TDHF Periodic Orbits and Nuclear Collective States

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Based on the calculation of collective motion on the periodic solutions of the time-dependent Hartric-Fock mean field, we propose a method to recover the stationary many-body wave functions for collective excitations. Results are presented for the monopole oscillation in the ^{16}O nucleus.

1 Introduction

Functional integrals provide a fundamental framework to describe the microscopic behavior of a quantum system systematically and consistently. The stationary-phase approximation (SPA) to an exact functional integral leads to the time-dependent Hartree-Fock (TDHF) equation[1]. It has been known for some time that in the SPA bound state energies of a many-body system can be determined from the periodic solutions of the TDHF equation through a Bohr-Sommerfeld quantization rule[2]

$$\int_0^\tau dt\ (\phi^P | i\partial_t | \phi^P) \ = \ 2\ n\ \pi,$$

where ϕ^P is the periodic solution with a period τ, and n is an integer. However, the numerical difficulty in solving periodic solutions held this approach in check until in recent years we developed a numerical algorithm[3,4] to construct periodic orbits for the TDHF equation using effective nucleon-nucleon interaction. The key element in the success is that the numerical algorithm preserves "exact" energy conservation in the TDHF evoltuion. Generally, the TDHF equation can be written as

$$i\frac{\phi(n+1) \ - \ \phi(n)}{\Delta t} \ = \ (\ h(n{+}1/2) - \lambda\ )\ \frac{\phi(n+1) \ + \ \phi(n)}{2}\ ,$$

where

$$h(n+1/2) \ = \ K \ + \ w(n+1/2),$$

is the single-particle hamiltonian and K is the kinetic energy operator. For a density ρ-dependent Skyrme force with an energy functional

$$E \ = \ (\ \phi\ |H|\ \phi\ )$$

where

$$H \ = \ K \ + \ \nu(\rho)\ ,$$

it can be proved that the appropriate hamiltonian which preserves the total energy reads

$$w(n + 1/2) \ = \ \frac{\rho_{n+1}\ \nu(\rho_{n+1}) \ - \ \rho_n\ \nu(\rho_n)}{\rho_{n+1} \ - \ \rho_n}$$

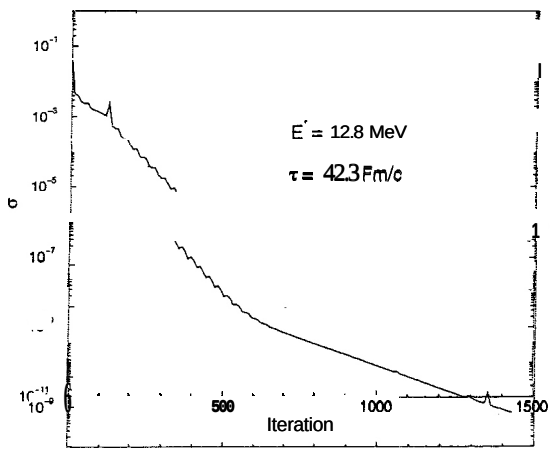

Figure 1: The standard deviation in the periodic wave function, as a function of iteration number for a cycle of ^{16}O. The excitation energy and the period are on the figure.

In ref. 4, we reported an iterative procedure which leads to convergence to the perodic TDHF solutions. Fig.1 shows a typical convergence sequence for the monopole vibration of ^{16}O at an excitation energy of 12.8 MeV, where σ is defines as

$$\sigma \ = \ \sqrt{\frac{1}{N\ M}\sum_m |\phi(m, N+1) \ - \ \phi(m,1)|^2},$$

where N is the number of time steps, and m is the space index for a total number of M mesh points. We applied the quantization rule to the nucleus of ^{16}O to determine its monopole excitation[5].

Fig.2 shows the HF ground state density and the TDHF densities at the times t_1 and t_2, which correspond to the maximum and minimum rms radius, respectively. It was the first time that the TDHF periodic orbits with multiple single particle wave functions were ever calculated for a nuclear system heavier than ^4He.

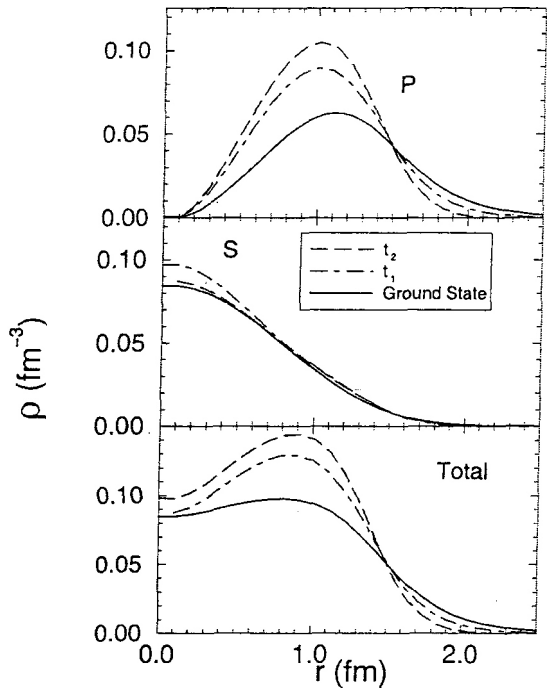

Figure 2: The HF ground state density of ^{16}O compared to the periodic TDHF density at two times: t_1 at which the rms radius is maximum; and t_2 at which it is minimum. The cycle is chosen *so* that the quantization condition is satisfied. The contributions to the total density from the s–wave and the p–wave components are compared separately.

2 Requantization

It is a dream for nuclear theorists to find a microscopic foundation for nuclear collective phenomena, in which many nucleons act coherently. The progress we have made can be considered as the first step towards a fully quantum theory for nuclear collective motion. In the TDHF approximation, the many-body wave function is like a wave packet, which undergoes large variations with time. The restriction that the wave function is a Slater determinant brings a classical element into the picture. If we consider that a Slater determinant represents a certain shape for the nucleus in a shape space, the stationary wave function of a collective excitation carries the amplitudes for a whole variety of shapes. The restricted class of wave functions does not include such stationary collective states. Therefore, the TDHF approximation is capable of describing a special type of collective motion for the wave packet, but not the more general type of wave functions. When we apply the TDHF approximation to the collective motion of nuclei we must recover the fully quantum picture contained in the time-dependent motion, i.e. requantization for the periodic orbits is necessary.

Now we will report some preliminary work on a requantization procedure for TDHF periodic orbits[6]. In this approach, the TDHF periodic orbits provide us a family of many-body wave functions (Slater determinants), which is highly related to the collective motion in study. This set of Slater determinants and the HF ground state wave function form a basis for the generator coordinate method (GCM). We can calculate the matrix elements between the states for the exact Hamiltonian operator (in the form of second quantization), and they form an effective Hamiltonian matrix in the subspace. The GCM diagonalization of the effective Hamiltonian matrix in the subspace leads to a set of eigenstates, which provides a good approximation to the collective excitations. This is what we mean by the procedure of "requantization".

There exist two types of periodic orbits. For one type of periodic orbits, the orbit is invariant under the time-reversal transformation. We call this type of collective motion vibrations. For the other type of periodic orbits, the orbits show up in conjugate pairs, and the time-reversal transformation leads from one to the other. Rotations belong to this type of collective motion. Here, we only consider the collective motion of vibrations. Similar GCM procedure can be formulated for rotations.

For practical purpose we chose a set of Slater determinants uniformly distributed on the periodic orbit. It can be proved from the TDHF equation that for vibrations, there exists a moment when the wave function is real (upto an overall phase factor), which corresponds to an extreme in the shape space. Generally, for this type of periodic orbits, if a wave function is on the periodic orbit, its complex conjugate (upto an overall phase factor) is also on the same orbit. The chosen set of wave functions consists of a real wave function and pairs of complex conjugate wave functions $\{\phi(j)\}$, $j = 1, 2, ..., 2J+1$. This basis is neither orthogonal nor complete, i.e.

$$(\phi(i) \mid \phi(j)) = \beta_{ij}$$

where $i, j = 1, 2, ..., 2J+1$. These Slater determinants span a subspace highly related to the collective excitation in study. The effective Hamiltonian matrix $H_{eff} = \{ H_{ij} \}$ is hermitian where its matrix elements are

$$(\phi(i) \mid H \mid \phi(j)) = H_{ij}.$$

The diagonalization of the H_{eff} matrix leads to the Hill-Wheeler equation

$$H_{eff} |\alpha) = E_\alpha \, |\alpha),$$

where

$$|\alpha) = \sum_j a_{\alpha j} \, |\phi(j)).$$

Table 1: Given in the table are the excitation energies for the first excited state as a function of the number (J) of pairs of wave functions in the GCM basis taken from the periodic orbit satisfying the quantization rule.

J	Excitation Energy (MeV)
1	37.6048
2	31.4024
4	30.4302
6	30.3023
8	30.2944
12	30.3576
16	30.3493

To be more specific, the Hill-Wheeler equation reads

$$\sum_j H_{ij}\, a_{\alpha j} = E_\alpha \sum_j a_{\alpha j}\, \beta_{ij}.$$

The diagonalization of the hermitian matrix leads to a set of eigenstates with real wave functions, which provides a good approximation to the stationary states of collective excitations. The new quantization method has been tested on a few simple systems and appears very promising.

Table 1 gives a convergence sequence of the excitation energy as a function of J for the monopole vibration of ^{16}O. It shows that it converges very quickly with increasing J. In the meantime, the diagonalization also recovered a ground state with energy about half an MeV lower than that of the HF ground state. Once the convergence is reached we can recover the many-body wave function for the lowest excitation, and therefore, calculate all the properties of the excitation state.

The main conclusion from our work is that it is possible to extend periodic solutions of the TDHF equation into the nonlinear region in a systematic, reliable, and accurate way. Thus we have accessed all those nonlinear phenomena which lie beyond the RPA. The new quantization method opens up an approach leading to the stationary many-body wave functions for nuclear collective excitations. Now we intend to extend these results to heavier nuclei and to other collective modes. The code in two space dimensions for nuclear collective motion with cylindrical symmetry is in progress, and has produced preliminary results for periodic orbits. We expect to see more interesting collective phenomena in the near future.

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