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Mass dispersions from giant dipole resonances using the Balian–Vénéroni variational approach

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Abstract

The Balian–Vénéroni variational approach has been implemented using a three-dimensional time-dependent Hartree–Fock (TDHF) code with realistic Skyrme interactions and used to investigate the mass dispersions from giant dipole resonances in ^{32}S and ^{132}Sn decaying through particle emission. The fluctuations obtained are shown to be quantitatively larger than the standard TDHF results.

1. Introduction

The time-dependent Hartree–Fock (TDHF) approach can be used to determine the expectation values of single-particle observables, such as fragment mass, in nuclear reactions and decays but is known to underestimate the fluctuations in these values [1]. This is due to the one-body nature of TDHF and the fact that it neglects two-body correlations [2]. This problem has previously been studied by Balian and Vénéroni [3–5], who derived a general variational theory for the determination of expectation values, correlations and fluctuations. They found that, given the state of a system described, at the time t_0, by the one-body density matrix, $\rho(t_0)$ (a Slater determinant satisfying $\rho^2 = \rho$), the fluctuation, ΔQ, in a one-body observable, Q, at some later time t_1, is given by

$$(\Delta Q_{\mathrm{BV}})^2|_{t_1} = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon^2} \mathrm{Tr}[\rho(t_0) - \sigma(t_0, \varepsilon)], \tag{1}$$

where $\sigma(t, \varepsilon)$ is a one-body density matrix related to $\rho(t)$ through the boundary condition

$$\sigma(t_1, \varepsilon) = \exp(\mathrm{i}\varepsilon Q)\rho(t_1)\exp(-\mathrm{i}\varepsilon Q), \tag{2}$$

and where the time evolution of $\rho(t)$ and $\sigma(t, \varepsilon)$ is given by the usual TDHF equation. This result is significantly different from the standard TDHF result

$$(\Delta Q_{\mathrm{TDHF}})^2|_{t_1} = \mathrm{Tr}[Q\rho(t_1)Q(1 - \rho(t_1))], \tag{3}$$

in that it depends on the initial time, t_0, with the final time, t_1, entering only through the boundary condition (2). The other key feature of this result is that it contains, through (2), the observable Q such that this method is specifically tuned to the determination of the fluctuation of the observable of interest.

A practical implementation of (1) requires that a Hartree–Fock calculation be performed to determine the initial state, $\rho(t_0)$. The system is then excited by a suitable external excitation, and a TDHF calculation performed from $t_0 \to t_1$ to determine $\rho(t_1)$. This is used to obtain $\sigma(t_1, \varepsilon)$ using (2), and a second TDHF calculation is then performed with the TDHF code run backwards, $t_1 \to t_0$, to obtain $\sigma(t_0, \varepsilon)$. The transformation (2) and the second TDHF calculation must be repeated for a range of values of ε to allow ΔQ_{BV} to be determined by extrapolation to $\varepsilon \to 0$.

The large number of computations required to evaluate (1) and the complexity of these calculations means that only a handful of calculations have been performed using this method and those calculations which have been performed have used simplified interactions and made use of symmetries (either spherical [6] or axial [7, 8]) to render the problems tractable. However, advances in computing power mean that this approach can now be implemented using fully three-dimensional TDHF codes with full Skyrme interactions [9–12].

We consider the mass dispersion in a bounded region of space around a giant dipole resonance (GDR), which decays through particle emission, and calculate the mass (number of nucleons) in the nucleus according to

$$N(R_c) = \sum_{m<\epsilon_F} \int \mathrm{d}\bar{r} |\phi_m(\bar{r})|^2 \theta(R_c - |\bar{r}|), \tag{4}$$

where R_c is the cutoff radius used to define the bounded region of space.

The nucleus was excited by multiplying the ground-state wavefunctions from the HF calculation by a dipole boost given by

$$B_D(x, y, z) = \exp(\mathrm{i}FC(A_x x + A_y y + A_z z)) \tag{5}$$

with

$$C = \sqrt{\frac{5}{4\pi}} \frac{1}{1 + \exp(\sqrt{x^2 + y^2 + z^2})} \tag{6}$$

and where, for protons, $F = 1/Z$, and for neutrons, $F = -1/(A - Z)$, where A is the atomic mass number of the nucleus under investigation and Z is its charge. A_x, A_y and A_z determine the strength of the boost applied to the nucleus.

Written in terms of the single particle wavefunctions (1) becomes [7]

$$(\Delta N_{\mathrm{BV}})^2|_{t_1} = A - \lim_{\varepsilon \to 0} \frac{f(\varepsilon)}{\varepsilon^2}, \qquad f(\varepsilon) = \sum_{m,n<\epsilon_F} \int \mathrm{d}\bar{r} |\langle \psi_m(t_0, \bar{r}, \varepsilon) | \phi_n(t_0, \bar{r}) \rangle|^2. \tag{7}$$

The wavefunctions $|\phi_n(t, \bar{r})\rangle$ were obtained from the results of a static Hartree–Fock calculation, whilst the wavefunctions $|\psi_m(t, \bar{r}, \varepsilon)\rangle$ result from the backward TDHF calculations and are related to the wavefunctions $|\phi_n(t, \bar{r})\rangle$ through the boundary condition

$$\psi(t_1, \bar{r}, \varepsilon) = \exp(\mathrm{i}\varepsilon\theta(R_c - |\bar{r}|))\phi(t_1, \bar{r}). \tag{8}$$

2. GDR in ^{32}S

We first consider a GDR in ^{32}S calculated using the Skyrme interaction with the SLy6 [13] parametrization. All calculations were performed in a cubic model space of size $32 \times 32 \times 32$ fm^3 discretized in steps of 1 fm. The initial HF calculation gave a ^{32}S ground state with a total binding energy of 260.36 MeV (compared with the experimental value of 271.78 MeV [14]) and a prolate deformation ($\beta_2 = 0.11$).

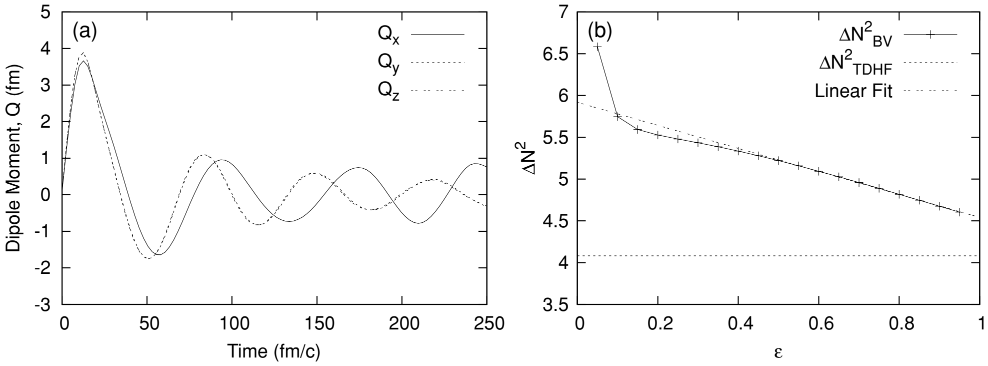

Figure 1. (a) The dipole moments (Q_x, Q_y and Q_z) plotted as a function of time for a GDR in ^{32}S. The difference between Q_x, Q_y and Q_z is consistent with a calculation using a prolate deformed ground state where x is the long axis. (b) $\Delta N^2_{\rm BV}$ plotted as a function of ε and extrapolated back to $\varepsilon = 0$. The standard TDHF result (calculated at t_1 and independent of ε) is shown for reference.

At the beginning of the dynamic calculation the ground-state wavefunctions were boosted in accordance with (5) and with $A_x = A_y = A_z = 112.5$ fm^{-1}. The simulation was allowed to run from an initial time $t_0 = 0$ fm/c to $t_1 = 250$ fm/c in steps of 0.2 fm/c. The emitted nucleons were reflected back from the boundary of the box and would, were the simulation allowed to run long enough, re-enter the region occupied by the de-exciting nucleus causing unphysical interactions. An analysis of the density and of $\langle N(R_c)\rangle$ as a function of time was used to verify that the number of nucleons in the nucleus had stabilized well in advance of the time t_1 and that the radiated flux had not had enough time to be reflected back and to interact with the nucleus. The problem of flux being reflected back from the boundary can be reduced by the use of absorbing boundary conditions [15]. However, absorbing boundary conditions cannot be used in this calculation since the evaluation of (1) requires the calculation to be reversible.

The dipole moments, Q_x, Q_y and Q_z, were obtained as a function of time using [11]

$$Q_i = \frac{(A-Z)Z}{A}\left(\langle x_i^P\rangle - \langle x_i^N\rangle\right), \tag{9}$$

where $i = 1, 2, 3$ denotes x, y and z, and $\langle x_i^P\rangle$ and $\langle x_i^N\rangle$ are the expectation values for position calculated using the proton and neutron single-particle states respectively. This is shown in figure 1(a). Due to the prolate deformation of the ^{32}S nucleus, the Q_y and Q_z values are identical and differ from the Q_x values. The periodicity of Q_x, Q_y and Q_z allows the excitation energies for the oscillations along each of the three primary axes to be estimated. In this instance we obtain, for Q_x, a period of ≈71 fm/c giving an excitation energy $E_x \approx$ 17.5 MeV and, for Q_y and Q_z, a period of ≈68 fm/c giving an excitation energy $E_y \approx E_z \approx$ 18.3 MeV.

The final state gave $\langle N\rangle = 26.65$ with $\Delta N^2_{\rm TDHF} = 4.08$ using $R_c = 8$ fm which represents the emission of ≈5 nucleons. R_c was chosen so that the bounded region fully enclosed the nucleus but omitted, as much as possible, the extended (or dissipated) components of the wavefunctions. We note from [2] that there is a theoretical upper limit on the mass dispersion that can be obtained using the standard TDHF approach

$$\left(\Delta N^2_{\rm TDHF}\right)_{\max} = \langle N\rangle\left(1 - \frac{\langle N\rangle}{A}\right), \tag{10}$$

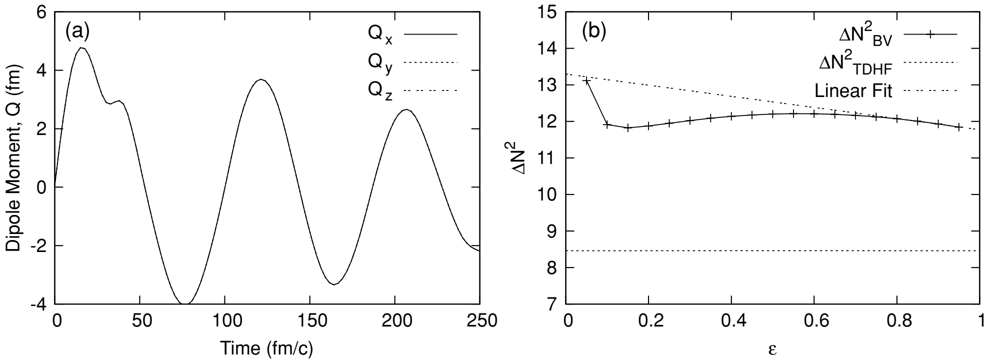

Figure 2. (a) The dipole moments (Q_x, Q_y and Q_z) plotted as a function of time for a GDR in ^{132}Sn. Q_x, Q_y and Q_z as a result of the ground state being spherical. The shoulder at ≈40 fm/c is a consequence of the 8 fm cutoff radius. (b) ΔN^2_{BV} plotted as a function of ε and extrapolated back to $\varepsilon = 0$. The standard TDHF result (calculated at t_1 and independent of ε) is shown for reference.

which gives, in this instance, $(\Delta N^2_{\mathrm{TDHF}})_{\mathrm{max}} = 4.46$. This limit has no physical basis and is due only to the assumptions of single-particle behaviour inherent in the TDHF approach. The transformation (8) was applied and the TDHF code was run in reverse. This process was repeated for ε values in the range $0.05 \leqslant \varepsilon \leqslant 0.95$ in steps of 0.05. At the end of each time-reversed calculation the fluctuation, $\Delta N^2_{\mathrm{BV}}(\varepsilon)$, was estimated using (7). These values were plotted (see figure 1(b)) and a straight line was fitted to the linear section of the graph and extended back to $\varepsilon = 0$ to obtain $\Delta N^2_{\mathrm{BV}} = 5.92$ which represents a 20% increase in ΔN using the BV approach compared with the standard TDHF result and exceeds the TDHF upper limit, $\left(\Delta N^2_{\mathrm{TDHF}}\right)_{\mathrm{max}}$. This graph is typical of those obtained using this approach and is linear for larger values of ε increasing asymptotically as $\varepsilon \to 0$ due to the $1/\varepsilon^2$ term in (1). Often, as in this case, the curve decreases for intermediate values of ε where the reduced value of ε means that the transformation (8) only has a small effect making the numerator in (1) numerically approximately zero and dominant over the ε^2 denominator.

This calculation has been repeated for $R_c = 8.5$ fm and $R_c = 9$ fm to test the stability of this approach. The results showed small changes in the observables consistent with the region of interest enclosing increasing amounts of the tails of the wavefunctions; however, the essential behaviour and trends remained unchanged as did the relative difference between the mass dispersions calculated using the TDHF and BV approaches.

3. GDR in ^{132}Sn

These calculations have been repeated for the doubly magic nucleus ^{132}Sn. All the calculations were carried out using the same model space and interaction as the ^{32}S calculation. The HF calculation produced a spherical ground state with a binding energy of 1099.71 MeV (compared with the accepted value of 1102.85 MeV [14]). The ground-state single-particle wavefunctions were boosted at the start of the TDHF calculation in accordance with (5) and with $A_x = A_y = A_z = 600$ fm^{-1}, and the calculation was run from $t_0 = 0$ fm/c to $t_1 = 250$ fm/c as in the previous calculation. The dipole moments were plotted as a function of time and are shown in figure 2(a). The graph shows Q_x, Q_y and Q_z to be identical as expected for a spherical nucleus and gives the periodicity of the dipole moments as ≈88 fm/c which corresponds to a resonance energy of ≈14.1 MeV. This is close to the experimentally measured value of 16.1(7) MeV [16].

The standard THDF calculation gave, at the time t_1, $\langle N\rangle = 121.02$ and $\Delta N^2_{\mathrm{TDHF}} = 8.46$ representing the emission of 11 nucleons. From (10) we obtain $\left(\Delta N^2_{\mathrm{TDHF}}\right)_{\max} = 10.07$. A series of transformations and time-reversed TDHF calculations were carried out as previously. The resulting graph, and linear fit, is shown in figure 2(b) which gives $\Delta N^2_{\mathrm{BV}} = 13.30$, which is significantly larger than $\left(\Delta N^2_{\mathrm{TDHF}}\right)_{\max}$ and represents a 25% increase in ΔN compared with the standard TDHF result.

4. Conclusions

The Balian–Vénéroni approach has been implemented for the first time using a three-dimensional TDHF code with the full Skyrme interaction. Calculations have been performed for GDRs in ^{32}S and ^{132}Sn and have demonstrated that the BV approach does produce quantitatively larger results for the fluctuations of one-body operators. This approach is now being applied to heavy-ion collisions.

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