Testing a Variational Method for Fluctuations

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Abstract. A variational approach for many-body systems due to Balian and Vénéroni, which goes beyond the Hartree-Fock mean field, has been implemented in the case of nuclear Skyrme effective interactions used in examining large amplitude collective motion. An evaluation of the numerical issues involved with the method is presented, in which it is found that the effect of model parameters is generally under control, but long-time running leads to unphysical results.

1. Introduction
A variational approach which is optimised to reproduce the expectation values of two-body observables while retaining a one-body density matrix representation of the physical state was proposed by Balian and Vénéroni [1, 2, 3] and implemented [4, 5, 6] in the 1980s. The first implementations in nuclear collisions and resonances necessarily featured restrictions in the realisation due to computational limitations. Since then, Time-Dependent Hartree-Fock (TDHF) capabilities, upon which the Balian-Vénéroni technique relies, have become more sophisticated [7, 8, 9, 10]. Recently, we have revisited the approach and implemented it in a symmetry-unrestricted way with full Skyrme forces [11, 12, 13, 14, 15].

Despite the fact that fuller calculations are now computationally feasible, there are still many numerical issues of concern, and some of these are addressed in the present paper.

2. The Method
The key point behind the Balian-Vénéroni approach is that the variational principle should include in it any observable whose expectation value is to be optimised, and that one can do this with two-body observables, even if one uses one-body density matrices as the trial states. One still improves upon those variational principles in which such considerations are not made.

The two-body observable studied in our work is the fluctuation of the number operator, which is applied to counting the number of nucleons in a spatial region identified with one nucleus or fragment. We have considered the excitation and subsequent decay of giant resonances, and heavy ion collisions of a deep inelastic and a fusion-evaporation nature. The application of the Balian-Vénéroni procedure leads to an expression for the fluctuation of a one-body observable, $\hat{N}$, of the form

$$\Delta N^2(t_1) = \lim_{\epsilon \to 0} \frac{1}{2\epsilon^2} \text{Tr} \left[ (\rho(t_0) - \sigma(t_0))^2 \right]$$

(1)

where

$$\sigma(t_1) = e^{i\epsilon \hat{N}} \rho(t_1) e^{-i\epsilon \hat{N}}.$$  

(2)
Figure 1. $\Delta N^2(t_1)$ plotted as a function of $\epsilon$ for different values of the cutoff radius $R_c$. The TDHF results, calculated at $t_1$ (and independent of $\epsilon$) are shown for comparison.

The implementation of this approach consists of running a TDHF code from $t = 0$ to some finite end time $t_1$, apply the transformation (2) to only the remnant nucleus and not any dripped flux, run the code backwards to time $t = 0$ and evaluate (1). The procedure should be performed for a series of values of $\epsilon$ and extrapolated back to $\epsilon = 0$.

Various numerical issues arise in this process, the TDHF process being a rather computationally intensive one. It is important to ensure that the process of extrapolation of $\epsilon$ is as well-controlled as possible, that the transformation is applied to only the daughter nucleus, that parameters related to the spatial box in which the wavefunctions are represented, and the choice of end time are all as free from giving ambiguous physical results as possible. We explore these issues in the next section.

3. Results
All examples given here use as a test case the excitation of a large-amplitude giant dipole resonance in $^{32}$S. As a check of the stability of results as a function of parameters in the procedure, we look at the dependence on the cutoff radius $R_c$ inside which we consider the daughter nucleus to exist. This has previously been reported in less detail [15]. In figure 1, values of the number fluctuation are given for different cutoff radius sizes; 8fm, 8.5fm and 9fm from the centre of the daughter nucleus. The number fluctuation does change as a function of cutoff radius, as more of the tail of the nuclear wavefunction is included, but only in the same way that there is an increase in TDHF, leaving the percentage change in fluctuation between the TDHF and the (better) Balian-Véroni answer quite constant. One should run the code in a region where the sensitivity to cutoff radius is smallest.

In figure 1, the range of sizes of $\epsilon$ for which a linear extrapolation can be made is clear. The range is actually quite large, but one must be careful. The flat region is only so large when one evaluates the $\rho(t_0)$ in (1) by evolving the system forward in time to $t_1$ and then backwards to
4.3 Application of the Balian-Vénéroni approach to a GDR in 32S 61

Figure 4.9 is an extended version of figure 4.3.

...interference and interactions with the nucleus and other emitted flux.

Figure 2. A schematic view of the radial dependence (plotted outwards from the centre-of-mass of the nucleus) of the step function, $\chi_1(|\vec{r} - \vec{r}_{CM}|, R_c, R_t)$, and the linear function, $\chi_2(|\vec{r} - \vec{r}_{CM}|, R_c, R_t)$, used in place of the theta function.

Table 1. The dependence of $\langle N \rangle$, $\Delta N_{TDHF}$ and $\Delta N_{BV}$ on the form of the spatial cutoff function (and on $R_c$ and $R_t$). The function $\theta(R_c - |\vec{r} - \vec{r}_{CM}|)$ provides a sharp cutoff at $r = R_c$. The function $\chi_1(r, R_c, R_t)$ provides a cutoff which decreases in steps whilst the function $\chi_2(r, R_c, R_t)$ provides a linear cutoff. $R_t$ controls the sharpness of the cutoff functions $\chi_1(r, R_c, R_t)$ and $\chi_2(r, R_c, R_t)$ as shown schematically in figure 2. These results values were all calculated for $t_1 = 250$ fm/c using the SLy6 parameterisation of the Skyrme force.

|          | $R_c$ (fm) | $R_t$ (fm) | $\langle N \rangle|_{t_1}$ | $\Delta N_{TDHF}|_{t_1}$ | $\Delta N_{BV}|_{t_1}$ | Change  |
|----------|------------|------------|-----------------------------|--------------------------|-------------------------|---------|
| $\theta(R_c - r)$ | 8.0        | -          | 26.6366                    | 2.0218                   | 2.3506(0)               | +16%    |
| $\chi_1(r, R_c, R_t)$ | 8.0        | 0.25       | 26.6244                    | 2.0234                   | 2.3346(0)               | +15%    |
| $\chi_2(r, R_c, R_t)$ | 8.0        | 0.25       | 26.6295                    | 2.0226                   | 2.3387(0)               | +16%    |
| $\theta(R_c - r)$ | 9.0        | -          | 26.8975                    | 1.9875                   | 2.2924(0)               | +15%    |
| $\chi_1(r, R_c, R_t)$ | 9.0        | 0.25       | 26.9044                    | 1.9877                   | 2.2689(0)               | +14%    |
| $\chi_2(r, R_c, R_t)$ | 9.0        | 0.25       | 26.8951                    | 1.9885                   | 2.2758(0)               | +14%    |

$t_0$ without performing the Balian-Vénéroni transformation on it. This ensures that systematic errors are eliminated from the process of finding the difference between two small values in (1).

The form of the spatial cutoff in figure 1 is a sharp step function. It is not obvious that this is the best choice. We have examined other function, such as a multistep function and a linear function to lessen the sudden break between nucleus and environment.
Figure 3. Mean number $\langle N \rangle$ and the fluctuation in TDHF and BV methods as a function of end time $t_1$.

Figure 2 shows the spatial form of the different cutoff functions used, and Table 1 the results from using these different functions to split the system between the daughter nucleus (in which the transformation (2) is applied) and the environment (where it is not). The table shows that the differences between the different methods are slight, with the numbers being physically reasonable given that the stepping and linear functions actually feature a little less of the discretisation. These variations were negligible.

Finally, we look at the dependence of the final time, $t_1$. In principle, one should aim to perform a calculation in which the daughter nucleus has completely decayed and all flux that has left the nucleus has gone far off into the environment away from the nucleus. In practice, one is limited in box size and the customary boundary conditions (reflecting or periodic) result in unphysical interference with the emitted particles and the daughter nucleus. This means that one must pick an intermediate value of $t_1$; large enough that the system has approached its asymptotic state, but small enough that numerical problems are not starting to rear their head.

Calculations as a function of end time $t_1$ are shown in figure 3. It shows that the Balian-Vénéroni calculation of the number fluctuation increases significantly at large times. This happens after the number of nucleons in the daughter nucleus starts to rise again due to reflections and is an indication of numerical problems. The results are at least reasonably stable for a large range of times, and the numbers at any of those times can be taken as a good value for the fluctuation at that time. In the long run, better boundary conditions at the edge of the box will be needed to allow for better long time behavior.

Other numerical aspects have been studied too; the effect of variation of time step and spatial discretisation. These variations were negligible.
4. Conclusion
We have presented an analysis of some of the numerical issues related to implementing the Balian-Vénérond variation procedure in nuclear collective motion. Parameters related to the separation of the system between nucleus and environment give rise to slightly different answers (as they do in TDHF), but in a physical way. Long-time behaviour is problematic and will require improved boundary conditions.

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