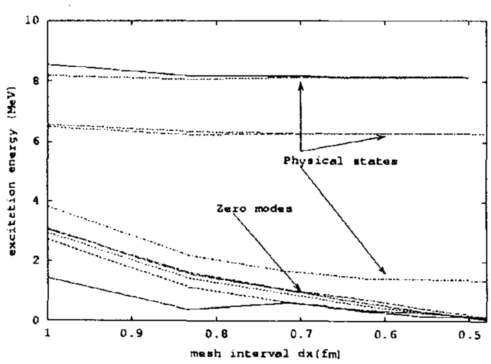

Fig. 2. Excitation energies of ^{20}Ne as a function of mesh interval dx in the nuclear mean-field model with simplified interaction. Convergence of excitation energies is plotted against the iteration number in the conjugate gradient method.

To demonstrate how the proposed method works, we first take an example for nuclear mean-field model with simplified interaction (BKN-like interaction). The following single-particle Hamiltonian [4] will be used

$$h[\rho] = -\frac{\hbar^2}{2m}\nabla^2 - \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^3 \tag{1·1}$$

with $t_0 = -1132.4$ MeV fm^3 and $t_3 = 23610.4$ MeV fm^6. For each spatial orbital, four nucleons are assumed to occupy. We apply our method for two nuclei, ^{16}O as an example of spherical nuclei, and ^{20}Ne for axially-deformed nuclei.

First the ground states are constructed with the imaginary time method. The ground state of ^{20}Ne nuclei shows prolate deformation with reflection symmetries in this model, although it is known that the octupole deformation appears in the calculation of variation after parity projection. [5]

In Fig. 1, we show convergence behavior of the RPA excitation energies in the conjugate gradient method. The grid points inside a box area of $10 \times 10 \times 10$ fm^3 with grid spacing of 0.5 fm are employed.

For ^{16}O nuclei, seven excited states corresponding to 3^- level are obtained at the excitation energy of 8 MeV. The next five levels at around 13 MeV composes 2^-. For ^{20}Ne nuclei, there is one level at very low excitation energy, at about 1.7 MeV. In both calculations, converged results are obtained with 100-200 iterations.

1.2. *Light nuclei with Skyrme III interaction*

Next, we calculate the low-lying states of the nuclei ^{16}O and ^{24}Mg with Skyme III interaction [2]. We omit the Coulomb terms and spin-orbit terms for simplicity. The mesh interval is 0.8fm in 6.4 fm $\times$ 6.4 fm $\times$ 6.4 fm rectangular box. Results are shown in Table 1.2. For ^{16}O nuclei, three zero-mode states (0.71 MeV) and seven excited states 3^- (12.58 $\sim$ 12.59 MeV) are obtained. We also calculate the low lying states of ^{24}Mg. The present results of the low lying states of ^{24}Mg are tentative, because the recutangular box size (6.4 fm $\times$ 6.4 fm $\times$ 6.4 fm) is small compared with the calculation with BKN-like interaction (10 fm $\times$ 10 fm $\times$ 10 fm).

Table I. Excitation energies and zero-mode energies of ^{16}O and ^{24}Mg with Skyrme III interaction

^{16}O		^{24}Mg	
levels	Excitation Energies(MeV)	levels	Excitation energies(MeV))
10	12.59		
9	12.59		
8	12.59	8	2.95
7	12.58	7	2.95
6	12.58	6	0.88
5	12.58	5	0.79
4	12.56	4	0.67
3	0.71	3	0.64
2	0.71	2	0.36
1	0.71	1	0.20

§2. Summary

We have presented a method to solve RPA equation directly in the three-dimensional grid representation. Representing RPA equation with grid points as particle indices, the conjugate gradient algorism works efficiently to obtain a few low-lying solutions.
BKN-like interaction and Skyrme III interaction is used. Now we are developing our method and making the program of HFB+QRPA with Skyrme interaction. We are going to apply our method to low-lying states of unstable nuclei.

References

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