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Collective Periodic Orbits in a Model Nucleus

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Periodic orbit families are calculated for a one-dimensional nuclear model in the mean field approximation. Phase space is 20-dimensional. The essential element which makes the calculation possible is the fact that the two conservation laws (probability and energy) are still exactly satisfied after the discretization of the equations of motion.

I. INTRODUCTION

One of the motivations for this work arose in a conversation I had with Chris and Mike about five years ago. They had done a calculation of a nuclear collision in the mean field approximation, and they showed me on the Macintosh some striking oscillations that the compound system was going through. They had plotted various characteristics as functions of time. One of them was the quadrupole moment. And the oscillations were so nearly perfect that they said: "There is bound to be a periodic orbit very close in the vicinity. Do you think you could find it for us?"

This was near the beginning of my involvement with periodic orbits, and it took me a while to get oriented in this complicated business, but the reason that I am here today is to tell Chris that I have found it. More precisely, I have a method which seems sturdy and reliable, and which can find periodic orbits for general time-dependent mean field situations. I believe this, because I have found a whole bunch of them in a particularly simple case.

I shall speak as a nuclear physicist. The same sort of thing can be done for atomic problems. For instance, Klaus Richter and Dieter Wintgen calculated many periodic orbits for the helium atom. But I am more used to the nuclear case. I shall begin by defining the problem for you. Then I shall show some results. I shall examine some of the fine points which make the problem soluble in practice. And, I shall discuss the connections with chaos theory and nuclear theory.

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II. A MODEL NUCLEUS

I have taken a model, which is grossly oversimplified from the point of view of a nuclear physicist, but which would be considered extremely complicated by a specialist of dynamical systems. It is a one-dimensional nucleus which I take in the mean field approximation, suitable for the study of its collective motion. All the particles of this nucleus are in the same one-body wave function $\psi(x, t)$, which obeys the time-dependent Schrödinger-like equation

$$i \frac{\partial \psi}{\partial t} + \frac{\partial^2 \psi}{\partial x^2} - f(\rho) \psi = 0. \quad (1)$$

In this equation, $f(\rho)$ is a time-dependent mean field, which is a function of ρ , the density of particles

$$\rho = A |\psi|^2, \quad (2)$$

and A is the number of particles. The wave function is normalized in the usual way

$$\int dx |\psi(x, t)|^2 = 1, \quad (3)$$

which means that this is not field theory, but many-body quantum mechanics.

The problem is to calculate the periodic orbits of this object. Actually, there are none; the normalization condition (3) kills them (there would be some in field theory). But there are quasi-periodic orbits, i.e. orbits obeying the condition

$$\psi(x, t + \tau) = e^{-i\theta} \psi(x, t) \quad (4)$$

where θ is a constant phase, and they are just as useful as the true periodic ones. Defining $\lambda = \theta/\tau$, we can consider the function

$$\phi(x, t) = e^{i\lambda t} \psi(x, t) \quad (5)$$

which is truly periodic of period τ

$$\phi(x, t + \tau) = \phi(x, t) \quad (6)$$

and which obeys the equation

$$i \frac{\partial \phi}{\partial t} + \frac{\partial^2 \phi}{\partial x^2} + [\lambda - f(\rho)] \phi = 0. \quad (7)$$

This equation differs from (1) by the term $\lambda\phi$; it is the price we have to pay for demanding a fixed normalization. Of course ϕ is normalized the same way as ψ

$$\int dx |\phi(x, t)|^2 = 1 \quad (8)$$

and λ acts as a Lagrange multiplier for the normalization. It is real and is called the quasi-energy.

The true energy of the system (the expectation of the many-body hamiltonian) is given by

$$\mathcal{E} = \int dx \left[A \left| \frac{\partial \phi}{\partial x} \right|^2 + F(\rho) \right], \quad (9)$$

where $F(\rho)$ is the primitive of $f(\rho)$

$$f(\rho) = dF/d\rho. \quad (10)$$

Of course, the total number of particles is

$$\mathcal{N} = \int dx A |\phi|^2 \quad (11)$$

FIG. 1.

which is A . Both $\mathcal{E}$ and $\mathcal{N}$ are conserved quantities, a fact which will be very important later.

The functions $f(\rho)$ and $F(\rho)$ should look as in Fig. 1 so that nuclear matter will saturate for a finite density. Their actual form was chosen by Negele and Vautherin in conformity with the well-known Skyrme force. It is

$$F(\rho) = -F_1 \rho^2 + F_2 \rho^{2+\sigma} \quad (12)$$

$$f(\rho) = -f_1 \rho + f_2 \rho^{1+\sigma} = dF/d\rho. \quad (13)$$

The 3 parameters f_1 , f_2 , and σ were chosen to fit the energy and density of nuclear matter and the thickness of the nuclear surface. The unit of length was chosen to make the density of nuclear matter equal to unity. The number of particles, A , was taken to be 10.

With these choices, the function $\phi(x)$ for the ground state looks as in Fig. 2. Therefore I have chosen to carry the search for periodic orbits under the space boundary conditions $\phi(x, t) = 0$ for $x = \pm 10$. This means that I am putting 10 particles inside a space which, in nuclear matter, would contain 20. In addition, I have looked so far only for solutions which possess ($x \longleftrightarrow -x$) symmetry.

In the limit of very small amplitude, the periodic solutions are relatively easy to find, because one can just linearize the equations of motion in the vicinity of the ground state. Therefore I use this limit, known in nuclear physics as the random phase approximation (RPA), as my starting point in the extension to large amplitude periodic motion. I shall discuss in a moment the method used for this extension. The number

The Ground State

FIG. 2.

FIG. 3.

of RPA modes of small oscillation is of course infinite, but one expects the lowest-frequency mode to be a “breathing mode.” Fig. 3a shows what $\rho(x)$ for the breathing mode would look like at quarter-period intervals. The next lowest x -symmetric RPA mode would look like Fig. 3b, with small x and large x moving in opposite directions. This gives the oscillations a much shorter wave length than for the first mode, and therefore a much higher frequency. These two modes should be the most “collective” of all the RPA modes, and they are the only ones whose extension to large amplitude I have followed so far.

Fig. 4 shows my results for the energy of the breathing mode as a function of its period. The amplitude is indicated by the numbers next to the curve, which are $(R_{\max} - R_{\min})/R_{\text{ave}}$, R being the root mean square radius. This quantity goes up to .80, implying truly large amplitude collective motion. The RPA yields only the bottom point on the curve, $\tau = 13.2$, $E/A = -1.006$. An attempt to improve the RPA by perturbation theory would be accurate only for the tiny linear portion below $E/A = -1.00$. Everything else is entirely unexpected, not to say shocking. Note the sudden turn taken by the curve just above $E/A = -1.00$; the complicated bifurcation around $E/A = -0.93$, the details of which are shown in the insert; and the tight loop at $E/A = -0.73$, accompanied by a decrease in oscillation amplitude. At this last point, having watched the energy per particle increase rapidly and the period increase also, I expected the breathing nucleus to break apart, but instead it tightened up and turned around. This curve, and also the bifurcation, should be followed further, of course, but the work is extremely time-consuming and I have not had time to get to the end of this tantalizing story. I have followed the second RPA excitation part of the way also, and I have found equally dramatic phenomena, including several bifurcations.

III. CALCULATING PERIODIC ORBITS

The method used is in principle quite simple: you make a guess for the periodic orbit $\phi(x, t)$, you linearize the equations of motion in the vicinity of this guess, and you solve these linear equations, thus generating a new guess. You repeat the procedure until you have obtained convergence to the desired accuracy. This is the principle of the Newton-Raphson method for solving systems of non-linear equations. In all applications to periodic orbit calculations for Hamiltonian systems, you have at least one constant of the motion, the energy, given in the present case by Eq. (9). The constants of the motion act as free parameters (in the language of dynamical systems, “control parameters”), the variations of which define “families” of periodic orbits. For generic systems, when energy is the only constant of the motion, the plot of energy vs. period is

FIG. 4.

called the “ (E, τ) plot.” Fig. 4 is an example. On the (E, τ) plot, the families are represented by continuous lines, which can only begin and end at equilibrium states and at bifurcations. There are several kinds of bifurcations, including period-multiplying, and the stability of the periodic orbit often changes at these points. The continuous lines in the (E, τ) plot are calculated by moving along them in small steps. Once a point has been found, i.e. a periodic orbit with a certain E and a certain τ , then one calculates a nearby point by using the first one as initial guess. The position of the second point is defined by fixing either its E or its τ , and the other variable comes out of the calculation. Sometimes it is necessary, in order not to lose the convergence, to proceed by very, very small steps. This is the time-consuming aspect of the work, and for it no automated program can really match the skill of an experienced human guide. When convergence is present, it is usually quite good, involving 3 or 4 iterations at the most. The number of Newton-Raphson equations can be very large, since both the space variable x and the time variable t have to be put on a fine enough mesh. A total of a few hundred equations and variables, or even a few thousand, is quite normal. Hence some thought must be given to the best way of solving these linear equations. Three methods are available: (1) brute force, viable only in the low-range of a few hundred variables; (2) the monodromy method, much quicker but more sensitive to convergence problems and involving more programming; (3) Fourier selection. In the present work I have used brute force. Most of my past work was with the monodromy method.

The above procedure provides the method for following the periodic families in a continuous fashion. But two questions remain: how to get started, and what to do when one reaches a bifurcation? To get started, one begins in the vicinity of the ground state, using the RPA. As for bifurcations, they can be predicted from the eigenvalues of the monodromy matrix, and then the eigenvectors of that same matrix provide the starting directions for the bifurcated families.

This completes the discussion of the general method. I shall now outline briefly the implementation for the problem at hand, the search for periodic solutions of Eq. (7). I assume a total of M space points, labeled by the subscript m , and N time points, labeled by the subscript n . For a start, I chose $M = 10$ (this is for $x > 0$ only) and $N = 16$. The wave function $\phi(x, t)$ is specified in terms of its modulus and its phase, $\phi = Qe^{iS}$. Thus I have 160 variables Q_{mn} and 160 variables S_{mn} . The next task is to discretize the equations of motion, writing them in terms of Q_{mn} and S_{mn} . At this point, however, a very important requirement intervenes: it is absolutely essential, for reasons outlined later, that the conservation laws be obeyed *exactly* by the discretized version of the problem. There are two conservation laws: conservation of probability

$$\frac{\partial \gamma}{\partial t} + \frac{\partial j}{\partial x} = 0 \quad (14a)$$

$$\gamma = Q^2 \quad j = 2\gamma \frac{\partial S}{\partial x} \quad (14b)$$

and conservation of energy

$$\frac{\partial \Gamma}{\partial t} + \frac{\partial J}{\partial x} = 0 \quad (15a)$$

with

$$\Gamma = \left(\frac{\partial Q}{\partial x} \right)^2 + \gamma \left(\frac{\partial S}{\partial x} \right)^2 + \frac{1}{A} F(\rho) - \lambda \gamma \quad (15b)$$

$$\rho = A\gamma \quad (15c)$$

$$J = -2 \frac{\partial Q}{\partial x} \frac{\partial Q}{\partial t} - 2\gamma \frac{\partial S}{\partial x} \frac{\partial S}{\partial t}. \quad (15d)$$

γ and j are the probability density and current, respectively. Γ and J are the energy density and current. It is essential that the problem be discretized in such a way that the space integrals of the two densities

$$\sum_m \gamma_{mn} \quad \text{and} \quad \sum_m \Gamma_{mn} \quad (16)$$

are automatically independent of the time label n . This can indeed be done, although it is a little complicated and I skip the details. But the possibility of doing this is the real reason for having chosen Q and S as the primary variables, rather than the real and imaginary parts of ϕ . This requirement also led me to adopt Eqs. (14a) and (15a) as the primary equations of motion, rather than the more straightforward Eq. (7).

FIG. 5.

IV. SLIDING

Why this emphasis on obeying conservation laws exactly? The reason lies in a peculiarity of the search for periodic orbits, for any dynamical problem, in a way which I shall now endeavor to explain. Consider in full generality a periodic orbit for an arbitrary system. It is denoted by a function $x(t)$ with the property $x(t + \tau) = x(t)$. Depending on the system, x is a collection of M variables, in sufficient number to define completely the state of the system at time t , i.e. x is some M -dimensional vector (the meaning of M is now different from earlier). The function $x(t)$ parametrizes a closed curve in M -dimensional space, which is the periodic orbit considered. If M happens to be 2, this might look like Fig. 5a. However, to do any numerical calculation we must discretize the time. Let the period τ be divided into N equal intervals. Then we do not have a continuous curve $x(t)$ any more, but a set of N discrete points as in Fig. 5b, $x_0 x_1 x_2 \cdots x_{N-1}$, with x_N being the same as x_0 . We have therefore MN variables x_n . We must look now at the number of equations, and there we encounter two possibilities.

If the number of distinct equations is also equal to MN , then the system has discrete solutions. This may mean, for instance, that if the circles in Fig. 5c are a solution, then the stars, which look equally good, are not. In other words, the discrete points are not allowed to slide along the continuous orbit. But this is very strange! What criterion could possibly make a certain set of discrete points better than some other? This is contrary to the original translational symmetry of the problem in time. Moreover, if MN is very large, it can be extremely confusing for the computer program. This is because, although the circles are the only exact solutions of the discretized equations, the stars are certainly very close to solutions if N is sufficiently large. Thus the computer is being asked to distinguish between exact solutions and nearly-exact solutions, which is something it finds very difficult to do, and consequently it may display erratic behavior and refuse to converge: a very unclean situation!

If on the other hand the number of equations is $MN - 1$, one less than the number of variables, then there is a continuous degree of freedom left. It will turn out to be the sliding freedom, the ability of the N points to slide along continuously together without ceasing to be an exact solution. This is much more reasonable than the previous situation. Moreover, it is what is needed from the computer's point of view. To make the problem soluble, we only need to add an extra equation. One way to do this is to give arbitrarily one of the M coordinates of one of the points, say x_0 . This "pins down" the solution, which is then completely incapable of sliding. The solution is truly unique, the computer has no reason to get confused, and convergence is assured.

The question is then: which of these two situations occurs in practice? And the answer is: if you discretize the problem without taking any particular care, you will generally be in the first case. But if there is a conservation law, and if your discretization treats it exactly, then you will be in the second case. I shall now illustrate how this works on a simpler example, with much lower dimensionality than my model nucleus.

Consider a simple 4-dimensional flow with Hamiltonian $H(p_1 p_2 q_1 q_2)$, whose numerical value is the conserved energy E . We must discretize the equations of motion, which could be Hamilton's equations. Suppose,

however, that we include among the $4N$ equations of motion the following N equations, which express conservation of energy (the subscript is the time index n)

$$H_0 = H_1 \quad H_1 = H_2 \quad H_2 = H_3 \quad \cdots \quad H_{N-1} = H_0. \quad (17)$$

We see that these equations are not independent. Adding them all up leads to an identity, and therefore there are only $N - 1$ equations there, instead of N . This is our extra freedom, the sliding freedom for the orbit, which allows us to pin the orbit down any way we wish.

Returning to the model nucleus now, we have two conservation laws, probability and energy. They provide two sliding freedoms. One of them is time-sliding, which we just examined. The other is phase-sliding: the phase S is undetermined by an arbitrary additive constant and needs to be pinned down too. Without a correct treatment of these two symmetries, attempts at numerical solution of such a high-dimensional problem get hopelessly mired in poor convergence. Such a treatment is the real key to the success of the method.

V. DISCUSSION

One can make two kinds of comments about the calculation I have done, depending on whether one takes the point of view of a chaos specialist or that of a nuclear physicist.

To chaos specialists, the search for periodic orbits is one of the best and time-honored ways of studying a chaotic system. Every stable periodic orbit is at the center of a regular region. Every unstable one is at the center of a chaotic region. By classifying systematically the periodic orbits in order of increasing complexity, one obtains a view of the chaotic system on successively finer scales. In this respect, the interesting aspect of the present calculation is its high dimensionality, which is 20, since there are 10 Q variables and 10 S variables. Most periodic orbit calculations done so far for conservative systems have been either 2-dimensional, for conservative maps, or 4-dimensional, for Hamiltonian flows. Here is a chance, therefore, to extend one's experience to a completely different realm of dimensionality and to see whether qualitative ideas obtained from the lower realm should be modified by new learning. The systematic exploration of a 20-dimensional space is difficult and highly time-consuming, but it can be done, and it may be well worth it in some carefully chosen cases.

For nuclear physicists, on the other hand, this problem is about the calculation of collective motion. The simplicity of collective motion comes from the fact that many particles act together, or do the same thing. These high numbers introduce a classical aspect to the phenomenon, which is evident both in the way we talk about it and in the way we calculate it. We talk about, and we think of, rotations, vibrations, collisions between heavy ions, . . . as if they were classical, of course. When we calculate them, after having realized that it is totally impossible to solve the many-body Schrödinger equation exactly, we usually introduce a classical element somewhere: some quantity, some function, which varies as a function of time like a classical variable and is not quantized. For example, a popular approach is the time-dependent Hartree-Fock approximation, in which there is a mean field which is handled classically: it evolves as a function of time the way a classical field does, while a quantal field would have to have an associated wave functional, obeying a Schrödinger functional equation. As another example, consider a rotating nucleus. You think of it as having a certain deformation. This deformation is a number which you try to measure. True, it does have small fluctuations, but basically it is a classical quantity.

Thus, the best that we can do about collective motion, in most cases, is to calculate solutions to a classical problem, classical trajectories. The question is then: how can we go from there to quantities which can be compared with experiment, like energy levels or transition probabilities, which are quantum mechanical quantities, given that a solution of the full many-body Schrödinger equation is impossible? This is the quantization problem: how to go from the classical results, the trajectories, to the quantal results, with a minimum of theoretical backtracking, or with no backtracking at all? How to write the quantal data directly in terms of classical data without going back to the beginning, the Hamiltonian, the commutation relations, etc. . . ? For one-dimensional systems, the solution is well-known: the WKB method answers all questions. For multidimensional systems, if the classical motion is regular, there is an extension of WKB called EBK (Einstein-Brillouin-Keller). But if the classical motion is chaotic, there is no EBK. Since most interesting collective motion problems are at least 2-dimensional, and since all 2-dimensional classical problems are at least partially chaotic except for a set of measure zero, clearly we must look elsewhere. This problem, the quantization of chaotic systems, is one of the outstanding problems in quantum chaos theory today. It has

been occupying the minds of most workers in the field for decades, and it is still far from being entirely solved. Some very important ideas have emerged, however, and one of them is the importance of classical periodic orbits, first stated by Gutzwiller in 1969 when he wrote his famous trace formula. In fact, all methods proposed so far for quantizing chaotic motion do it in terms of classical periodic orbits. This is the best justification for the kind of work I have reported here, the calculation of periodic orbits in the mean field approximation to collective motion. With the knowledge that we have today, it is a necessary step on the way to the quantal solution, except for trivial one-dimensional or other integrable cases.

Of course, I am still very far from having pushed this approach all the way. In addition, there are obvious difficulties due to the fact that the number of periodic orbits, for a given energy, is infinite. Clearly, only a few can be calculated, and one expects that the simpler ones, those with shorter periods, will be the important ones. But there is another problem. According to quantum chaos theory, most of the properties of the system, including the energy levels, are given by infinite sums over classical periodic orbits. These sums, however, do not seem to converge, so that even if we had all the periodic orbits we would not know what to do. Both of these difficulties disappear if we decide to be satisfied with calculating short-time properties of the quantal system, i.e. smoothed energy level densities and other energy-smoothed observables. Then, for smoothing parameter ΔE , we only need to include in the sums orbits whose periods do not exceed $\hbar/\Delta E$ in order of magnitude. The sums, then, become finite, and even quite short in most cases, and the whole enterprise becomes tractable. Besides, such a smoothing procedure is quite appropriate for collective motion, which usually underlies large numbers of energy levels split for other reasons.

I hope to have convinced you that this approach to collective motion, stimulated in part by Chris, is interesting and worth pursuing.