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Monopole collective motion in helium and oxygen nuclei

J.-S. Wu,[1] M. R. Strayer,[2] and M. Baranger[3]
[1]*Department of Natural Sciences, Fayetteville State University, Fayetteville, North Carolina 28301*
[2]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*
[3]*Center for Theoretical Physics and Laboratory for Nuclear Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*

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We review the rationale for basing the calculation of collective motion on the periodic solutions of the time-dependent Hartree-Fock mean field. With suitable discretization, we find a family of these solutions and we apply a simple quantization rule. Results are presented for ^{4}He and ^{16}O. [S0556-2813(99)04009-1]

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I. INTRODUCTION

In a previous paper [1], we reported some preliminary calculations of the quasiperiodic solutions of the nonlinear time-dependent Hartree-Fock (TDHF) equations for the monopole oscillations of the ^{4}He nucleus. The present paper reports some additional results, with some improvements in the method, for both ^{4}He and ^{16}O.

The TDHF approximation for nuclear phenomena [2] is a particular example of a very general method for dealing with many-body and field-theoretical problems, namely, the mean field approximation [3]. The essence of the mean field approach is the assumption that there exists a single function of space and time, as well as other coordinates, the mean field, which is the approximate, average result of the quantum fluctuations undergone by the system. For instance, in the nuclear TDHF case, the mean field is the single-particle (SP) potential which constitutes the major part of the interaction seen by each particle. One aspect of all mean field approximations is that the mean field is treated like a classical quantity, a *c* number. For the nuclear TDHF example, once again, the SP potential can be plotted as a function of $\mathbf{r}$ and t (possibly nonlocal), doing whatever it does when the nucleus rotates, or changes its shape, or breathes, or when two nuclei collide, just like our classical eye and our classical brain would have it do.

The consequence of such an approach is that, once it has been carried out, one has to requantize somehow. The lack of requantization is the basic reason why TDHF theory does not work for predicting all of the results of heavy ion collisions, for instance. We are not claiming here that TDHF theory treats a nucleus completely classically. Certainly not; the SP wave functions are still Schrödinger probability amplitudes, of course. But having made one object classical, the mean field, is enough to require repair. Thus every successful TDHF application is followed by a second stage, the requantization. This stage is always present, explicitly or implicitly.

The TDHF approximation is nonlinear. When it is linearized in the vicinity of the ground state, it becomes the random phase approximation (RPA), a small amplitude limit [3]. The RPA has been used extensively to describe nuclear collective motion [4], but the accuracy of such an approach is open to question. Excitation energies and transition probabilities can be fitted as long as one allows for adjustable parameters. But our calculations show the TDHF equations to be highly nonlinear at the energies of interest for the type of nuclear collective motion we are studying here.

In the present work we are dealing only with bound collective motion, starting with monopole vibrations of closed-shell nuclei. Our first step consists in finding families of periodic solutions of the TDHF equations [3]. Our second step is to requantize. Why periodic solutions? Actually, it is not necessary to go through periodic solutions; it is just a convenience. The periodic solutions, which we also call cycles, come to mind for at least two reasons. The first is that they are the classical objects that share one important property with the quantal stationary states: they are invariants of the motion. This leads one to think that there might be some connection between the stationary states and the cycles. The second reason is that they are finite in duration; after one period, they just repeat themselves. If, on the other hand, one tries to quantize a nonperiodic TDHF solution, one will have the problem of deciding how much of this infinitely long function of time is necessary for quantization, and therefore how much of it one must calculate.

Little will be said in this paper about quantization. We use the Bohr-Sommerfeld formula, derived in this context by a variety of authors long ago [5]. Actually, this formula is only a very rough approximation. We are actively engaged in working out a much better quantization method.

The present work constitutes only the early steps in what is expected to be a large endeavor, extending to many kinds of collective motion and to all sorts of nuclei, including heavy ones. In keeping with this situation, we are using for this beginning a simple version of the Skyrme potential [3], spin and isospin independent, with an attractive term proportional to the density and a repulsive term proportional to the square of the density. It contains two arbitrary coefficients which can be fitted to give a fairly good account of the periodic table [6]. It is also possible, for each closed-shell nucleus, to choose these coefficients so as to give correctly the total energy and the nuclear radius.

Section II of the paper reviews this nuclear model. Section III examines the cycles (which are actually *quasiperiodic*) and sets down the quantization rule. Section IV discusses the space and time discretizations which are necessary for a numerical calculation. This includes the necessity of obeying exactly the conservation laws for energy and probability. Section V gives some details of the numerical method. Section VI presents results for ^{4}He and ^{16}O. Section VII contains some conclusions and outlook.

II. MODEL

One way to derive the TDHF equations is by using the time-dependent variational principle with a Slater determinant trial function [7]. Let the latter be made up of the SP wave functions $\psi_\alpha(\mathbf{r},t)$, each with degeneracy g_α. Degeneracy is possible because we are ignoring the spin and isospin degrees of freedom. For instance, for ^{4}He there is but a single $\psi(\mathbf{r},t)$, with $g=4$. Under these assumptions, the quantity to be varied, which generalizes Hamilton's action, is written

$$\mathcal{S}[\psi^*,\psi]=\int dt\left[\sum_\alpha g_\alpha\int d^3r\ \psi_\alpha^*(\mathbf{r},t)\,i\partial_t\psi_\alpha(\mathbf{r},t) - \mathcal{H}[\psi^*,\psi]\right], \tag{1}$$

where $\mathcal{H}$ is the many-body Hamiltonian. We follow the usual classical mechanics convention of calling this quantity $\mathcal{H}$, the Hamiltonian, when it is considered as a function of the independent variables, and of calling it E, the energy (i.e., the total many-body energy), when it is considered as a simple number. We use units such that $\hbar=c=m=1$. The wave function ψ_α and its complex conjugate ψ_α^* must be treated as independent variables in the variation.

Before writing the Skyrme Hamiltonian $\mathcal{H}$, we introduce the nuclear density

$$\rho(\mathbf{r},t)=\sum_\alpha g_\alpha|\psi_\alpha(\mathbf{r},t)|^2. \tag{2}$$

We define also the kinetic energy operator K:

$$\int d^3r\ \psi^*(\mathbf{r},t)K\psi(\mathbf{r},t)=\frac{1}{2}\int d^3r\ |\nabla\psi(\mathbf{r},t)|^2 = -\frac{1}{2}\int d^3r\ \psi^*(\mathbf{r},t)\nabla^2\psi(\mathbf{r},t). \tag{3}$$

Then $\mathcal{H}$ has the form

$$\mathcal{H}[\psi^*,\psi]=\int d^3r\sum_\alpha g_\alpha\psi_\alpha^*(\mathbf{r},t)[K+\mathcal{V}\{\rho(\mathbf{r},t)\}]\psi_\alpha(\mathbf{r},t), \tag{4}$$

which can also be written

$$\mathcal{H}[\psi^*,\psi]=\int d^3r\left[\frac{1}{2}\sum_\alpha g_\alpha|\nabla\psi_\alpha|^2+\rho\mathcal{V}(\rho)\right]. \tag{5}$$

The many-body potential $\mathcal{V}(\rho)$ is given by

$$\mathcal{V}(\rho)=-\alpha\rho+\beta\rho^2. \tag{6}$$

The two positive constants α and β are connected as follows to the usual [3] Skyrme parameters t_0 and t_3:

$$\alpha=-\frac{3}{8}t_0,\qquad \beta=+\frac{1}{16}t_3. \tag{7}$$

(Note that the definitions of α and β differ from those we used in [1].) The variation of $\mathcal{S}$ with respect to the ψ's and ψ^*'s yields the Hamilton-like equations

$$i\partial_t\psi_\alpha(\mathbf{r},t)=\frac{\delta\mathcal{H}}{\delta\psi_\alpha^*(\mathbf{r},t)},$$

$$-i\partial_t\psi_\alpha^*(\mathbf{r},t)=\frac{\delta\mathcal{H}}{\delta\psi_\alpha(\mathbf{r},t)},$$

which are the TDHF equation and its complex conjugate. The explicit form of the former is

$$i\partial_t\psi_\alpha(\mathbf{r},t)=H(\mathbf{r},t)\psi_\alpha(\mathbf{r},t), \tag{8}$$

with the SP Hamiltonian H given by

$$H(\mathbf{r},t)=K+w[\rho(\mathbf{r},t)] \tag{9}$$

and the one-body potential

$$w(\rho)=\frac{d}{d\rho}[\rho\mathcal{V}(\rho)]. \tag{10}$$

With expression (6) for $\mathcal{V}$, this is

$$w(\rho)=-2\alpha\rho+3\beta\rho^2. \tag{11}$$

We note in passing that a nonlinear Schrödinger equation very similar to Eq. (8), with a density-dependent potential, was used by one of us [8] in an exploration of nuclear hydrodynamics.

There are two conservation laws associated with TDHF motion, and they play an important role in the search for cycles. They are the conservation of the overlaps between SP wave functions and the conservation of the total many-body energy. The former follows in the usual way from the Hermiticity of the SP Hamiltonian (9). It implies that the motion of the Slater determinant is unitary and that the normalizations are conserved separately for each ψ_α. To show the conservation of the total energy E, which is expression (5), let us calculate its time derivative

$$\frac{dE}{dt}=\int d^3r\left[\frac{1}{2}\sum_\alpha g_\alpha\partial_t|\nabla\psi_\alpha|^2+\frac{d}{d\rho}\{\rho\mathcal{V}(\rho)\}\partial_t\rho\right]. \tag{12}$$

By Eq. (10) this can be rewritten

$$\frac{dE}{dt}=\sum_\alpha g_\alpha\int d^3r\left[\frac{1}{2}\partial_t|\nabla\psi_\alpha|^2+w(\rho)\partial_t|\psi_\alpha|^2\right]. \tag{13}$$

And this last expression vanishes, separately for each α, as a consequence of the TDHF equation and its complex conjugate. Indeed, it can be written

$$\langle \partial_t \psi_\alpha | H | \psi_\alpha \rangle + \langle \psi_\alpha | H | \partial_t \psi_\alpha \rangle,$$

which vanishes by virtue of

$$i | \partial_t \psi_\alpha \rangle = H | \psi_\alpha \rangle \quad \text{and} \quad -i \langle \partial_t \psi_\alpha | = \langle \psi_\alpha | H.$$

Note, however, that the SP energies are not conserved and, as usual, the total energy is not the sum of the SP energies.

III. CYCLES

The TDHF equation (8) does have truly periodic solutions. In general, however, such a solution does not have the ψ_α's correctly normalized. This is because the equation is nonlinear, and one cannot simply multiply a solution by an arbitrary constant. If we were doing field theory instead of many-body physics, these solutions would be perfectly acceptable. But here we require unit normalizations. The price of this requirement is that we have to be satisfied with quasiperiodic solutions, i.e., solutions which repeat themselves after period τ except for a phase factor

$$\psi_\alpha(\mathbf{r},t+\tau) = e^{-i\theta_\alpha} \psi_\alpha(\mathbf{r},t). \tag{14}$$

The angle θ_α is sometimes called the Floquet index. We can then define a new function ϕ_α by the formula

$$\psi_\alpha(\mathbf{r},t) = e^{-i\lambda_\alpha t} \phi_\alpha(\mathbf{r},t), \tag{15}$$

and by choosing λ_α such that

$$\lambda_\alpha \tau = \theta_\alpha, \tag{16}$$

we can make ϕ_α truly periodic:

$$\phi_\alpha(\mathbf{r},t+\tau) = \phi_\alpha(\mathbf{r},t). \tag{17}$$

The cost now is that the TDHF equation contains an additional real term λ_α, which we call the quasienergy. The equation is

$$i\partial_t \phi_\alpha(\mathbf{r},t) = [K + w\{\rho(\mathbf{r},t)\} - \lambda_\alpha] \phi_\alpha(\mathbf{r},t). \tag{18}$$

We can also think of λ_α as a Lagrange multiplier that we introduce to satisfy the constraint on the normalization of ϕ_α. The density ρ and the SP potential w are truly periodic, and ψ_α is a true Floquet solution in this periodic potential. Moreover, the SP density matrix and, hence, the expectations of all SP operators are also periodic. Hence it is reasonable to think of these solutions as periodic and to drop the ''quasi'' qualifier. From now on we deal only with the wave functions ϕ and we call the solutions cycles.

As in all generic Hamiltonian problems, the cycles occur in one-parameter families. See Ref. [9] for an example. Along such a family, the energy changes continuously, and so do the period, the action, and other observables. A common way of looking at things is to represent each family by a line in the (E,τ) plane. This is known as an (E,τ) plot. On this (E,τ) plot, one can follow how the various families connect to each other through bifurcations of many kinds. The existence of bifurcations is one of the signatures of nonlinearity and chaos. One aim of our work could be to understand exactly what bifurcations there are and how much nonlinearity there is in nuclear collective motion. We have not progressed very much in that direction yet, but we expect to work on it in the future. The figures of Sec. VI do not show any bifurcations, but this does not mean that they do not exist.

For a generic Hamiltonian problem in classical mechanics, the number of cycle families is infinite. In fact, the cycles are dense in phase space. But the number of cycles whose period is smaller than some given τ, and with a given energy, is finite. These shortest cycles are the most important ones. They organize phase space around themselves. Stable cycles lie at the center of regular regions and unstable cycles at the center of chaotic regions. One knows a lot about the system already if one knows only a few of its shortest cycles. For our case of many-body collective motion, the situation is exactly the same with one possible difference. Collective motion is often especially slow compared to other possible motions of the system. This slowness leads to longer periods. Hence the cycles of interest in collective motion are not necessarily the absolute shortest. For instance, in the RPA treatment of the monopole oscillations of a closed-shell nucleus, the breathing mode is the solution with the longest period. The possible interaction between one long-period family of collective cycles and a number of other families of shorter periods is one of the causes of dissipation.

For the present paper we have calculated only one family of cycles, which is obviously a collective family. We know that other families exist because we have seen them numerically, and in any case they are present in the linear limit of the RPA. But we are not prepared to talk about them at this time.

Once the families (or family) of cycles have been found, the second step in the approach is quantization. As we said in Sec. I, our provisional recipe for this is the Bohr-Sommerfeld formula. For the future, we are working on a much better method. The Bohr-Sommerfeld formula [5] involves the reduced action J^P, which is the same as the familiar $\oint \mathbf{p}\cdot d\mathbf{q}$, but calculated for the periodic part ϕ of the wave function, rather than ψ itself:

$$\begin{aligned} J^P &= i\int_0^\tau dt \sum_\alpha g_\alpha \int d^3r\, \phi_\alpha^*(\mathbf{r},t)\partial_t \phi_\alpha(\mathbf{r},t) \\ &= -i\int_0^\tau dt \sum_\alpha g_\alpha \int d^3r\, [\partial_t \phi_\alpha^*(\mathbf{r},t)] \phi_\alpha(\mathbf{r},t). \end{aligned} \tag{19}$$

Then the quantization rule is

$$J^P = nh, \tag{20}$$

where n is an integer and Planck's constant h is 2π in our units. The reduced action (19) increases smoothly along the (E,τ) line, beginning at the value 0 for the ground state, where ϕ_α is independent of t. The Bohr-Sommerfeld rule says that the energy of the first excited state is the energy at which J^P reaches 2π.

IV. DISCRETIZATION

We use only the simplest possible discretizations, so that we may reserve the major fraction of the numerical power for obtaining the cycles. The angular part of the calculations is usually completely standard and in fact, for the present paper, trivial. Hence, the wave functions to be discretized have two variables, the radius and the time. We replace $\phi(r,t)$ by ϕ_{mn}, where m is a space index and n a time index. The interesting discretization problems concern the time dependence; they arise because we want ϕ to be periodic. The space discretization does not matter.

We have used two kinds of space discretization, which we call *end point* and *midpoint*. They seem to be comparable in accuracy. Consider a function $f(r)$ defined for $0 \leqslant r \leqslant R$ and required to vanish at both ends, as is the case with the radial wave functions we shall need. Let the interval be divided into equal subintervals of size σ. In the end point method, f_m is the value of $f(r)$ at one of the points separating two subintervals. If there are $M+1$ subintervals, there are M variables f_m, with $1 \leqslant m \leqslant M$. We may also introduce f_0 and f_{M+1}, but they vanish. The three formulas needed to do all the calculations are

$$\int_0^R dr f(r) = \sigma \sum_{m=1}^{M} f_m, \tag{21}$$

$$\left(\frac{d^2 f}{dr^2}\right)_m = \frac{1}{\sigma^2}(f_{m+1} - 2f_m + f_{m-1}), \tag{22}$$

for m on the interval $(1 \leqslant m \leqslant M)$, and

$$\int_0^R dr \left(\frac{df}{dr}\right)^2 = \frac{1}{\sigma} \sum_{m=0}^{M} (f_{m+1} - f_m)^2. \tag{23}$$

It is important to note that the relation

$$\int_0^R dr \left(\frac{df}{dr}\right)^2 = -\int_0^R dr f \left(\frac{d^2 f}{dr^2}\right) \tag{24}$$

remains true after the discretization; otherwise, the Hermiticity of the kinetic energy operator would be compromised. In the midpoint method, on the other hand, f_m is the value of $f(r)$ in the middle of a subinterval. Let there be M subintervals, this time, and M variables f_m, with $1 \leqslant m \leqslant M$. To express the fact that $f(r)$ vanishes at $r=0$ and $r=R$, we must introduce two more quantities

$$f_0 = -f_1 \quad \text{and} \quad f_{M+1} = -f_M. \tag{25}$$

Of the three formulas needed, the first two, Eqs. (21) and (22), are the same as before. But Eq. (23) is changed to

$$\int_0^R dr \left(\frac{df}{dr}\right)^2 = \frac{1}{\sigma}\left[2f_1^2 + \sum_{m=1}^{M-1} (f_{m+1} - f_m)^2 + 2f_M^2\right]. \tag{26}$$

Again, Eq. (24) remains true after discretization.

Now we consider the time discretization. When one calculates cycles for Hamiltonian systems with many degrees of freedom, it is very important to have a time discretization which conserves exactly the discretized approximations of all the constants of the motion. This is because the phenomenon known as *sliding* tends to make the computer algorithm very unstable otherwise [10]. In the present case, given the conservation laws mentioned in Sec. II, it is necessary first to make each step of the propagation strictly unitary and, second, to conserve the total energy. The discretization that we used in Ref. [1], which had been used much earlier in Ref. [11], does both. If n is the time index and ϵ is the size of the time step, unitarity is ensured by writing

$$|\phi_\alpha^{n+1}\rangle = U_\alpha(n+\tfrac{1}{2})|\phi_\alpha^n\rangle, \tag{27}$$

with

$$U_\alpha(n+\tfrac{1}{2}) = \frac{1 - \frac{1}{2} i\epsilon H_\alpha(n+\frac{1}{2})}{1 + \frac{1}{2} i\epsilon H_\alpha(n+\frac{1}{2})}. \tag{28}$$

Here $H_\alpha(n+\frac{1}{2})$ is the SP Hamiltonian of Eq. (18) taken at time $(n+\frac{1}{2})\epsilon$,

$$H_\alpha(n+\tfrac{1}{2}) = K + w[\rho(n+\tfrac{1}{2})] - \lambda_\alpha, \tag{29}$$

and since H_α is Hermitian, U_α is obviously unitary. The discretized equivalent of Eq. (10) is

$$w[\rho(n+\tfrac{1}{2})] = \frac{\rho_{n+1}\mathcal{V}(\rho_{n+1}) - \rho_n \mathcal{V}(\rho_n)}{\rho_{n+1} - \rho_n}. \tag{30}$$

With the potential (6), this becomes

$$w[\rho(n+\tfrac{1}{2})] = -\alpha(\rho_{n+1} + \rho_n) + \beta(\rho_{n+1}^2 + \rho_{n+1}\rho_n + \rho_n^2). \tag{31}$$

It is now easy to show conservation of energy, using again the reasoning used at the end of Sec. II to show it for continuous time. For this purpose, it is not necessary to discretize space explicitly; only time discretization is involved. The energy (4), discretized, becomes

$$E_n = \sum_\alpha g_\alpha \langle \phi_\alpha^n | K | \phi_\alpha^n \rangle + \int d^3r\, \rho_n \mathcal{V}(\rho_n). \tag{32}$$

Instead of the time derivative (12) we calculate

$$E_{n+1} - E_n = \sum_\alpha g_\alpha [\langle \phi_\alpha^{n+1} | K | \phi_\alpha^{n+1} \rangle - \langle \phi_\alpha^n | K | \phi_\alpha^n \rangle] + \int d^3r [\rho_{n+1}\mathcal{V}(\rho_{n+1}) - \rho_n \mathcal{V}(\rho_n)]. \tag{33}$$

By Eq. (30) this can be written

$$E_{n+1}-E_n=\sum_\alpha g_\alpha[\langle\phi_\alpha^{n+1}|K|\phi_\alpha^{n+1}\rangle-\langle\phi_\alpha^n|K|\phi_\alpha^n\rangle]$$
$$+\sum_\alpha g_\alpha\int d^3r[\phi_\alpha^*(\mathbf{r},n+1)\phi_\alpha(\mathbf{r},n+1)$$
$$-\phi_\alpha^*(\mathbf{r},n)\phi_\alpha(\mathbf{r},n)]w(\rho(\mathbf{r},n+\tfrac{1}{2}))\qquad(34)$$

or

$$E_{n+1}-E_n=\sum_\alpha g_\alpha[\langle\phi_\alpha^{n+1}|H_\alpha(n+\tfrac{1}{2})+\lambda_\alpha|\phi_\alpha^{n+1}\rangle$$
$$-\langle\phi_\alpha^n|H_\alpha(n+\tfrac{1}{2})+\lambda_\alpha|\phi_\alpha^n\rangle].\qquad(35)$$

The brackets in this last expression vanish for each α as a result of Eq. (27), since $U_\alpha(n+\frac{1}{2})$ and $H_\alpha(n+\frac{1}{2})$ commute. Hence $E_{n+1}=E_n$.

V. NUMERICAL METHOD

The numerical method is the same one we used in [1], with some improvements. Many of our results are new, however, including everything concerning ^{16}O. This is probably our last paper using this method. We already mentioned in [1], Sec. IV, that we were developing a much more powerful and stable method, based on the ideas of Ref. [10], and completely different from the present approach. The new method is now working well, and we are switching to it for future investigations.

Returning now to the old method, we use as a starting point a solution of the static Hartree-Fock problem in which the SP Hamiltonian is Eq. (9), with ρ independent of time, plus a constraining potential of the form γr^2. The values of γ range from 1.5×10^{-5} to 7×10^{-4} (in natural units), with higher γ's leading to higher energy cycles. These static equations are solved in imaginary time by iteration. Then we ''let loose'' this originally static Slater determinant by removing γr^2, and it propagates according to the TDHF equation (8) or (18). It has been known for some time [12] that the TDHF solution so obtained is almost periodic, at least for sufficiently low energies. Our job is then to modify it gently until it becomes rigorously so. We do this by successive approximations, which are complicated by the fact that the equations are nonlinear, and that τ, E, and λ all change with each iteration.

Some details are given in Sec. IV of [1]. The iteration procedure can be summarized as follows. Denote by $\phi_\alpha^{[k]}$, $\lambda_\alpha^{[k]}$, $\tau^{[k]}$ the values of ϕ_α, λ_α, τ for the kth trajectory, and by $U^{[k]}(t,t')$ the appropriate evolution operator. Then the steps are the following: (i) Define initial values $\tau^{[0]}$, $\lambda_\alpha^{[0]}$, and $\phi_\alpha^{[0]}(\mathbf{r},0)$ at a particular energy E. (ii) For the kth iteration, if the evolution $U^{[k]}(\tau^{[k]},0)$ is unity, then stop. Otherwise, (iii) evolve a complete trajectory, i.e. $\phi_\alpha^{[k]}(\mathbf{r},\tau^{[k]})=U^{[k]}(\tau^{[k]},0)\phi_\alpha^{[k]}(\mathbf{r},0)$. (iv) Compute values of τ, λ_α, and ϕ_α at the $(k+1)$th iteration from their values at the kth iteration. Although the evolution conserves the energy exactly, the process for defining an improved value of the state ϕ requires a projection to keep the energy constant, $\phi_\alpha^{[k+1]}(\mathbf{r},0)=\mathcal{P}_E[c_0\phi_\alpha^{[k]}(\mathbf{r},0)+c_1\phi_\alpha^{[k]}(\mathbf{r},\tau^{[k]})]$. Otherwise, at high excitations, the energy drops down uncontrollably. This projection is the most important difference with the method of Ref. [1]. Steps (ii)–(iv) must be repeated until convergence is achieved.

A few comments are in order. (a) 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 10^3 time steps, performed in double precision. For each time step the nonlinear equations must be solved. We solve them by successive approximations, which may involve 10–20 iterations. At the end of the run we find that the total particle number has been preserved up to 1 part in 10^{15} and the total energy up to 1 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. (b) As explained in Ref. [10], the conservation of particle number and energy reduces the total number of equations by $A+1$, which allows us to impose $A+1$ additional crucial equations, the *phase* condition for each single-particle wave function and the *antisliding* condition. In our realization of these conditions, we impose the *phase* condition by requiring that the first space component at time 0 for each α, $u_\alpha(1,0)$, be real. The *antisliding* condition is realized by keeping the real part of $u_\alpha(1,0)$, for one α only, fixed within certain appropriate bounds. Our experience shows that an adjustment of this value may accelerate the convergence of the iterative procedure. (c) The convergence of the periodicity is measured by the standard deviation of the difference between the space components of the wave functions at $t=0$, and $t=\tau$,

$$\sigma^2=\frac{1}{MA}\sum_{m,\alpha}|u_\alpha(m,1)-u_\alpha(m,N+1)|^2,\qquad(36)$$

where M is the number of mesh points in space. This is significantly more sensitive than simply looking at the initial and final values of $\langle r^2\rangle$.

VI. RESULTS

We have applied the above model and method to the calculation of monopole vibrations in ^{4}He and ^{16}O, disregarding the Coulomb interaction between the protons. In helium there is only one wave function (only one α) with degeneracy $g=4$. In oxygen there are two α's, one s wave with degeneracy $g_s=4$ and one p wave with $g_p=12$ (recall that our Skyrme interaction has no spin dependence). As usual we can write $\phi_\alpha(\mathbf{r},t)$ in terms of a radial wave function $u_\alpha(r,t)$ and a spherical harmonic, times a spin-isospin function which we do not need to show,

$$\phi_\alpha(\mathbf{r},t)=\frac{1}{r}u_\alpha(r,t)Y_{l_\alpha m}(\hat{r}),\qquad(37)$$

and u_α must vanish at $r=0$ and at some large box radius $r=R$. The normalization is $\int dr|u_\alpha(r)|^2=1$ and the density is given by

TABLE I. The parameters t_0 and t_3 defining the interaction, the Hartree-Fock ground state energy and rms radius, the Bohr-Sommerfeld monopole excitation energy, and the period for the nuclei ^{4}He and ^{16}O.

	^{4}He	^{16}O
t_0 (MeV fm^3)	−1090.0	−1132.4
t_3 (MeV fm^6)	17288.0	23610.4
$E_{\mathrm{g.s.}}$ (MeV)	−33.24	−128.0
$a_{\mathrm{g.s.}}$ (fm)	1.732	2.710
E_m^* (MeV)	26.49	29.49
τ_m (fm/c)	48.16	42.88

$$\rho(r,t)=\frac{1}{4\pi r^2}\sum_\alpha g_\alpha|u_\alpha(r,t)|^2. \tag{38}$$

In terms of the radial wave function, the TDHF equation (18) becomes

$$i\partial_t u_\alpha(r,t)=-\frac{1}{2}\partial_r^{\,2}u_\alpha(r,t)+\left[\frac{l_\alpha(l_\alpha+1)}{2r^2}+w\{\rho(r,t)\}-\lambda_\alpha\right]u_\alpha(r,t). \tag{39}$$

The parameters t_0 and t_3 are given in Table I for each nucleus. For ^{4}He, they are the parameters of Ref. [6]. For ^{16}O, they are fitted in the HF ground state to the rms radius and the binding energy. We have calculated one family of cycles for each nucleus, going from the breathing mode RPA solution of the TDHF equation at low energy, up to the excitation energy where the reduced action J^P equals 2π, which is the energy where the Bohr-Sommerfeld rule would locate the first excited state.

We begin by showing in Fig. 1 a typical rate of convergence for the iteration procedure. This is for a cycle of ^{16}O partway up to the first excited quantized energy. Figure 2 displays three properties of the ^{4}He family. The bottom graph is the (E,τ) plot, from the RPA to the Bohr-Sommerfeld excited state. The middle graph is the reduced action, which goes from 0 to 2π. And the top graph is the quasienergy.

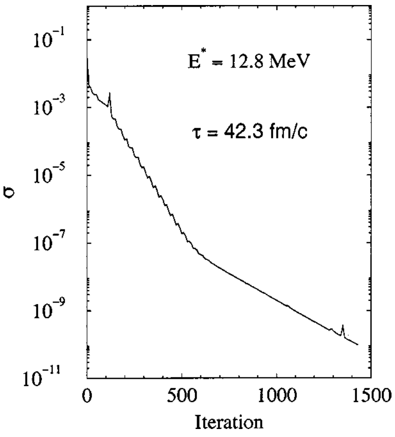

FIG. 1. The standard deviation in the periodic wave function, Eq. (36), as a function of iteration number for a cycle of ^{16}O. The excitation energy and the period are on the figure.

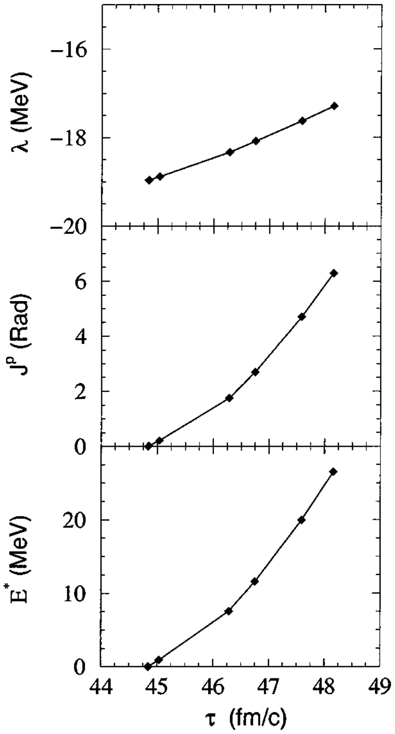

FIG. 2. The excitation energy E^*, the reduced action J^P, and the quasienergy λ as functions of the period for the monopole vibrations in the nucleus ^{4}He.

Figure 3 is the same for ^{16}O. This time there are two quasienergies, one for the s state and one for the p state. We note that the oxygen plots are much more linear than those for helium. This is presumably due to the much larger number of particles in oxygen, which makes the motion much more collective for a given excitation energy.

Figure 4 demonstrates that, in helium too, the (E,τ) plot can be perfectly linear at sufficiently low energy. These considerations lead us to surmise that problems due to nonlinearity and chaos will be more severe in cases of not-very-collective motion. Of course, from the point of view of monopole collective motion, helium is the least interesting nucleus. But it is also the easiest to calculate, which makes it a precious entity to test new methods on.

The coordinate space behavior of the helium cycle whose reduced action is 2π is illustrated in Fig. 5. Shown in the figure are the Hartree-Fock ground-state density and snapshots of the periodic density at two times: t_1, the time at which the rms radius is a maximum, and t_2, when it is a minimum. An important feature of this figure is the large amplitude of the spatial oscillation of the central density. In this case the collective motion is very far removed from the approximations that validate the RPA method. For large amplitude oscillations the local density is far from harmonic. It

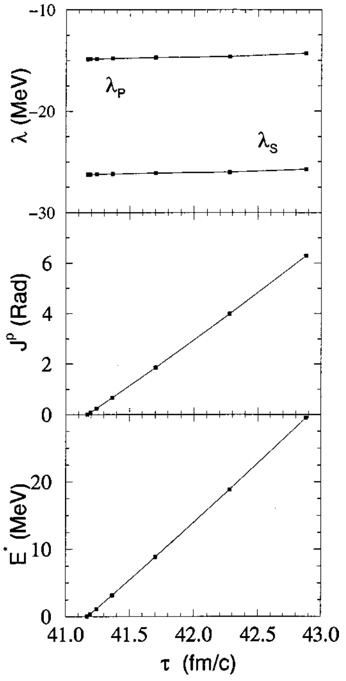

FIG. 3. The excitation energy E^*, the reduced action J^P, and the quasienergies λ_s and λ_p as functions of the period for the monopole vibrations in the nucleus ^{16}O.

is more difficult to compress the central nuclear matter than to stretch it.

Similar plots for oxygen are in Fig. 6. Again we compare the ground state density with that of the cycle whose reduced action is 2π. Here we observe that the difference between the ground state density and the periodic density comes mainly from the p-wave contribution and peaks in the surface. As with ^{4}He, the amplitude of the periodic motion is large and not calculable with the RPA method. For both nuclei, it appears that the motion undergone by the excited

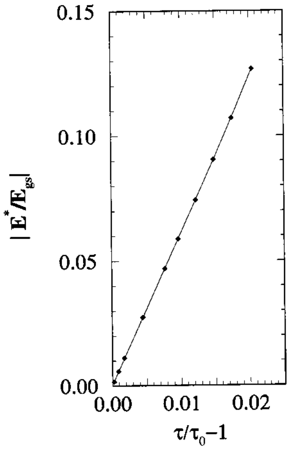

FIG. 4. The (E,τ) plot for the low-excitation cycles of ^{4}He, illustrating the linear behavior from which the RPA period can be extrapolated. The curves are scaled by the Hartree-Fock ground state energy $E_{\mathrm{g.s.}} = -33.24$ MeV and by the RPA period $\tau_0 = 44.77$ fm/c.

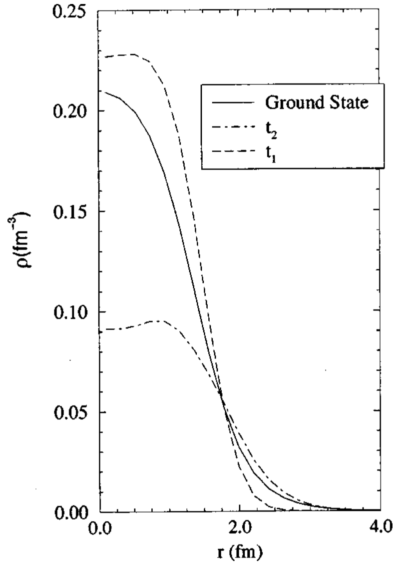

FIG. 5. The nuclear density vs r in ^{4}He in the ground state and in the TDHF cycle whose reduced action is exactly 2π. The times t_1 and t_2 correspond to maximum and minimum rms radius, respectively, and they are half a period apart.

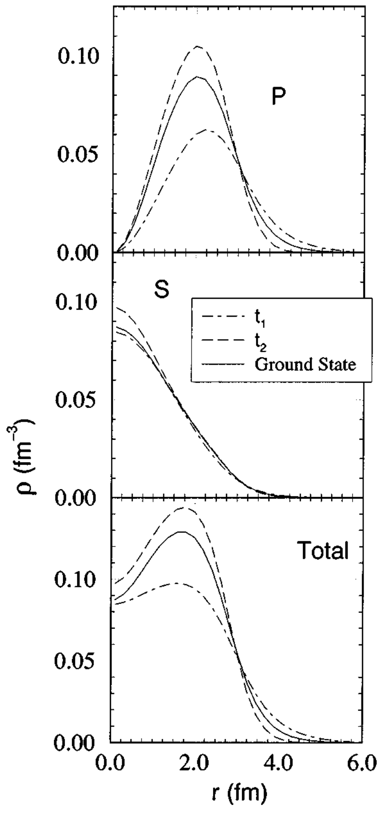

FIG. 6. The HF ground state density of ^{16}O compared to the periodic TDHF density at two times: t_1, at which the rms radius is maximum, and t_2, at which it is minimum. The cycle is chosen so that the reduced action is exactly 2π. The contributions to the total density from the s-wave and the p-wave components are compared separately.

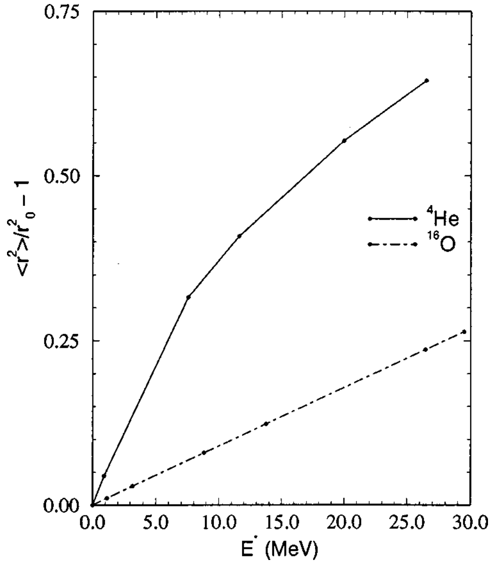

FIG. 7. The fractional change in the time-averaged mean square radius, $(\langle r^2\rangle / r_0^2) - 1$, as a function of excitation energy for the cycle families in ^{4}He and ^{16}O. The radius of the Hartree-Fock ground state is r_0.

state is rather complex, though this cannot be seen directly from the (E, τ) plot. As more and more energy goes into exciting periodic motion, the nucleus appears to undergo stretching at the surface, as seen in Fig. 7, which shows the time average of the mean square radius as a function of the excitation energy for both ^{4}He and ^{16}O. Again we would like to emphasize that the periodic motion consists of large amplitude collective behavior and is very different from the small amplitude linear response of the nucleus as calculated with the RPA. One would expect that the quantized solution from this approach would be especially meaningful for nuclei with a double-well structure of the energy surface in configuration space, when the large amplitude oscillations would be dramatically different from the oscillations around a single local minimum, and the RPA approximation would be totally invalid.

VII. CONCLUSION AND OUTLOOK

The main conclusion is that it is possible to extend periodic solutions of the time-dependent Hartree-Fock 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. Until now, these had been handled in a piecemeal fashion which always seemed to contain an element of guesswork and wishful thinking. So far, we have applied the method to helium and oxygen. This is the first time that periodic TDHF orbits have been calculated in ^{16}O [13]. Now we intend to extend the results to heavier nuclei and to other collective modes. We have done much additional work on helium, which is not reported here because it uses our new numerical method, and this work shows the nonlinear effects in this nucleus to be huge. It is likely that similarly large nonlinear effects will occur in some other nuclei for some other collective modes.

Two important improvements are in the offing, and we plan at least two other publications in the near future. One will be about the new numerical method — faster, more accurate, and more robust than the one used here. The development work on it is finished; time is needed only to port it to faster computers and to generate more data. The other big improvement is the new quantization method. It has been tested on a few simple systems and appears very promising. It is not fully developed for nuclear collective motion yet.

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