GIANT RESONANCES FROM TDHF

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A method of calculating giant resonance strength functions using Time-Dependent Hartree-Fock techniques is described. An application to isoscalar giant monopole resonances in spherical nuclei is made, thus allowing a comparison between independent 1-, 2- and 3-Dimensional computer codes.

1. Theory of Calculating Giant Resonances

It is well-known that the Random Phase Approximation (RPA) is equivalent to Time-Dependent Hartree-Fock (TDHF) to first order in the density fluctuations from the static Hartree-Fock ground state.\(^1\) Therefore either approach may be used to calculate giant resonance states in nuclei. Historically, the RPA approach has been more popular, particularly working directly in the response function formalism.\(^2\) This has especially been the case because of computational complexity of TDHF calculations. Nevertheless, successful calculations of giant resonances using TDHF have been made, including those of Stringari and Vautherin,\(^3\) and Chomaz et al.\(^4\)

Recently there has been renewed interest in TDHF calculations of giant resonances,\(^5\) motivated by the better scaling to calculations with no assumptions on the spatial symmetry of the system. In such cases, it is the TDHF calculations which afford easier computation. Such relaxation of the symmetry assumptions are necessary for the proper calculation of deformed systems and resonances. It is also advantageous to use TDHF if one wishes to explore different effective interactions,
such as finite range forces. Once one has a static HF code it is, at least conceptually, trivial to program a TDHF code. Also, since RPA is a limiting case of TDHF, TDHF makes a natural choice for exploring beyond-RPA (nonlinear) approaches.

To calculate giant resonance states, the TDHF equations

\[ [\hat{h}(t), \rho(t)] = [\hat{h}_{HF}(t), \rho(t)] + \hat{h}_{ext}(t), \rho(t)] = i\hbar \dot{\rho} \]

are solved. This is achieved by solving the static HF equations

\[ [\hat{h}_{HF}, \rho] = 0 \]

for the initial single-particle wavefunction \( \{ \psi_i(t = 0) \} \). These are then evolved in time under the action of the unitary operator

\[ U(t, t + \Delta t) = e^{-i\hat{h}\Delta t/\hbar} \]

which is realised in the TDHF code by a Taylor expansion. The external perturbation used in the TDHF part consists of a spatial part with a time profile, which couples to the density

\[ \hat{h}_{ext}(t) = \int d^3r \rho(r, t) F(r) f(t) \]

Here, \( F(r) \) is the spatial form of the external perturbation, which determines the kind of resonance which gets excited. For the present purposes isoscalar monopole (ISGMR) excitations are considered and \( F(r) = W_0 \sum_i r_i^2 \), i.e. a harmonic oscillator potential acting on all particles. The function \( f(t) \) describes the time profile of the external perturbation, which is taken to be gaussian in the following calculations.

The physically interesting observable is the strength function, defined as

\[ S(E) = \sum_\nu |\langle \nu | F |0 \rangle|^2 = -\frac{1}{\pi} \text{Im} \int \frac{1}{\hbar - E + i\delta} F |0 \rangle \]

which is extracted from the TDHF calculation as the Fourier transform of the fluctuation of the expectation of the spatial operator inducing the excitation divided by the Fourier transform of the time profile of the external perturbation.

\[ S(\omega) = -\frac{1}{\pi} \text{Im} \int d^3r \frac{\delta(F(r, \omega))}{f(\omega)} \]

2. Practical Calculations

There are several issues to address when using TDHF to make practical calculations. Perhaps the most important involves boundary conditions. With TDHF calculations in coordinate space, one necessarily works in a box of finite size. If one imposes the condition that wavefunctions vanish at the edge of the box then one obtains a discrete excitation spectrum caused by particle flux unphysically bouncing off the boundary and interfering with the outgoing flux. In this case, the number of discrete states found depends upon the size of the box.
One remedy is to use a box so large that even after evolving for a long time, flux has yet to reach the boundary. Even seventeen years ago, a box size of 720 fm, with a rather fine mesh (0.2 fm) was feasible for a spherically-symmetric (1D) TDHF calculation of a resonance state. Nowadays, much larger boxes can be easily used, at least in 1D. One can think of this kind of calculation where the maximum time evolved ($t_{\text{max}}$) is sufficiently low that the boundary is not explored to be equivalent to a continuum calculation. Of course, the value of $t_{\text{max}}$ determines the energy resolution of the calculated strength function.

For axially-symmetric (2-D) or triaxial (3-D) codes, with which one can look at more general kinds of resonance, a smaller box size is desirable for timely computation. The discretisation that results in the response function is unphysical, yet the discrete peaks lie in the correct region, and the total (integrated) strength agrees with the continuum result. One may therefore perform a smoothing procedure on the discretised results, and compare to the smoothed continuum result. The smoothing process is physically reasonable when one considers the experimental resolution of giant resonance strength and the effect of spreading caused by higher-order effects not included in RPA. In this work a gaussian convolution is employed to smooth the strength function.

In figure 1, the comparison is made between a continuum and discrete calculation. The continuum calculation is made in a 1000 fm box, and the discrete calculation in a 45 fm box. These are ISGMR calculations in 1-D using a BKN-like force. In both cases time evolution proceeded in steps of $\Delta t = 1$ Mev/c up to a maximum time of $t_{\text{max}} = 2^{11}$ Mev/c. The width of the smoothing gaussian is 1 MeV. The unsmoothed discrete result is shown as a histogram, which reveals the energy resolution commensurate with the chosen value of $t_{\text{max}}$. With higher-dimensional TDHF calculations, one is not restricted to monopole resonances. However, since it is difficult to perform true continuum calculations in
Fig. 2. Isoscalar Giant Monopole resonance strength function using SkM* Skyrme interaction for $^{16}\text{O}$. The 1-D calculations corresponds to spherical symmetry, and the 2-D to axial symmetry. The 1-D calculation was performed in a 24fm radius spherical box, and the 2-D calculation in a cylinder of height 24fm and radius 24fm. Gaussian smoothing is used with a width of 1MeV.

In this case, it is instructive to compare the results of a monopole calculation from a code which allows deformation to a spherically symmetric calculation. This is a way to validate the independent 1-, 2- and 3-D codes. This is presented in figure 2. In this case a more realistic Skyrme force, SkM*, is used, also to calculate the ISGMR in $^{16}\text{O}$. The close agreement between the 1-D and 2-D calculations is encouraging and suggests that the approach of using modest box sizes along with smoothing is a feasible technique for calculating giant resonances with TDHF.

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