Mass Dispersions from giant dipole resonances using the Balian-Vénérioni variational approach

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Abstract. The Balian-Vénérioni variational approach has been implemented using a 3-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.

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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 1-body nature of TDHF and the fact that it neglects 2-body correlations \[2\]. This problem has previously been studied by Balian and Vénéroni \[3, 4, 5\], 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 1-body density matrix, \(\rho(t_0)\) (a Slater determinant satisfying \(\rho^2 = \rho\)), the fluctuation, \(\Delta Q\), in a 1-body observable, \(Q\), at some later time \(t_1\), is given by

\[
(\Delta Q_{BV})_1^{t_1} = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon^2} \text{Tr} \left[ \rho(t_0) - \sigma(t_0, \varepsilon) \right],
\]

where \(\sigma(t, \varepsilon)\) is a 1-body density matrix related to \(\rho(t)\) through the boundary condition

\[
\sigma(t_1, \varepsilon) = \exp(i\varepsilon Q) \rho(t_1) \exp(-i\varepsilon Q),
\]

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

\[
(\Delta Q_{TDHF})_1^{t_1} = \text{Tr} \left[ Q\rho(t_1) Q (1 - \rho(t_1)) \right],
\]

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 \(\varepsilon\) to allow \(\Delta Q_{BV}\) 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, modern advances in computing power mean that this approach can now be implemented using fully 3-dimensional TDHF codes with full Skyrme interactions \[9, 10, 11, 12\].

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

\[
N(R_c) = \sum_{m < \epsilon_F} \int d\bar{r} \left| \phi_m(\bar{r}) \right|^2 \theta(R_c - |\bar{r}|),
\]
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

\[
B_D (x, y, z) = \exp \left( iFC (Ax x + A_y y + A_z z) \right)
\]  

(5)

with

\[
C = \sqrt{\frac{5}{4\pi^2}} \frac{1}{1 + \exp \left( \frac{1}{\sqrt{x^2 + y^2 + z^2}} \right)}
\]  

(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]

\[
(\Delta N_{BV})^2 \bigg|_{t_1} = A - \lim_{\varepsilon \to 0} \frac{f(\varepsilon)}{\varepsilon^2},
\]

(7)

\[
f(\varepsilon) = \sum_{m,n<\varepsilon} \int d\vec{r} \left| \langle \psi_m (t_0, \vec{r}, \varepsilon) | \phi_n (t_0, \vec{r}) \rangle \right|^2.
\]

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

\[
\psi (t_1, \vec{r}, \varepsilon) = \exp \left( i\varepsilon \theta (R_c - |\vec{r}|) \right) \phi (t_1, \vec{r}).
\]

(8)

2. GDR in \(^{32}\text{S}\)

We consider first a GDR in \(^{32}\text{S}\) calculated using the Skyrme interaction with the SLy6 [13] parametrisation. All calculations were performed in a cubic model space of size \(32 \times 32 \times 32 \text{ fm}^3\) discretised in steps of 1 fm. The initial HF calculation gave a \(^{32}\text{S}\) 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 \((\beta_2 = 0.11)\).

At the beginning of the dynamic calculation the ground state wavefunctions were boosted in accordance with (5) and with \( A_x = A_y = A_z = 112.5 \text{ fm}^{-1} \). The simulation was allowed to run from an initial time \( t_0 = 0 \text{ fm/c} \) to \( t_1 = 250 \text{ fm/c} \) 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 stabilised 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 increasing the size of the model space or through the use of absorbing boundary conditions [15]. However, absorbing boundary conditions cannot be used in this
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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 \(Q_x\) and \(Q_y\) and \(Q_z\) is consistent with a calculation using a prolate deformed ground state where \(x\) is the long axis. (b) \(\Delta N_{BV}^2\) plotted as a function of \(\epsilon\) and extrapolated back to \(\epsilon = 0\). The standard TDHF result (calculated at \(t_1\) and independent of \(\epsilon\)) is shown for reference.

calculation since the evaluation of (1) requires the calculation to be reversible. Increasing the size of the model space is possible but would increase the time taken by the TDHF calculations which is particularly problematic for this application where the TDHF code must already be run many times during each calculation.

The dipole moments, \(Q_x\), \(Q_y\) and \(Q_z\), were obtained as a function of time using

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

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 \(Q_z\) allow 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 \(\approx 71\) fm/c giving an excitation energy \(E_x \approx 17.5\) MeV and, for \(Q_y\) and \(Q_z\), a period of \(\approx 68\) 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 \(\Delta N_{TDHF}^2 = 4.08\) using \(R_c = 8\) fm which represents the emission of \(\approx 5\) 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 the relative simplicity of the observable \(N \langle R_c \rangle\) means that there is a theoretical upper limit on the mass dispersion that can be obtained using the standard TDHF approach

\[
\left( \Delta N_{TDHF}^2 \right)_{max} = \langle N \rangle \left( 1 - \frac{\langle N \rangle}{A} \right),
\]

which gives, in this instance, \(\left( \Delta N_{TDHF}^2 \right)_{max} = 4.46\). 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 \(\epsilon\) values in the range \(0.05 \leq \epsilon \leq 0.95\) in steps of 0.05. At the end of each time-reversed calculation the fluctuation, \(\Delta N_{BV}^2(\epsilon)\), 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 \( \Delta N^2_{BV} = 5.92 \) which represents a 20\% increase in \( \Delta N \) using the BV approach compared with the standard TDHF result and exceeds the TDHF upper limit, \( (\Delta N^2_{TDHF})_{max} \). This graph is typical of those obtained using this approach and is linear for larger values of \( \varepsilon \) 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 \( \varepsilon \) where the reduced value of \( \varepsilon \) means that the transformation (8) only has a small effect making the numerator in (1) numerically approximately zero and dominant over the \( \varepsilon^2 \) 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 \(^{132}\text{Sn}\)

These calculations have been repeated for the doubly magic nucleus \(^{132}\text{Sn}\). All the calculations were carried out using the same model space and interaction as the \(^{32}\text{S}\) calculation. The HF calculation produced an 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 \( \approx 88 \) fm/c which corresponds to a resonance energy of \( \approx 14.1 \) 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 \( \Delta N^2_{TDHF} = 8.46 \) representing the emission of 11 nucleons. From (10) we obtain \( (\Delta N^2_{TDHF})_{max} = 10.07 \). A series of transformations and time-reversed TDHF calculations were carried out as previously. The resulting graph, and linear fit, are shown in figure 2(b) which gives \( \Delta N^2_{BV} = 13.30 \) which is significantly larger than \( (\Delta N^2_{TDHF})_{max} \) and represents a 25\% increase in \( \Delta N \) compared with the standard TDHF result.

4. Conclusions

The Balian-Véronéroni approach has been implemented for the first time using a 3-dimensional TDHF code with the full Skyrme interaction. Calculations have been performed for GDRs in \(^{32}\text{S}\) and \(^{132}\text{Sn}\) and have demonstrated that the BV approach does produce quantitatively larger results for the fluctuations of 1-body operators. This
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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. $Q_x$ and $Q_y$ and $Q_z$ as a result of the ground state being spherical. The shoulder at $\approx 40 \text{ fm/c}$ is a consequence of the 8 fm cutoff radius. (b) $\Delta N_{BV}^2$ plotted as a function of $\varepsilon$ and extrapolated back to $\varepsilon = 0$. The standard TDHF result (calculated at $t_1$ and independent of $\varepsilon$) is shown for reference.

approach is now being applied to heavy ion collisions.

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References