New Results from Skyrme-TDHF: Giant Resonances and Collisions

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We summarise the time-dependent Hartree-Fock technique and describe its practical application to nuclear giant resonance and collision applications. With the availability of a fully symmetry-unrestricted (3+1)-dimension code, new results such as the deformation splitting of resonances in triaxial isotopes, and energy loss mechanisms in collisions are presented.

Introduction

The Time-Dependent Hartree-Fock (TDHF) method is a mean-field approach which is able to describe some aspects of oollective motion in nuclei. Although first described by Dirac, it became practical for somewhat realistic calculations about 30 years ago (for summary see [Neg82], [Dav85]). With the advent of more powerful computers, the technique has been recently revisited by several groups [Ste04,Mar05,Mar06,Nak05,Uma06]. Here were give a summary of some of the calculations that have been undertaken with the most modern codes.

TDHF Theory

TDHF is a time-dependent generalisation of standard HF, in which the single particle states making up the Slater Determinant Ansatz are allowed to be time-dependent:

$$\Phi(x_1\cdots x_n,t)=\frac{1}{\sqrt{n!}}\begin{vmatrix}\phi_1(x_1,t) & \phi_2(x_1,t) & \cdots & \phi_n(x_1,t)\\ \phi_1(x_2,t) & \phi_2(x_2,t) & \cdots & \phi_n(x_2,t)\\ \vdots & \vdots & \ddots & \vdots\\ \phi_1(x_n,t) & \phi_2(x_n,t) & \cdots & \phi_n(x_n,t)\end{vmatrix}. \quad (1)$$

The single particle states satisfy the following generic equation

$$i\hbar\frac{\partial\phi}{\partial t}=\hat{h}\phi \quad (2)$$

where the single particle Hartree-Fock Hamiltonian is itself time-dependent. The $t=0^-$ boundary conditions are the that single particle states are those of the static Hartree-Fock problem for the nucleus of interest. At early times in the solution of the TDHF equations an external perturbation is added to initiate the collective motion of interest, specifics of which are given later.

In our work the TDHF equations (2) are solved using a series expansion of the formal solution

$$\phi(x,t+\Delta t)\approx\sum_n\frac{(-i\Delta t)^n}{n!}\hat{h}^n\phi(x,t) \quad (3)$$

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which is exact in the limit $\Delta t \to 0$ and an infinite number of terms in the sum used. In practice, we limit the number of terms in the sum to around 4, and the timestep to around 1/8 fm/c, which we find suitable accurate to allow evolution to long times.

Our wavefunctions are represented spatially on a discretised coordinate grid, either in fully a fully unrestricted 3-D code, or a spherically symmetric 1-D code. In the 3-D code, grid spacings of 1 fm in each of the Cartesian axes give reasonably well converged solutions.

Effective Interaction

We use the Skyrme effective interaction, including time-odd terms. The Skyrme interaction can be written as an energy functional, schematically as follows

$$\mathrm{E} = \mathrm{E}_{kin} + \int d^3r\left(\varepsilon_{Sk} + \varepsilon_{Sk}^{ls}\right) + \mathrm{E}_C \qquad (4)$$

where E_{kin} is the kinetic energy, E_C the coulomb energy, and the Skyrme energy densities are

$$\begin{aligned}\varepsilon_{Sk} &= \frac{b_0}{2}\rho^2 + b_1(\rho\tau - \vec{j}^2) - \frac{b_2}{2}\rho\nabla^2\rho + \frac{b_3}{3}\rho^{\alpha+2} \\ &- \sum_q \left[\frac{b'_0}{2}\rho_q^2 + b'_1(\rho_q\tau_q - \vec{j}_q^2) + \frac{b'_2}{2}\rho_q\nabla^2\rho_q + \frac{b'_3}{3}\rho^\alpha\rho_q^2\right]\end{aligned} \qquad (5)$$

for the regular Skyrme energy density, and

$$\varepsilon_{Sk}^{ls} = -b_4\left(\rho\nabla\cdot\vec{J} + \vec{\sigma}\cdot(\nabla\times\vec{j})\right) + b'_4\sum_q(\rho_q\nabla\cdot\vec{J}_q + \sigma_q\cdot(\nabla\times\vec{j}_q)) \qquad (6)$$

for the spin-orbit density. The densities and currents have their usual meanings – for further details, see [Ben03].

Giant Resonances

To excite giant resonances within TDHF, an external perturbation is applied to the ground state HF Slater Determinant of a nucleus in the form of an instantaneous, or quick-acting multipole field.

If F(x) is the spatial form of the multipole operator, then the principle observable of giant resonances is the strength function, defined as

$$S(E) = \sum_\nu \left|\langle\nu|F|0\rangle\right|^2 \delta(E - E_\nu) \qquad (7)$$

where the state vectors labelled with ν denote the eignemodes of the nuclear oscillations. The strength function can be written in the spectral representation by expressing the delta function by its Fourier integral

$$S(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t \sum_\nu \left|\langle\nu|F|0\rangle\right|^2 e^{i(E-E_\nu)t}. \qquad (8)$$

This integral can be performed separately for positive and negative *t* by inclusion of appropriate infinitesimal convergence factors:

$$S(E) = \sum_{\nu} \left| \langle \nu | F | 0 \rangle \right|^2 \left(\frac{1}{E - E_{\nu} + i\delta} - \frac{1}{E - E_{\nu} - i\delta} \right). \quad (9)$$

The bracketed term arising from the integration is a *c*-number which can be placed inside the matrix element, the energy eigenvalues replaced with the Hamiltionan and the unit dyadic removed to give

$$S(E) = \frac{1}{2\pi} \langle 0 | F \left(\frac{1}{E - H + i\delta} - \frac{1}{E - H - i\delta} \right) F | 0 \rangle . \quad (10)$$

Dirac's formula states

$$\frac{1}{x - x' \mp i\varepsilon} = \mathrm{P} \frac{1}{x - x'} \pm i\pi\delta(x - x') \quad (11)$$

so that from (10), the strength function is given by twice the imaginary part of either term:

$$S(E) = -\mathrm{Im} \frac{1}{\pi} \langle 0 | F \left(\frac{1}{E - H + i\delta} \right) F | 0 \rangle \quad (12)$$

From the linear response theory approach to TDHF [Fet71], which also corresponds to the small amplitude or RPA limit, it can be shown that the strength function is related to the Fourier transform of the time-dependent fluctuation of the expectation value of the operator *F* divided by the Fourier transform of the time profile of the external perturbation:

$$S(\omega) = -\frac{1}{\pi} \mathrm{Im} \int \mathrm{d}x \frac{\delta \langle F(x, \omega) \rangle}{f(\omega)} \quad (13)$$

which is directly calculable from the time-dependent Hartree-Fock calculations.

Note that the function *F* that is used to create the intitial excitation is also the same used in (13) to follow the time evolution. This gives rise to the normal strength function (7) which has a matrix element squared of a given *F*. One can also, in the TDHF approach, look at performing an initial excitation of one type (e.g. of one multipole) and observing the resultant change in another type of excitation mode to look at nonlinearities and mode-coupling [Alm05].

As an example calculation is shown in Figure 1, in which an ^{16}O nucleus is subjected to a isoscalar monopole (breathing mode) excitation and its evolution followed as a function of time. One sees the rapid damping of the oscillations, which correspond to a broad strength function.

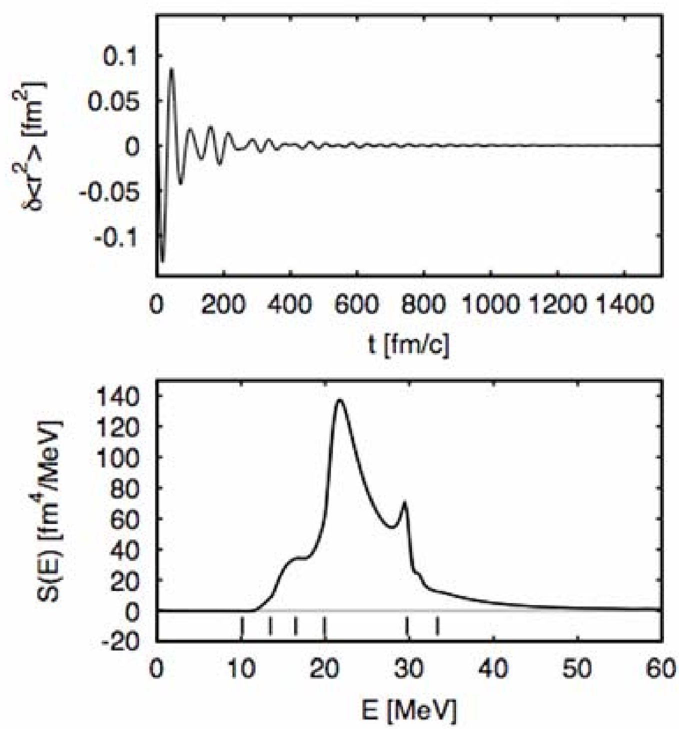

Figure 1: Time-dependent expectation value of isoscalar monopole operator (top panel) in ^{16}O, following an isoscalar monopole kick, and the associated strength function (lower panel). The single particle energies from the underlying static Hartree-Fock calculation are shown below the strength function. The Skyrme force SkM* was used.

Part of the width associated with the giant resonance comes from the emission of particles, as the resonance energy lies above the particle emission threshold. In practical TDHF calculations this causes a problem when the flux of emitted nucleons reaches the edge of ones coordinate space box. In practice there are several methods around this problem. In the case of monopole calculations of spherical nuclei, as shown in Figure 1, the box can be made sufficiently large that the outgoing flux never reaches the edge in the time of the calculation. For all other cases, absorbing boundaries or other smoothing techniques must be used [Nak05, Rei06]. Note that the small imaginary part in (12) is realised in a finite box calculation as an imaginary potential at the boundary which absorbs outgoing flux.

As an example of new calculations with the fully deformed code, Figure 2 shows calculations [Mar05] of the isovector giant dipole resonance in a series of neodymium isotopes for which experimental data are available. Starting from a (calculated) spherical nucleus in the bottom left, the strength function contributions from oscillations in the (x,y) and z-directions are identical. As one increases N, and increases the prolate deformation, the motion in the z-direction (i.e. the long axis of the prolate spheroid) becomes lower in energy, until by the moderately deformed ^{150}Nd isotope the splitting in energies of the resonance peaks is enough to be seen experimentally.

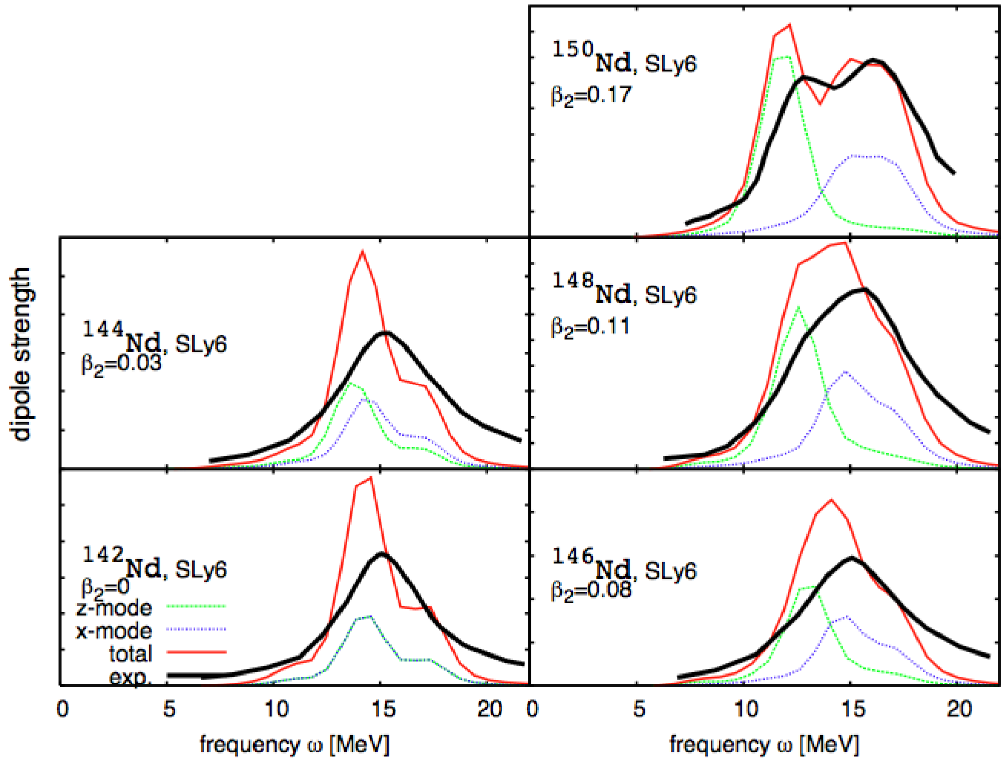

Figure 2: Giant dipole resonance in Nd isotopes calculated with SLy6, showing evolution of deformation splitting.

Collisions

Rather than set up an initial condition in which one nucleus is subjected to a multipole perturbation, one may set up two (or more) nuclei and give them an initial translational boost to set them on a collision course. This has historically been one of the more successful situations in which TDHF can be used. As an example, we show in Figure 3 snapshots from a simulations in which a ^{16}O and ^{48}Ca nucleus were collided just above the fusion barrier so that the resulting compound nucleus oscillated and deexcited into a fused daughter.

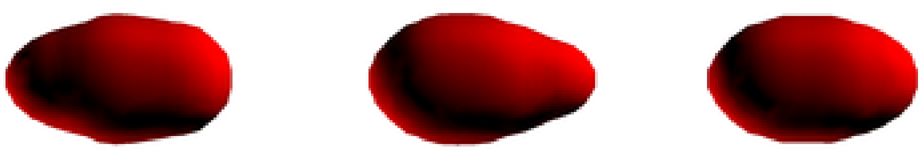

Figure 3: Three snapshots during a time-dependent calculation of the fusion between a ^{16}O and ^{48}Ca nucleus.

By having a completely symmetry-unrestriced code, new modes of energy transfer have been seen for the first time. [Mar06] and Figure 4 show how the incident kinetic energy of colliding nuclei is transferred into a toroidal current. This happens due to the time-odd parts of the Skyrme functional, and an experimental determination of its existence would play a valuable constraint on the many available Skyrme functionals.

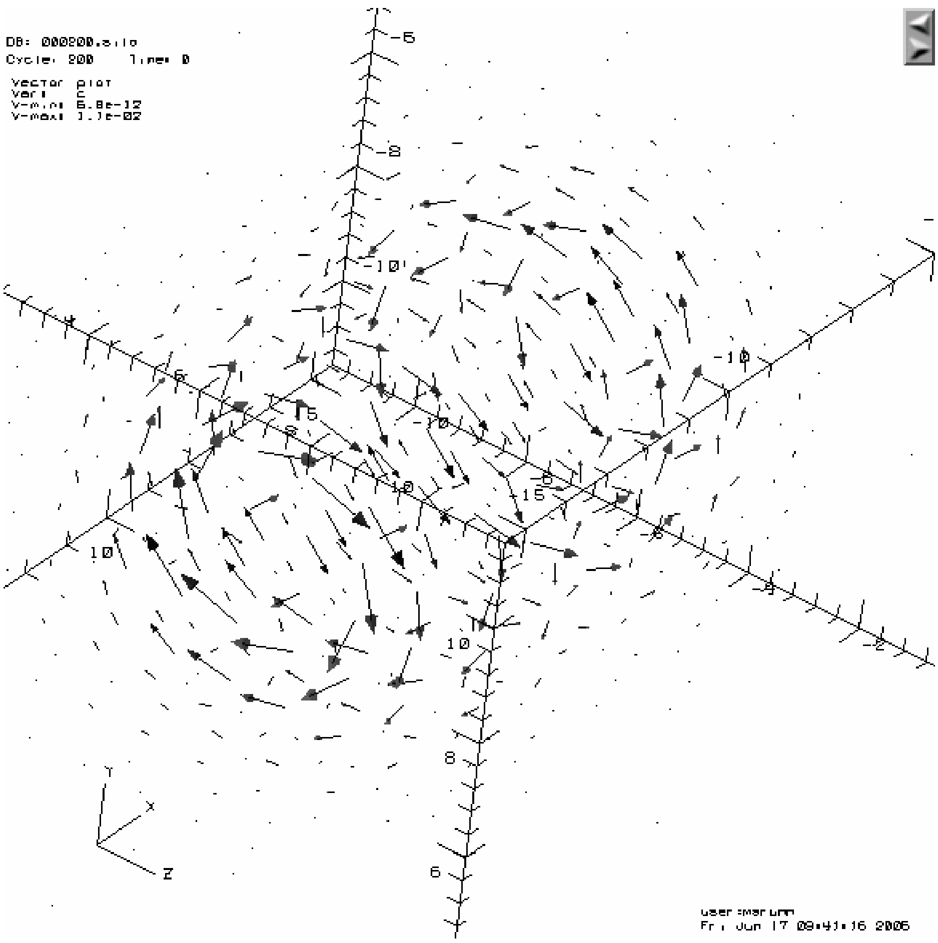

Figure 4: Current density in two colliding oxygen nuclei, showing the toroidal current that is induced by the Skyrme functional

Conclusions

TDHF is a powerful method for describing collective motion in nuclei. It provides a good quantitative description of giant resonances and collisions. Modern calculations with no symmetry restrictions show, for example, proper deformation splitting in giant resonances, and a more complete picture of internal motion during the collision process.

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