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The Continuum Time-Dependent Hartree-Fock Method

C.I. Pardi, **P.D. Stevenson**

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

Abstract. Time-dependent approaches are useful in tackling dynamic processes in nuclei, such as collective motion of a single nucleus, and collisions between nuclei. The basic mean-field approach is the time-dependent Hartree-Fock (TDHF) method. It has been widely applied to giant resonances, fusion, deep-inelastic collisions and transfer reactions. In all or most applications of nuclear TDHF, the processes occur above particle emission threshold. With wave functions represented on a spatial grid, the boundary conditions at the edge of the calculation region become a significant issue as particles are emitted. The simple conditions of periodic or reflecting boundaries can cause unphysical artefacts in observables. Methods to mitigate unphysical behaviour include the use of extended regions of complex absorbing potentials or masking functions. These methods can be made to work, with some computational cost, by judicious tuning of parameters, but are never exact for arbitrary outgoing flux. We present an exact method for implementing outgoing wave boundary conditions, based on a Laplace Transformation approach. We apply it to the case of giant monopole resonances in light doubly-magic nuclei, showing that the results agree exactly with computationally-punitive calculations performed in extremely large boxes. We discuss perspectives for application in other resonances, other forms of collective motion, and with more sophisticated interactions.

1 Introduction

The time-dependent Hartree-Fock (TDHF) method, as it applies to nuclear physics, has developed to a stage in recent years to be free of most constraining assumptions about the geometry of a problem, or the limiting forms of the effective interaction [1–37]. This has allowed a rather realistic calculation of phenomena such as reactions [15, 20] and giant resonances [1, 19, 30]. Essentially all practical calculations of nuclear TDHF have used versions of the Skyrme effective interaction [38], and perform their calculations in coordinate space of limited size. Since all physical phenomena tackled by time-dependent methods are by definition not stationary states, and given the weak-binding of nuclei, essentially all nuclear TDHF calculations run into the problem of dealing with boundary conditions at the edge of the spatial box. It is the purpose of the method presented here to show one way to give an essentially exact solution

to the problem, albeit with some very well controlled approximations along the way.

2 Time-Dependent Hartree Fock

TDHF calculations begin by the calculation of an initial condition - typically the ground state of a nucleus calculated via a static Hartree-Fock (HF) calculation, though other states may be prepared such as via a constrained HF approach. This is then augmented usually by some kind of boost operator, to give the nucleus some kind of collective momentum in such a way that it is no longer in a stationary state.

The time-consuming part of the HF calculation is then the repetitive stepping forward in time of the TDHF equations, which take the form of coupled non-linear Schrödinger equations for each single particle state present. While time-consuming by sheer repetition, the TDHF approach is conceptually simple, and implementations, while they have their pitfalls and subtleties, are quite straightforward, being essentially the solution of a simple, first-order differential equations. In other words, once the somewhat complicated coupled non-linear static problem is solved for the initial condition, the time-dependent problem is, on the face of it, quite simple.

Being differential equations, both the static and time-dependent Schrödinger equations must be solved along with their boundary conditions. Specialising now to the case of spherical symmetry, which we use in the present work for giant monopole resonances, we can write the full TDHF equation in the form

$$i\hbar\frac{\partial Q_{n,l}(r,t)}{\partial t} = \Big[-\frac{\hbar^2}{2m}\frac{\partial}{\partial r^2} + V_q(r,t,\rho_n,\rho_p) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\Big] Q_{n,l}(r,t). \quad (1)$$

Here, Q represents the *reduced* wave function, $Q = r\phi$, as often used in spherical problems to simplify the centrifugal part. We have made explicit that the potential is dependent on the densities (whence the non-linearity, since they are built of the wave functions) as well as the spatial *and* time coordinates. The potential is always time dependent in TDHF, except for the trivial case of stationary states. This comes from the dependence of the potential on the densities, which change over time. This allows the nucleus to explicitly explore the properties of the Hamiltonian away from the static HF density, in a way that the random phase approximation does by looking at a Taylor expansion of the interaction. The subscript q on the potential indicates that it depends on the charge of the state on which it acts (though one may write it in terms of isospin projection operators to equivalently omit particle-type subscripts).

For the nuclear part of the potential, we take a simplified version of the Skyrme force that is often used in exploratory work [39], retaining only two terms:

$$V(r,t,\rho_n,\rho_p) = t_0\left(\rho_{\bar{q}} + \frac{1}{2}\rho_q\right) = \frac{t_3}{4}\rho_{\bar{q}}\left(\rho_{\bar{q}} + 2\rho_q\right). \quad (2)$$

Here t_0 and t_3 are adjustable constants, and this expression for the potential derives from the normal Skyrme interaction when only these coefficients are non-zero [40]. In the case of the proton states, we also include the Coulomb potential in the typical case of exact treatment of the Poisson equation for the direct part of the mean field, and the Slater approximation [41] for the exchange part.

3 Boundary Conditions in HF and TDHF

In solving the static HF equations, the physically appropriate boundary conditions for a the calculation of a bound state of a single nucleus are that the wave functions go to zero as the the distance away from the origin goes to infinity. This would correspond to the case of an isolated nucleus in an empty universe, which is of course not quite the same as the natural situation. In practice, calculations of single nuclei in static HF take "infinitely far away" in space as being at a suitable distance, and keep the zero wave function condition. This causes little practical problem, as the wave functions of bound nuclear states decay exponentially and it is quite possible to perform calculations in large enough spatial regions so that numerically, at least, the wave function really is zero at the edge of the box.

When solving the time-dependent part of the problem, the differential equation is first-order, and the only boundary condition of concern is the initial condition, which is well specified. However, in the action of the time-evolution operator, by which the time-dependent equation is solved, the Hamiltonian operator is applied to the wave functions, and the operator includes the kinetic energy part, with its second-order spatial derivative.

It is here, that the boundaries of the spatial box become important. The simplest method of treating them is to suppose that the wave function is zero outside the spatial region dealt with. This, however implies an infinite external potential and a perfectly reflecting box. The beginnings of this reflection in a time-dependent calculation can be seen in Figure 1, which also shows that for the static HF ground state calculation (at $t = 0$ fm c^{-1}), there is no need to worry about boundary conditions as long as a large-enough box is used. The density is numerically zero, in this example, well before the edge of the box is reached in the static calculation.

Overcoming this issue of the reflecting boundaries is not easy. Most nuclear TDHF calculations involve reflecting boundaries, and most RPA calculations of states in the continuum feature the equivalent case of finite bases built upon HF state built with fixed boundaries, which amounts to exactly the same thing, though we note that true Continuum RPA (CRPA) calculations have been developed [42]. It has been our intention to develop genuine Continuum Time-Dependent Hartree-Fock (CTDHF) calculations, which deal exactly with the boundary.

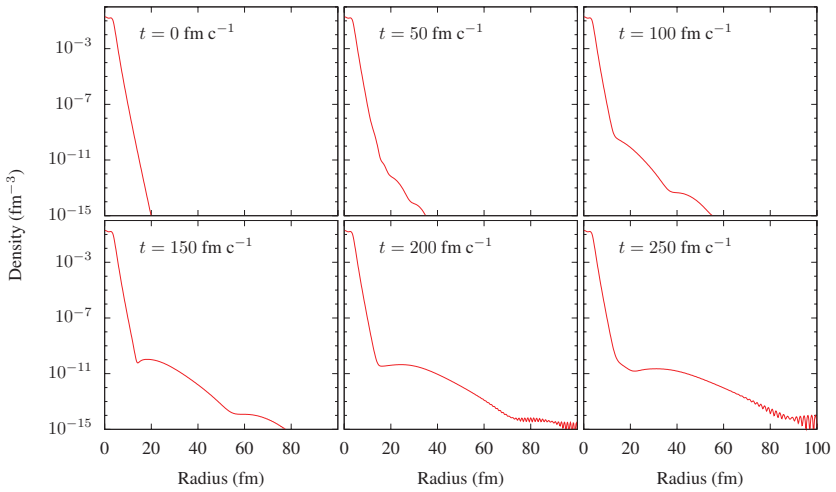

Figure 1. Plots showing the evolution in time of the isoscalar density of a calcium nucleus in a fixed box with reflecting boundaries, starting from a static HF calculation ($t = 0$ fm c^{-1}), at which point a monopole boost is applied. At subsequent time steps the emission of particles from the nucleus can be seen. The fluctuations of the nuclear density are too minuscule to observe on this scale. At the final two times, the reflected flux can be seen interfering with the outgoing flux in the form of waves forming in the density profile at the right-had side of the box.

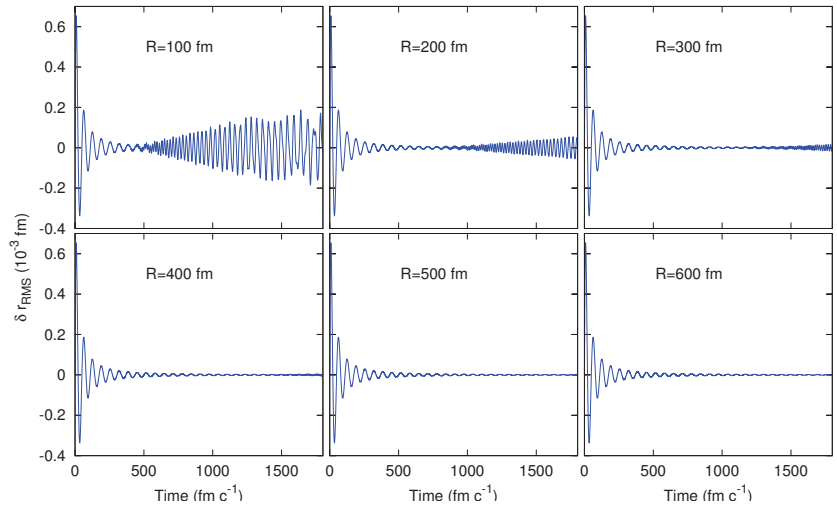

Figure 2. Plots showing the difference between the root mean square radius from that of the initial state of a helium nucleus. Each plot shows the evolution of this value through time for calculation with varying artificial boundaries.

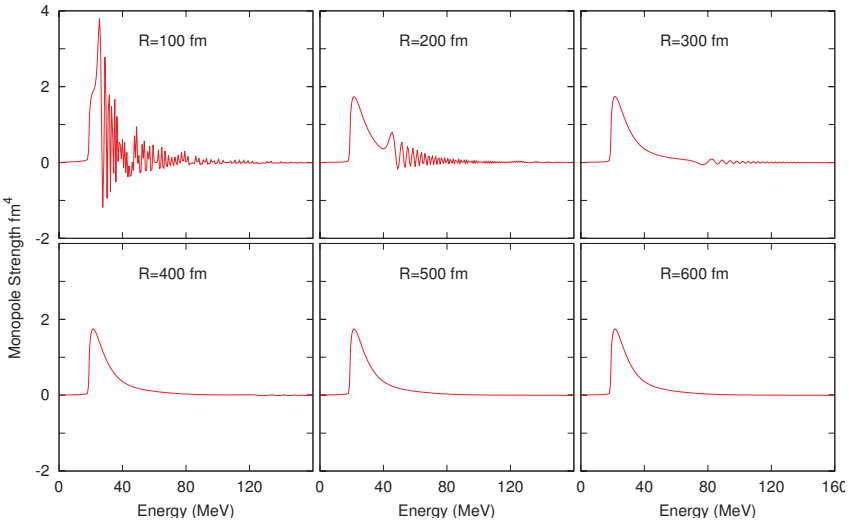

Figure 3. Monopole strength functions of He-4 nuclei as a function of the box size in which the calculations are performed.

Though the effect looks small in Figure 1, the effect upon the strength function, the key observable of interest in giant resonances [43], is pronounced [7, 12]. As an example, Figure 2 shows the fluctuating radius as a function of time the the response of a helium-4 nucleus to a monopole boost. Calculations in successively larger box sizes are shown, and it can be seen that as the spurious effect of reflection can be large, but can be pushed back to later and later times by increasing the box size to be orders of magnitude greater than the size of the nucleus. It is also possible to discern from the plots that the physical oscillations, though much damped, have not entirely died out after rather long times. Since very sharp resonances and quasi-stationary states may be excited in these kind of collective modes, the ability to calculate for a long time without reflection is desirable. The effect of the reflections on the strength functions can be seen in Figure 3.

The smallest radius in Figure 3 is 100 fm, which is already large on the scale of most practical calculations. The special case of monopole resonances in spherical nuclei presented here allows a practical exploration of much larger box sizes.

4 A Sketch of the Method

A full description of the CTDHF method is beyond the scope of this proceeding, and full details can be found elsewhere [32, 40, 44]. They key point is to deal separately with the TDHF equations in the so-called interior region, where the nuclear potential is finite, and a chosen exterior region, where only the Coulomb

and centrifugal potentials apply. By absorbing the physical constants in the variables in (1), the TDHF equation for the exterior region can be written

$$i\frac{\partial Q(r,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2 Q(r,t)}{\partial r^2} + \left(\frac{\sigma}{r} + \frac{l(l+1)}{2r^2}\right) Q(r,t). \tag{3}$$

The next step is then to take the Laplace transform of this equation, transforming the time coordinate to a Laplace conjugate variable, s:

$$\frac{1}{2}\frac{\partial^2 Q(r,s)}{\partial r^2} + \left(is - \frac{\sigma}{r} - \frac{l(l+1)}{2r^2}\right) Q(r,s) = 0, \tag{4}$$

where we have assumed that the wave function is initially zero in the exterior region (as indeed it is), so that the boundary term does not appear explicitly in the Laplace-transformed equation. By substituting $z = br\sqrt{s}$ with $b = -2i\sqrt{2i}$, the equation can be rendered in a form whose solution is well-studied and tabulated:

$$\frac{\partial^2 Q(r,s)}{\partial z^2} + \left(-\frac{1}{4} + \frac{\kappa(s)}{z} - \frac{\frac{1}{4}-\mu^2}{z^2}\right) Q(r,s) = 0. \tag{5}$$

Here $\kappa(s) = -\sigma/b\sqrt{s}$ and $\mu = l + 1/2$. The equation in this form has solutions in the form of the Whittaker M and W functions [45]. We keep the notation $Q(r,s)$ despite the use of z as the independent variable in the derivatives to make clear from the s that the Q in this equation is the Laplace-transformed version.

The boundary condition for large r, corresponding also to large z, requires that the M function be zero and we have that

$$Q(r,s) = BW_{\kappa,\mu}(br\sqrt{s}) \tag{6}$$

where B is a constant of integration. This equation may be divided by its derivative and rearranged to give

$$Q(r,s) = \frac{1}{b\sqrt{s}}\left(\frac{W_{\kappa,\mu}(br\sqrt{s})}{\frac{\partial W_{\kappa,\mu}(br\sqrt{s})}{\partial r}}\right)\frac{\partial Q(r,s)}{\partial r}. \tag{7}$$

Application of the convolution theorem, with the result evaluated at $r = R$ (the boundary position) gives a formal expression for the wave function at the boundary of

$$Q(R,t) = \int_0^t G_{\kappa,\mu}(R,\tau)\frac{\partial Q(R,t-\tau)}{\partial r}d\tau, \tag{8}$$

in which the integration kernel is the inverse Laplace transform of

$$G_{\kappa,\mu}(R,s) = \frac{1}{b\sqrt{s}}\left(\frac{W_{\kappa,\mu}(br\sqrt{s})}{\frac{\partial W_{\kappa,\mu}(br\sqrt{s})}{\partial r}}\right)\Bigg|_{r=R}. \tag{9}$$

To proceed, then, this inverse Laplace transformation must be evaluated to obtain the boundary value for the wave function, and the CTDHF equation is then discredized in time and space, with the time-dependent part being solved by the Crank-Nicholson algorithm.

Unfortunately, then inverse Laplace transformation is not available in analytic form, and instead a sum of poles approximation is used [44] which can be controlled to give an accuracy of any desired form. This involves expressing the kernel in a partial fraction expression, in which each term has a well-known tabulated inverse Laplace transformation, and the linear nature of Laplace Transformations is exploited.

Our results so far have shown that the method works extremely well for giant monopole resonances with small box sizes using this technique reproducing exactly the results of extremely large box sizes without the special boundaries. The time taken for the calculations is much less than that large-box reflecting calculations. One can see, however, from (8) that the expression for the wave function at the boundary at time t, requires knowledge of the entire history of the wave function from the start of the simulation. In principle, then, the calculation of each successive time step takes longer than the each previous one. In practice, a recursive method is used to ensure that the slow-down is negligible. Our results have been presented for the simplified Skyrme force, as above, initially ignoring the Coulomb force [32] but also now with the Coulomb force [44]. Our short-term plans are to use the full Skyrme force and make a study of the fine structure of giant monopole resonances, with a longer term aim to extend to more general spatial symmetries. This will be a challenge since there will be more than a single boundary point to consider, but our results thus far lead us to expect the challenge to be surmountable.

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