

# Mass Distributions Beyond TDHF

J. M. A. Broomfield and P. D. Stevenson

*Department of Physics, University of Surrey, Guildford, Surrey, GU2 7XH, UK*

**Abstract.** The mass distributions for giant dipole resonances in  $^{32}\text{S}$  and  $^{132}\text{Sn}$  decaying through particle emission and for deep-inelastic collisions between  $^{16}\text{O}$  nuclei have been investigated by implementing the Balian-Vénéroni variational technique based upon a three-dimensional time-dependent Hartree-Fock code with realistic Skyrme interactions. The mass distributions obtained have been shown to be significantly larger than the standard TDHF results.

**Keywords:** Balian-Vénéroni, TDHF, Mass Distributions, Giant Dipole Resonance, Nuclear Collision

**PACS:** 21.60.Jz, 24.30.Cz, 24.60.-k, 25.70.-z

## INTRODUCTION

The standard time-dependent mean-field methods used in nuclear physics (namely the time-dependent Hartree-Fock (TDHF) approach and its derivatives [1, 2]) have been successfully used to determine the expectation values for single-particle observables, such as fragment mass, in nuclear reactions and decays but severely underestimate the fluctuations in these values [3]. This was first observed by Davies et al. [4] in 1978 who performed TDHF calculations to investigate the full-width-half-maximum of the mass of the projectile-like fragment for the heavy-ion reactions  $^{84}\text{Kr}+^{208}\text{Pb}$  ( $E_{lab}=494$  MeV) and  $^{84}\text{Kr}+^{209}\text{Be}$  ( $E_{lab}=600$  MeV) and found that they underestimated the experimental results by about an order of magnitude. It is now well known that the TDHF method underestimates the fluctuation of any single-particle operator, or in fact the expectation value of any many-body operator, except the energy [3]. This is a consequence of the central assumption of the methods; the approximation of the full many-body state of the system as a Slater determinant, evolving in a mean-field, neglecting explicit two-body correlations.

This problem was studied by Balian and Vénéroni [5, 6, 7] in the 1980's, who produced a general variational theory optimised to the determination of the expectation values and fluctuations for arbitrary single-particle operators whilst the state of the system is given by a single Slater determinant. They found that, for a system described, at the time  $t_0$ , by the one-body density matrix,  $\rho(t_0)$ , the expectation value for the single-particle observable  $\hat{Q}$ , at the later time  $t_1$ , is given by  $\langle Q \rangle|_{t_1} = \text{Tr}[\hat{Q}\rho(t_1)]$ , in keeping with the usual TDHF approach, whilst the distribution, or standard deviation,  $\Delta Q$ , is given by

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

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

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

The time evolution of  $\rho(t)$  and  $\sigma(t, \varepsilon)$  is given by the usual TDHF equation. This latter result differs from the usual TDHF result

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

in that it depends explicitly on the initial time,  $t_0$ , with the final time,  $t_1$ , entering through the boundary condition (2). The boundary condition (2) also contains the operator  $\hat{Q}$  such that this approach is specifically tuned to the determination of  $\Delta Q$ . It has also been shown by Dasso [8] that, for simple operators such as mass (or, equivalently, charge), the single-particle nature of TDHF leads to an unphysical upper limit on the mass distributions that can be obtained from (3). It can be shown that

$$(\Delta N_{TDHF}^2)_{MAX} \Big|_t = \langle N(R_c) \rangle_t \left( 1 - \frac{\langle N(R_c) \rangle_t}{A} \right), \quad (4)$$

where  $A$  is the total number of nucleons in the system.

Solving (1) requires that a Hartree-Fock calculation be performed to determine the initial state,  $\rho(t_0)$  followed by a suitable instantaneous excitation of the system and a TDHF calculation from  $t_0$  to  $t_1$  to determine  $\rho(t_1)$ . The transformation (2) gives  $\sigma(t_1, \varepsilon)$  and a second TDHF calculation must then be performed, backwards from  $t_1$  to  $t_0$ , to obtain  $\sigma(t_0, \varepsilon)$ . These latter steps must be repeated for a range of values of  $\varepsilon$  to allow  $\Delta Q_{BV}$  to be determined from the extrapolation of  $\varepsilon$  to 0.

The large number of calculations required to evaluate (1), and their complexity, means that only a handful of calculations were performed using this method and those calculations used simplified interactions and symmetries (either spherical [9], or axial [10, 11]) to make the problems solvable. However, advances in computing power mean that this approach can now be implemented using fully three-dimensional TDHF codes with full Skyrme interactions [12, 13, 14, 15, 16].

Written in terms of the occupied single-particle states (1) becomes [10]

$$(\Delta N_{BV})^2 \Big|_{t_1} = A - \lim_{\varepsilon \rightarrow 0} \frac{f(\varepsilon)}{\varepsilon^2}, \quad (5)$$

where

$$f(\varepsilon) = \sum_{m,n < \varepsilon_F} \int d\vec{r} |\langle \psi_m(\vec{r}, t_0, \varepsilon) | \phi_n(\vec{r}, t_0) \rangle|^2, \quad (6)$$

and  $A$  is the number of nucleons in the system. The wavefunctions  $|\psi_m(\vec{r}, t, \varepsilon)\rangle$  are the wavefunctions from the backwards TDHF calculations and are related to the wavefunctions from the forwards calculations,  $|\phi_n(\vec{r}, t)\rangle$ , through the boundary condition

$$\psi(\vec{r}, t_1, \varepsilon) = \exp(i\varepsilon\hat{Q})\phi(\vec{r}, t_1). \quad (7)$$

In these calculations, as in Bonche and Flocard's earlier work [11], the wavefunctions  $|\phi_n(\vec{r}, t_0)\rangle$  were obtained by evolving the TDHF equations forwards and then backwards

without the transformation (7) being applied. This approach ensures that all the single-particle wavefunctions used in evaluating (5) result from the same number of computations and has been found to significantly reduce systematic numerical errors [16] allowing the extrapolation required in (5) to be extended to significantly smaller values of  $\epsilon$ .

We consider the mass distribution in a bounded region of space around a nucleus and calculate the mass (number of nucleons) in the nucleus according to

$$\langle N(R_c) \rangle_t = \sum_{m < \epsilon_F} \int d\bar{r} |\phi_m(\bar{r}, t)|^2 \theta(R_c - |(\bar{r} - \bar{r}_{CM})|), \quad (8)$$

where  $R_c$  is the cut-off radius used to define the bounded region of space and  $\bar{r}_{CM}$  is the centre-of-mass location of the nucleus.

### GDRS IN $^{32}\text{S}$ AND $^{132}\text{SN}$

We consider first a giant dipole resonance (GDR) in the deformed nucleus  $^{32}\text{S}$  decaying through particle emission. The calculations were all performed in a cubic spatial box of size  $32 \times 32 \times 32$  fm discretised in steps of 1 fm. The static Hartree-Fock calculation was carried out using the SLy6 parametrisation [17] of the Skyrme interaction and produced a ground state with prolate deformation ( $\beta_2 = 0.11$ ). A dipole excitation was induced by acting on each wavefunction at  $t = 0$  with a boost

$$B_D(x, y, z) = \exp(iFC(A_x x + A_y y + A_z z)), \quad (9)$$

where

$$C = \sqrt{\frac{5}{4\pi}} \frac{1}{1 + \exp\left(\sqrt{x^2 + y^2 + z^2}\right)}, \quad (10)$$

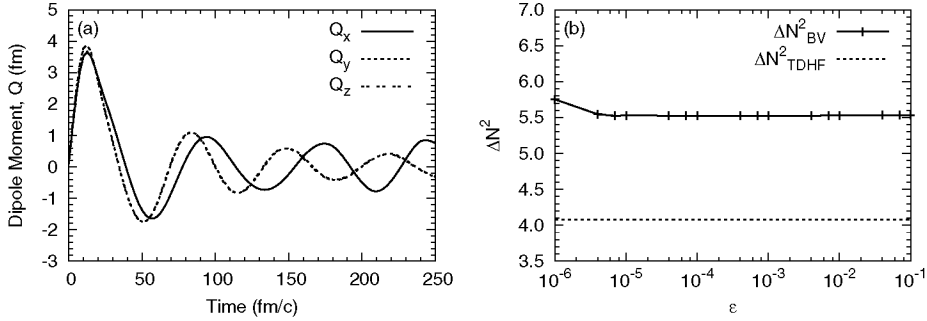
is a spatial cut-off, and where, for protons,  $F = 1/Z$ , and for neutrons,  $F = -1/(A - Z)$ , where  $A$  is the nucleus' atomic mass and  $Z$  is its charge. The  $A_x$ ,  $A_y$  and  $A_z$  parameters determine the strength of the applied boost and were set to  $112.5 \text{ fm}^{-1}$ .

In the present calculation, the system was evolved forward in time until  $t_1 = 250$  fm/c. Dirichlet boundary conditions were used at the edge of the spatial box, where the wavefunctions disappear. These lead to spurious reflections for sufficiently large  $t_1$  so the value chosen for  $t_1$  had to be kept sufficiently small, whilst ensuring that  $\langle N(R_c) \rangle_t$  had stabilised following the prompt de-excitation of the resonance by particle emission.

The dipole moments,  $Q_x$ ,  $Q_y$  and  $Q_z$ , as a function of time, are shown in figure 1(a), in accordance with [14]

$$Q_i = \frac{(A - Z)Z}{A} (\langle x_i^P \rangle - \langle x_i^N \rangle), \quad (11)$$

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. The prolate deformation of the  $^{32}\text{S}$  nucleus (with  $x$  the long-axis) results in  $Q_y$  and  $Q_z$  being



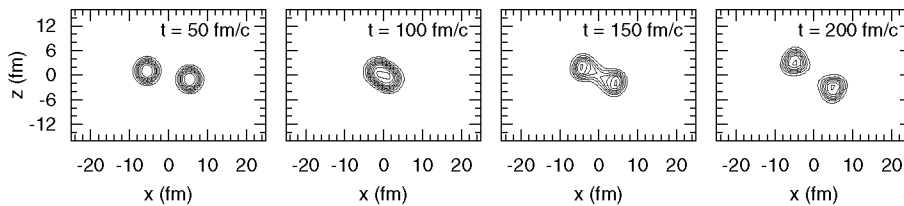
**FIGURE 1.** (a) The dipole moments  $Q_i$  ( $i=x, y, z$ ) as a function of time, for a GDR in  $^{32}\text{S}$ . The differences between  $Q_x$  and  $Q_y$  and  $Q_z$  are consistent with a prolate deformed ground state where  $x$  is the long axis. (b)  $\Delta N_{BV}^2$  as a function of  $\epsilon$ .  $\Delta N_{BV}^2$  is given by extrapolation to  $\epsilon \rightarrow 0$ . The  $x$ -axis has a logarithmic scale to emphasise that the values obtained are independent of  $\epsilon$  across several orders of magnitude. The standard TDHF result (calculated at  $t_1$  and independent of  $\epsilon$ ) is shown for reference.

identical whilst  $Q_x$  differs. The periodicity of  $Q_x$ ,  $Q_y$  and  $Q_z$  provides an estimate of the excitation energy for the oscillations along each of the three primary axes. For  $Q_x$ , a period of  $\approx 71$  fm/c is found, giving an excitation energy  $E_x \approx 17.5$  MeV and, for  $Q_y$  and  $Q_z$ , a period of  $\approx 68$  fm/c gives an excitation energy  $E_y \approx E_z \approx 18.3$  MeV.

Following the decay of the GDR in  $^{32}\text{S}$ , it was found that  $\langle N \rangle = 26.65$  and  $\Delta N_{TDHF}^2 = 4.08$  (using  $R_c = 8$  fm) representing 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 radiated components of the wavefunctions. From (4) we obtain  $(\Delta N_{TDHF}^2)_{MAX} = 4.46$ . Following evolution to  $t_1$ , the transformation (7) was applied and the system evolved back to  $t_0$  for  $\epsilon$  values down to  $10^{-6}$ . After each calculation the fluctuation,  $\Delta N_{BV}^2(\epsilon)$ , was calculated using (5) and the results plotted and extrapolated back to  $\epsilon = 0$ . The results are shown in figure 1(b), giving  $\Delta N_{BV}^2 = 5.52$  which represents a 16% increase in  $\Delta N$  and exceeds the TDHF upper limit,  $(\Delta N_{TDHF}^2)_{MAX}$ . Calculations were also performed for  $R_c = 8.5$  fm and  $R_c = 9$  fm and showed only small changes in the results consistent with the bounded region enclosing increasing amounts of the wavefunctions tails.

The calculations were repeated for the doubly magic nucleus  $^{132}\text{Sn}$  using the same spatial box and interaction as in the  $^{32}\text{S}$  calculation. An initial dipole boost (9) with  $A_x = A_y = A_z = 600$  fm $^{-1}$  induced the resonance, which was evolved from  $t_0 = 0$  fm/c to  $t_1 = 250$  fm/c as before. The dipole moments show a periodicity of  $\approx 88$  fm/c corresponding to a resonance energy of  $\approx 14.1$  MeV which is close to the experimental value of 16.1 (7) MeV [18].

The standard TDHF calculation gave, at the time  $t_1$ ,  $\langle N \rangle = 121.02$  and  $\Delta N_{TDHF}^2 = 8.46$  representing the emission of 11 nucleons. From (4) we obtain  $(\Delta N_{TDHF}^2)_{MAX} = 10.07$ . Again, the Balian-Vénéroni transformation was applied for different values of  $\epsilon$ , the extrapolation to  $\epsilon = 0$  yielding  $\Delta N_{BV}^2 = 11.29$ , representing a 14% increase in  $\Delta N$  compared with the standard TDHF result.



**FIGURE 2.** Density contour plots showing a deep inelastic collision ( $E_{CM} = 128$  MeV) between two  $^{16}\text{O}$  nuclei for an impact parameter  $b = 2$  fm ( $l \approx 14 \hbar$ ).

## $^{16}\text{O}+^{16}\text{O}$ COLLISIONS ( $E_{CM} = 128$ MEV)

The main application for this method will be heavy-ion collisions as mentioned in the introduction. As a test case using light nuclei, collisions between  $^{16}\text{O}$  nuclei at  $E_{CM} = 128$  MeV have been studied.

The dynamic calculations were carried out in a rectangular space of size  $50 \times 32 \times 50$  fm except the head-on calculation where, taking advantage of the symmetry a spatial box of size  $50 \times 32 \times 32$  fm was used. The nuclei were initially positioned at  $(\pm 10, 0, \pm b/2)$  where  $b$  is the impact parameter and the nuclei collide in the  $x$ - $z$  plane.

Calculations were performed for impact parameters  $b = 0, 1, 2$  and 4 fm. Contour plots showing the densities during a collision for  $b = 2$  fm are shown in figure 2. The calculations were run for 2000 timesteps (400 fm/c) until the scattered nuclei had clearly separated but before they reached the edge of the box. The exception was the calculation for  $b = 4$  fm where the nuclei fused with the compound nucleus decaying through particle emission and where the runtime was extended to 2000 fm/c to allow the excited compound nucleus time to decay and check that it did not undergo a delayed fission.

The mass distributions obtained from these calculations using the TDHF and BV approaches are given in table 1, showing the large increase (at least doubling in each case) of  $\Delta N$  in the BV case over TDHF.

**TABLE 1.** Mass distributions calculated for  $^{16}\text{O}+^{16}\text{O}$  at  $E_{CM} = 128$  MeV using the standard TDHF approach and the Balian-Vénéroni variational approach for a range of impact parameters (the equivalent angular momentums are also given).

$b$ (fm)	$l$ ( $\hbar$ )	$\langle N(R_c = 8 \text{ fm}) \rangle_{t_i=400 \text{ fm/c}}$	$\Delta N_{\text{TDHF}}$	$(\Delta N_{\text{TDHF}})_{\text{MAX}}$	$\Delta N_{\text{BV}}$	Change
0	0.00	14.96	1.37	2.82	2.84	+107%
1	7.02	14.90	1.38	2.82	2.87	+108%
2	14.05	14.83	1.44	2.82	3.17	+120%
4	28.10	25.10*	2.06	2.33	-†	-

\* After 2000 fm/c. The  $^{16}\text{O}$  nuclei fused to form an excited compound nucleus which decays by particle emission. The reduced value of  $(\Delta N_{\text{TDHF}})_{\text{MAX}}$  for  $b = 4$  fm is a consequence of the dependence of (4) on both the number of nucleons in the system,  $A$ , and on the number of nucleons in the nucleus of interest,  $\langle N(R_c) \rangle_l$ .

† Not calculated due to the extended runtime required for the compound nucleus to decay and to ensure that the compound nucleus did not fission.

## CONCLUSIONS

The Balian-Vénéroni approach has been implemented using a three-dimensional TDHF code with the full Skyrme interaction and calculations have been performed for GDR's in  $^{32}\text{S}$  and  $^{132}\text{Sn}$  and for collisions of  $^{16}\text{O}$  nuclei. The BV approach produces mass distributions which are quantitatively larger than those obtained using the usual TDHF approach. We are continuing to apply this approach to heavy ion collisions with a view towards performing calculations for heavier systems to allow a comparison with experimental data.

## ACKNOWLEDGMENTS

The authors are pleased to acknowledge the assistance of, and discussions with, Ph. Chomaz, R. Balian, J. S. Al-Khalili and E. B. Suckling. This work was supported by the UK Science and Technology Facilities Council (STFC).

## REFERENCES

1. D. Lacroix, S. Ayik and Ph. Chomaz, *Prog. Part. and Nucl. Phys* **52**, 497-563 (2004)
2. S. Ayik, *Phys. Lett. B* **658**, 174-179 (2008)
3. P.-G. Reinhard, R. Y. Cusson and K. Goeke, *Nuc. Phys. A* **398**, 141-188 (1983)
4. K. T. R. Davies V. Maruhn-Rezwani et al., *Phys. Rev. Lett.* **41**, 632-635 (1978)
5. R. Balian and M. Vénéroni, *Annals of Physics* **281**, 65-142 (2000)
6. R. Balian and M. Vénéroni, *Annals of Physics* **187**, 29-78 (1988)
7. R. Balian and M. Vénéroni, *Annals of Physics* **216**, 351-430 (1992)
8. C. H. Dasso, T. Døssing and H. C. Pauli, *Z. Physik A* **289**, 395-398 (1979)
9. T. Troudet and D. Vautherin, *Phys. Rev. C* **31**(1), 278-279 (1985)
10. J. B. Marston and S. E. Koonin, *Phys. Rev. Lett.* **54**(11), 1139-1141 (1985)
11. P. Bonche and H. Flocard, *Nucl. Phys. A* **437**, 189-207 (1985)
12. J. A. Maruhn, P.-G. Reinhard et al., *Phys. Rev. C* **74**, 027601 (2006)
13. A. S. Umar and V. E. Oberacker, *Phys. Rev. C* **74**, 024606 (2006)
14. C. Simenel, Ph. Chomaz and G. de France, *Phys. Rev. C* **76**, 024609 (2007)
15. T. Nakatsukasa and K. Yabana, *Nucl. Phys. A* **788**, 349c-354c (2007)
16. J. M. A. Broomfield and P. D. Stevenson, *J. Phys. G* **35**, 095102 (2008)
17. E. Chabanat, P. Bonche et al., *Nucl. Phys. A* **635**, 231-256 (1998)
18. P. Adrich, A. Klimkiewicz et al., *Phys. Rev. Lett.* **95**, 132501 (2005)