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Periodic numerical solutions of the time-dependent Hartree-Fock equations

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We propose a numerical algorithm for finding periodic solutions of the time-dependent Hartree-Fock equations. We show that this algorithm preserves the particle number and the total energy exactly. We demonstrate the method by calculating the periodic breathing mode of ^{4}He. We discuss the generalization to more realistic cases, including multidimensional periodic modes. [S0556-2813(97)05508-8]

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I. INTRODUCTION

It has been known for some time that approximate bound-state energies of many-body systems can be found from the periodic solutions of the time-dependent Hartree-Fock (TDHF) equations [1–3]. A quantization rule is needed to return to full quantum mechanics, since TDHF is partly classical. In the simplest cases (nonchaotic, one dimensional), this rule is usually analogous to Bohr-Sommerfeld quantization [4–6], and tests with simple models have been very encouraging [7,8]. An accurate calculation of the periodic TDHF solutions is a key element of the method. The work of Chomaz *et al.* [9] emphasizes this point and proceeds to construct periodic solutions to the one-body density matrix employing a symplectic theory. These solutions have been the most reliable to date using realistic nuclear interactions. However, as demonstrated in Ref. [10], a range of solutions having different periods is needed to use effectively the requantization method. Except for semianalytic model studies testing the requantization method, no calculations with realistic nuclear forces have been carried out [5,7,10].

In the present work we present an algorithm for accurately solving the periodic time-dependent Hartree-Fock equations. Our method is based on a discrete wave function approach which preserves the total energy exactly. A similar approach was used long ago in the study of nuclear collisions [11]. However, we differ from this earlier work in several respects, but most importantly in the treatment of unitarity. We present the method in Sec. II, and in Sec. III we describe the search procedures for obtaining the TDHF periodic orbits. We give the period of the breathing mode of ^{4}He as a function of its amplitude or of its energy. In Sec. IV we give a brief discussion of the stability of the algorithm and the generalization to more realistic cases, which include multidimensional periodic modes. Throughout the paper we shall employ units where $\hbar=c=m=1$.

II. PROBABILITY AND ENERGY CONSERVATION

The search for quasiperiodic solutions of the TDHF equations has been pursued for some time. Chomaz *et al.* [9] provided the first successful algorithm which might lead to general numerical solutions. However, difficulties in convergence prevented these authors from applying their method more widely. The problem was studied in detail by one of us [10], and it was shown that it is essential to use a discretization scheme which preserves exactly the conservation laws for energy and probability in the time evolution. In Ref. [10] this was done by using densities and currents, but there are other ways.

In our approach, we deal directly with the dynamics of the one-body wave functions governed by the TDHF equations. Our method is similar to that employed by one of us [12] for the evolution of nuclear hydrodynamics in terms of a nonlinear Schrödinger equation.

We begin by writing the one-body TDHF equations

$$i\,\frac{\partial}{\partial t}\,\psi_\alpha=-\tfrac{1}{2}\nabla^2\psi_\alpha+w(\rho)\psi_\alpha, \tag{1}$$

where $w(\rho)$ is the one-body potential, assumed to depend only on the local density ρ. We write the time-discretized form of these equations as

$$|\psi_\alpha^{n+1}\rangle-|\psi_\alpha^n\rangle=-i\epsilon H(n+\tfrac{1}{2})(|\psi_\alpha^n\rangle+|\psi_\alpha^{n+1}\rangle)/2, \tag{2}$$

where n is the index for the nth time step, whose size is ϵ. So far the space discretization is not explicit. The one-body Hamiltonian H, assigned the time $n+\frac{1}{2}$, has to be determined. One condition on H is that it be Hermitian, which insures unitarity and therefore conservation of probability. This is obvious if one writes Eq. (2) as

$$|\psi_\alpha^{n+1}\rangle = U(n+\tfrac{1}{2})|\psi_\alpha^n\rangle, \tag{3}$$

with

$$U(n+\tfrac{1}{2}) = \frac{1-\frac{1}{2}i\epsilon H(n+1/2)}{1+\frac{1}{2}i\epsilon H(n+1/2)}. \tag{4}$$

If H is Hermitian, then U is unitary, and the overlap matrix is constant in time:

$$\langle\psi_\alpha(n+1)|\psi_\beta(n+1)\rangle = \langle\psi_\alpha(n)|\psi_\beta(n)\rangle.$$

Therefore the total particle number $\Sigma_\alpha\langle\psi_\alpha^n|\psi_\alpha^n\rangle$ is conserved.

To determine $H(n+\frac{1}{2})$ more fully, we now invoke the time-discretized version of energy conservation. We are using an interaction of the Skyrme type; this is essential. The conserved energy E, which should be independent of n, is

$$E = \sum_\alpha \langle\psi_\alpha^{n+1}|K+\mathcal{V}(\rho_{n+1})|\psi_\alpha^{n+1}\rangle = \sum_\alpha \langle\psi_\alpha^n|K+\mathcal{V}(\rho_n)|\psi_\alpha^n, \tag{5}$$

where K is the kinetic energy, ρ is the density given by

$$\rho_n(\mathbf{r}) = \sum_\alpha |\langle\mathbf{r}|\psi_\alpha^n\rangle|^2,$$

and

$$\mathcal{V}(\rho) = -\frac{\alpha}{2}\rho + \frac{\beta}{2+\sigma}\rho^{1+\sigma}.$$

On the other hand, according to Eq. (1), the one-body Hamiltonian must have the form

$$H(n+\tfrac{1}{2}) = K + w(n+\tfrac{1}{2},\mathbf{r}).$$

In the continuous-time formulation, w is given by

$$w(\rho) = \frac{\delta}{\delta\rho}[\rho\mathcal{V}(\rho)]. \tag{6}$$

We shall derive a discretized-time $w(n+\frac{1}{2})$ which will reduce to this in the limit $\epsilon\to 0$. A similar result was obtained in Appendix B of Ref. [11], where TDHF was used to study heavy-ion collisions.

It should be obvious that the equation

$$\langle\psi_\alpha^{n+1}|H(n+\tfrac{1}{2})|\psi_\alpha^{n+1}\rangle = \langle\psi_\alpha^n|H(n+\tfrac{1}{2})|\psi_\alpha^n\rangle \tag{7}$$

follows from Eqs. (3) and (4) since $H(n+\frac{1}{2})$ and $U(n+\frac{1}{2})$ certainly commute. Summing Eq. (7) over α we get

$$\sum_\alpha \langle\psi_\alpha^{n+1}|K+w(n+\tfrac{1}{2},\mathbf{r})|\psi_\alpha^{n+1}\rangle = \sum_\alpha \langle\psi_\alpha^n|K+w(n+\tfrac{1}{2},\mathbf{r})|\psi_\alpha^n\rangle,$$

which we can compare with Eq. (5). When we subtract one equation from the other, the kinetic energy drops out and we get

$$\sum_\alpha \langle\psi_\alpha^{n+1}|\mathcal{V}(\rho_{n+1})-w(n+\tfrac{1}{2},\mathbf{r})|\psi_\alpha^{n+1}\rangle = \sum_\alpha \langle\psi_\alpha^n|\mathcal{V}(\rho_n)-w(n+\tfrac{1}{2},\mathbf{r})|\psi_\alpha^n\rangle,$$

which can be rewritten

$$\int d\mathbf{r}\{\rho_{n+1}[\mathcal{V}(\rho_{n+1})-w(n+\tfrac{1}{2},\mathbf{r})]\} = \int dr\{\rho_n[\mathcal{V}(\rho_n)-w(n+\tfrac{1}{2},\mathbf{r})]\}.$$

Even though this is a global condition on $\mathbf{r}$, it can be satisfied by adopting a simple local relation between the potential energies, namely

$$w(n+\tfrac{1}{2}) = \frac{\rho_{n+1}\mathcal{V}(\rho_{n+1})-\rho_n\mathcal{V}(\rho_n)}{\rho_{n+1}-\rho_n}, \tag{8}$$

which is indeed a discretization of Eq. (6). For the particular Skyrme $\mathcal{V}(\rho)$ mentioned above, this is

$$w(n+\tfrac{1}{2}) = -\frac{\alpha}{2}(\rho_{n+1}+\rho_n) + \frac{\beta}{2+\sigma}\frac{(\rho_{n+1}^{2+\sigma}-\rho_n^{2+\sigma})}{(\rho_{n+1}-\rho_n)}.$$

Overall, the advantage of our approach above is that fixing the total energy as a local condition, instead of a global condition, can be easily programed with an iterative procedure similar to the one in Ref. [13], and generalized to more complex systems. The details of the iterative algorithm are given in the next section.

III. NUMERICAL ALGORITHM

The solutions ψ_α that we seek for Eq. (1) are not really periodic; they are quasiperiodic in the Floquet sense [5]. Truly periodic functions ϕ_α can be defined by

$$\psi_\alpha(\mathbf{r},t) = e^{-i\lambda_\alpha t}\phi_\alpha(\mathbf{r},t),$$

with

$$\phi_\alpha(\mathbf{r},t+\tau) = \phi_\alpha(\mathbf{r},t).$$

The quantity λ_α is known either as the quasienergy or as the chemical potential. The equation satisfied by ϕ_α is

$$i\frac{\partial}{\partial t}\phi_\alpha = (H-\lambda_\alpha)\phi_\alpha. \tag{9}$$

We consider the monopole vibrations of ^{4}He, using a simple version of the Skyrme force, and we neglect the Coulomb interaction between protons. This definiteness leads to some simplifications in describing our algorithm. Generalizing to more complex many-body systems is straightforward and is discussed later. For the simple case, the spin and isospin degrees of freedom can be summed over, and the remaining wave function is the solution of a one-dimensional s-wave radial equation with fourfold degeneracy. If we define this wave function u by

$$\phi_\alpha(r,t) = \frac{u_\alpha(r,t)}{r}Y_{lm}(\hat{r})\chi_\alpha(\sigma)\chi_\alpha(\tau), \tag{10}$$

with the normalization $\int dr|u_\alpha(r)|^2 = 1$, then the TDHF equation becomes

$$i\frac{\partial}{\partial t}u_{\alpha}(r,t)=-\frac{1}{2}\frac{\partial^2}{\partial r^2}u_{\alpha}(r,t)+[w(\rho)-\lambda_{\alpha}]u_{\alpha}(r,t),\tag{11}$$

where $w(\rho)=(3/4)t_0\rho+(3/16)t_3\rho^2$ and where the density is

$$\rho(r,t)=\frac{1}{4\pi r^2}\sum_{\alpha}g_{\alpha}|u_{\alpha}(r,t)|^2.\tag{12}$$

For ^{4}He, there is only one occupied orbital and the degeneracy g_{α} equals 4. Hereafter we shall drop the subscript α for simplicity. The parameters t_0 and t_3 are given in Ref. [14] as $t_0=-1090.0$ MeV fm^3 and $t_3=17288.0$ MeV fm^6. The total energy is

$$E=g_{\alpha}\int_0^{\infty}dru^*(r)\left[-\frac{1}{2}\frac{d^2}{dr^2}u(r)+\mathcal{V}(\rho)u(r)\right],\tag{13}$$

where $\mathcal{V}(\rho)=(3/8)t_0\rho+(1/16)t_3\rho^2$.

In searching for the numerical solutions we first discretize this equation in space and time. With $n\epsilon$ denoting the time, Eq. (11) takes the form

$$|u^{n+1}\rangle-|u^{n}\rangle=-i\epsilon[K+w(n+\tfrac{1}{2})-\lambda](|u^{n}\rangle+|u^{n+1}\rangle)/2,\tag{14}$$

where $n=1,2\ldots N$ and the space index is again suppressed. The potential operator w is diagonal in space and given by Eq. (8). The iterative procedure we use to reach the periodic solution is quite general and can be summarized as follows. Here we specialize to the case of monopole nuclear motion.

Initialization. We obtain an initial guess for the period τ_0 and the parameter λ_0 from a trial wave function $|u_0^1\rangle$, which has a large component of an oscillating mode. In our calculation we use as initial trial wave function the ground state of the nucleus in a constraining potential field γr^2, i.e., we let

$$w(\rho)\rightarrow w(\rho)+\gamma r^2,\tag{15}$$

with $\gamma>0$. As in Ref. [15], we examine the trajectory of $\langle r^2\rangle$ in time with $\lambda=0$, and we determine an approximate period $\tau_0\simeq N\epsilon$. From the phase angle $\theta_0=\arg\langle u_0^{N+1}|u_0^1\rangle\simeq\lambda_0\tau_0$, we determine an initial value λ_0.

In the kth iteration of the procedure, we follow the time evolution of the trial wave function $|u_k^n\rangle$ using Eqs. (14) and (8). At the end of the time evolution we obtain a wave function $|u_k^{N+1}\rangle$. The perodicity condition should require $|u_k^1\rangle=|u_k^{N+1}\rangle$ a periodic solution. At each step of the iterations we use $\theta_k=\arg\langle u_k^{N+1}|u_k^1\rangle=\Delta\lambda_k\tau_k$ to correct the value of λ_k with

$$\lambda_{k+1}=\lambda_k+\Delta\lambda_k.$$

For the intermediate steps, Eq. (14) and (8) are exactly satisfied.

For a periodic solution there is one more equation to satisfy exactly,

$$|u_k^1\rangle-|u_k^N\rangle=-i\epsilon[K+w_k(N+\tfrac{1}{2})-\lambda_k](|u_k^1\rangle+|u_k^N\rangle)/2.\tag{16}$$

We use this equation to correct the trial wave function $|u_k^1\rangle$ and obtain a new wave function for the next iteration, $|u_{k+1}^1\rangle$. We first solve Eq. (16) for the wave function $|u_k^1\rangle'$ from the given $|u_k^N\rangle$ and the potential $w_k(N+\frac{1}{2})$, and then take a linear combination of $|u_k^1\rangle$ and $|u_k^1\rangle'$ as the new trial wave function $|u_{k+1}^1\rangle$. Again we analyze $\langle r^2\rangle$ and obtain a new estimate for the period τ_{k+1}.

We repeat the procedure given above until the desired precision for the periodic solution is reached.

IV. DISCUSSION

The search for periodic orbits is different from the search for static solutions, where there exists a definite static solution at a definite energy. For the TDHF periodic orbits the energy range starts with the ground-state energy and increases continuously, and they form a continuously infinite set of solutions. This leads to the following possible difficulty. The iterative procedure starts with a trial wave function, and this wave function needs to be modified at the end of each iteration. When we modify the wave function, this may modify the period or the energy. Thus, even though we have imposed the periodicity condition, we are unable to control the convergence of the approximate solution to some imposed value of the period or of the energy. Consequently we may end up with an iteration procedure which keeps modifying the period or the energy without ever converging. To avoid this problem we have to change our strategy. The new strategy will be referred to hereafter as fine tuning. In fine tuning, instead of fixing the period and the antisliding point (to be discussed shortly), we allow them to change toward the trial wave function at the end of each iteration. Figure 2 shows the effect of fine tuning turned on at the 100th iteration. At that point we see a significant improvement in the periodicity, and from then on the wave function converges rapidly and consistently.

Our calculations show that this procedure is stable and good convergence is reached. A few comments are in order. (i) The conservation of energy and particle number is built into our algorithm at each time and iteration step. We have tested this aspect of our algorithm numerically. A typical run may contain 10^4 time steps, performed in double precision. For each time step the nonlinear equation (14) must be solved. We solve it by successive approximations, which may involve 10 to 20 iterations. At the end of the run we find that the total particle number has been preserved up to one part in 10^{15}, and the total energy up to one part in 10^{13}. Because the iterative procedure preserves the total particle number and the total energy, it is quite stable and the stability is not affected by the number of iterations at each step. (ii) As explained in Ref. [10], the conservation of particle number and energy reduces the total number of equations by 2, which allows us to impose two additional crucial equations, the *phase* condition and the *antisliding* condition. In our realization we impose the *phase* condition by requiring that the first space component of the wave function $u_k^1(1)$ be real. The *antisliding* condition is realized by keeping the real part of $u_k^1(1)$ fixed within certain appropriate bounds. Our experience shows that an adjustment of this value may accelerate the convergence of the iterative procedure. When the

TABLE I. Four of the periodic solutions studied in the present work. Given in the table are the period, the frequency, and the excitation energy for each case. Note that these are members of a continuous family of periodic solutions, obtained from particular initial conditions as described in the text.

Solution	Period (fm/c)	Frequency (MeV/h)	Excitation energy (MeV)
1	44.847	27.646	0.056
2	45.035	27.531	0.913
3	45.500	27.250	3.01
4	46.280	26.790	7.57

convergence slows down, we modify this quantity to a value between $u_k^1(1)$ and $u_k^{N+1}(1)$. (iii) For the periodic orbits at different energies, we have used different magnitudes for the parameter γ of the constraining potential field, ranging from 1.5×10^{-5} to 7×10^{-4} (in natural units). The higher the energy, the stronger the potential strength. (iv) The convergence of the periodicity is measured by the standard deviation of the difference between the space components of the wave functions $|u_k^1\rangle$ and $|u_k^{N+1}\rangle$, i.e.,

$$\sigma_k = \sqrt{\frac{1}{M}\sum_j |u_k^1(j) - u_k^{N+1}(j)|^2},$$

where M is the number of mesh points in space. This is significantly more sensitive than the difference of the positions on the $\langle r^2\rangle$ trajectory.

In order to test this algorithm, we have studied the monopole vibrations of ^{4}He. A set of periodic solutions corresponding to different γ values of the constraining field are given in Table I. However, there is in fact a continuous spectrum of periodic solutions [10]. The trajectory of the squared radius for the mode labeled solution 1 in the table is plotted in Fig. 1 for more than ten periods. The variations observed in this figure give a good idea of the size of the monopole vibrations. No deviation from periodicity can be observed here at all; the difference between two wave functions separated by a period is less than one part in 10^8. The standard deviation is a much more stringent test of periodicity and is shown in Fig. 2 for solution 1, as the equations are iterated to convergence. In this case the convergence parameters require periodicity to one part in 2×10^8. The shape of the vibrations, i.e., the variation of $\rho(r)$, is plotted in Fig. 3.

In Fig. 4 we show the excitation spectrum as a function of the period. We note that the period varies linearly with the

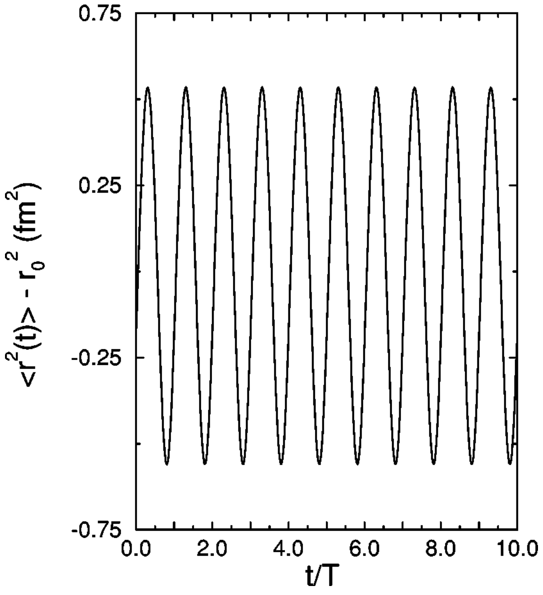

FIG. 1. The trajectory $\langle r^2(t)\rangle$ of monopole vibrations in Helium as a function of time for the case $\tau = 44.847$ fm/c. The constant, $r_0 = 1.797$ fm, is the value of the ground-state rms radius.

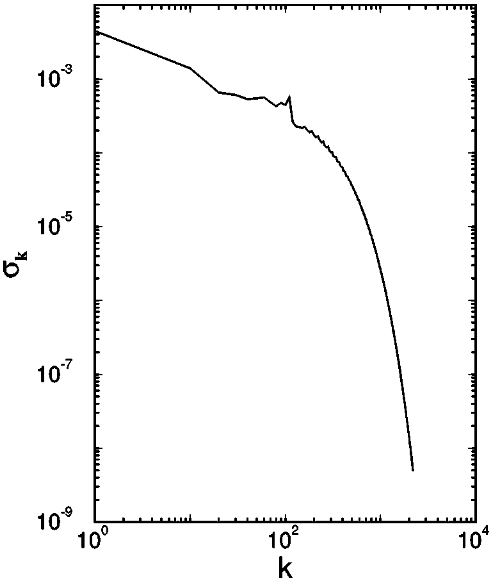

FIG. 2. The standard deviation in the periodic wave function as a function of iteration number for the periodic solution shown in Fig. 1. The structure at iteration number 100 represents the point when the algorithm begins reevaluating the period at each iteration.

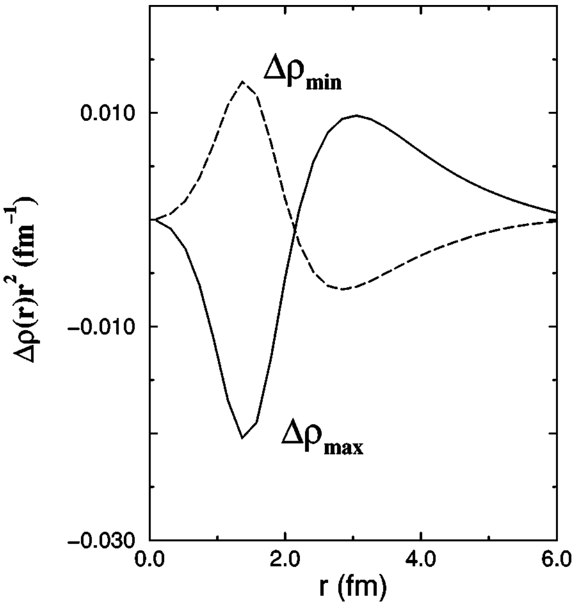

FIG. 3. The difference between the density at time t and the density at time 0 plotted for two different times as a function of r. The two times correspond to maximum (full line) and minimum (dashed line) values of $\langle r^2(t)\rangle$. Note that the densities are weighted with the factor r^2 for display purposes.

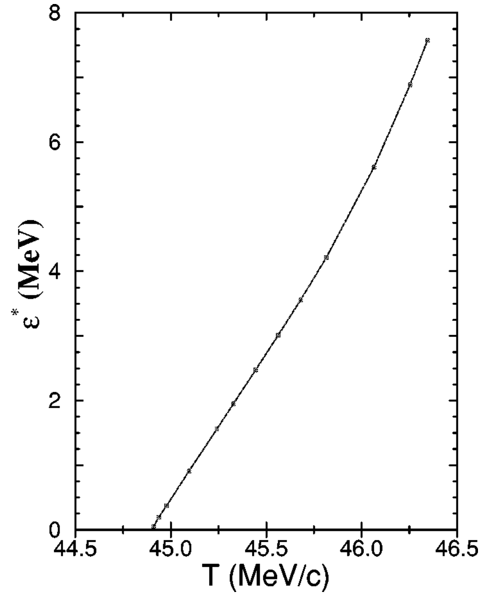

FIG. 4. The *classical-like* excitation spectrum for the monopole vibrations in ^{4}He. Here the spectrum is shown over the limited range calculated for the present paper.

excitation energy when the latter is low; at higher energy the plot acquires some curvature. The RPA frequency can be easily extrapolated from this figure. In order to requantize these solutions, calculations over a broader range of periods or energies would be needed.

For heavier nuclei we need more than one wave function to describe the collective states. We have extended the above formulation to the spherical nuclei ^{16}O and ^{40}Ca. For the case of ^{16}O we used two wave functions, s wave and p wave. For ^{40}Ca we also added a d wave and a second s wave. The orthonormality of the two s waves is ensured by using Gramm-Schmidt orthonormalization at each modification of the wave functions. The above approach can be simply generalized to such systems with multiple wave functions. Our preliminary runs have shown that the iterative procedure works well and gives good results for the TDHF periodic orbits of systems such as ^{16}O and ^{40}Ca.

The Skyrme force used here represents the short range nature of the strong interaction. For an extension of the algorithm to a full Skyrme Hamiltonian for heavy nuclei, the numerical algorithm preserving exact energy conservation is still a major issue. The spin-isospin dependence will not introduce further complications directly, except for an increase in the number of wave functions required. It is the momentum dependence of the Skyrme force which needs to be reconsidered, since it introduces nonlocal interactions in the picture. The problem can be solved, but there is a cost in higher complication.

Spherical symmetry only works for spherical nuclei and monopole excitations. Monopole excitations mainly serve as a testing ground for the algorithm. More interesting physics lies in giant resonances and quadrupole excitations. In these cases we have to replace the spherical symmetry by a rotational symmetry, and we have to describe the nucleus in two or even three space dimensions. Even though the algorithm may not change, the increase in space dimensions will cause a dramatic increase in needed computational resources, since it involves an increase in the number of variables by a dimension factor, accompanied in all likelihood by a slowdown of the convergence sequence. The increase in computation is often measured by the square of the dimension factor.

It seems, therefore, that moving up in space dimensions cannot be done unless we can achieve a radical improvement in the speed of convergence of our algorithm. Such an improvement, based on the ideas of Ref. [10], is in fact being implemented right now and we hope to report on the results in the near future.

V. CONCLUSION

In this article we have proposed a numerical algorithm which preserves the total particle number and the total energy. These conservation laws are essential for the calculation of large amplitude periodic orbits. We have demonstrated the use of the algorithm for the monopole vibrations in ^{4}He, employing simple Skyrme forces. As has been widely discussed in the literature, these periodic solutions may have great relevance to the collective excitations of a many-particle system. We will apply the method developed here to realistic quantum systems in nuclear physics and molecular physics.

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