

Semiclassical calculation of bound states in a multidimensional system. Use of Poincaré's surface of section*

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A method utilizing integration along invariant curves on Poincaré's surfaces of section is described for semiclassical calculation of eigenvalues. The systems treated are dynamically nonseparable and are quasiperiodic. Use is also made of procedures developed in the previous paper of this series. The calculated eigenvalues for an anharmonically coupled pair of oscillators agree well with the exact quantum values. They also agree with the previous semiclassical calculations in this laboratory, which instead used integrations along the caustics. The present paper increases the number of systems capable of being treated. Using numerical counter examples for nondegenerate systems, it is also shown that an alternative view in the literature, which assumes that periodic trajectories alone suffice, leads to wrong results for the individual eigenvalues.

I. INTRODUCTION

The calculation of bound state properties using semiclassical concepts has been of interest for many years. This problem has a well-known WKB solution¹ for systems permitting separation of variables. Recently, in a previous paper of this series,² a practical method was developed (for the first time) for calculating eigenvalues semiclassically for systems which had smooth potentials and which did not permit separation of variables. The method yielded an evaluation of the topological independent phase integrals (two in the case studied) associated with each trajectory. The analysis of the trajectories then yielded the eigenvalues (and other properties) associated with bound states.

In the present work a second method of evaluating the phase integrals is described in Sec. II, one which increases the range of application. The eigenvalues are calculated and compared in Sec. III with the exact quantum mechanical results² and with the previous semiclassical calculation in this laboratory.² They are shown to agree well.

In Sec. IV the role of the periodic trajectories is considered. It has been argued³⁻⁵ from a Feynman propagator analysis that the evaluation of a single phase integral along a periodic trajectory suffices to locate the eigenvalues. In Sec. IV this idea is shown to yield wrong numerical values for the individual eigenvalues. (A different role of certain periodic trajectories is referred to later.^{6,7}) The reason is that the evaluation of only one phase integral is not sufficient for determining the eigenvalue in the nondegenerate case in a two or more dimensional system.

Various arguments, beginning with Einstein's⁸ have pointed to the need for evaluating N topologically independent phase integrals, when there are N coordinates and the system is nondegenerate, to calculate eigenvalues. (If the state is intrinsically r -fold degenerate, only $N-r$ integrals are needed to obtain the eigenvalues.) Arguments were based on "old quantum theory"⁸ and later on WKB-type semiclassical theory.^{9,10} Specifically, the quantum conditions are (in units of $\hbar = 1$)

$$2\pi(n_i + \frac{1}{2}) = \int_{C_i} \sum_{k=1}^N p_k dq_k, \quad (i = 1 \text{ to } N) \quad (1.1)$$

where the $\frac{1}{2}$ applies to a system of nondegenerate oscillators but can be replaced by other (known) values for other kinds of systems.¹¹ The n_i are integers, and the q_k and p_k are the coordinates and their canonically conjugate momenta, respectively. The C_i are topologically independent closed paths. These paths C_i need not be along actual trajectories.⁸⁻¹⁰

Eastes and one of us was able to find a method of evaluating these phase integrals for nonseparable systems with smooth potentials²: a system where $N=2$ was considered, and the caustics were located, they forming the envelope of a single long time trajectory as in Fig. 1. Semiclassically, the caustics separate the classically allowed from the classical nonallowed regions. Integration along each of two sides of the four-sided caustic (e.g., in Fig. 1 from A to B and then back to A, and similarly A to D to A) yielded the two independent phase integrals. The eigenvalues were determined by requiring both n_1 and n_2 in Eq. (1.1) to be integers. The topologically independent paths are indicated in Fig. 2. The latter can be made to lie along the caustics AB and AD, respectively, the basic idea used in Ref. 2.

This method was successful for trajectories which gave rise to an obvious caustic. However, in some systems, such as nearly periodic ones, the behavior near the caustic was not quite as simple (tendency to form foci, etc.) and another method is needed. The one we have devised utilizes an integration along closed paths in Poincaré's surfaces of section. It applies to the previously treated case as well as to this more complex one. These closed paths are not in themselves the actual trajectories. Rather they are as defined below.

Many years ago Poincaré introduced the "surface of section" concept in which, to take the case of $N=2$ as an example, the behavior in the phase plane (x, p_x) at a constant value of y is examined.^{12,13} Each time the trajectory passes some plane, $y=0$, say, in a given direction, a point at the value of x and p_x is marked. After many cycles of the trajectory, some pattern of points

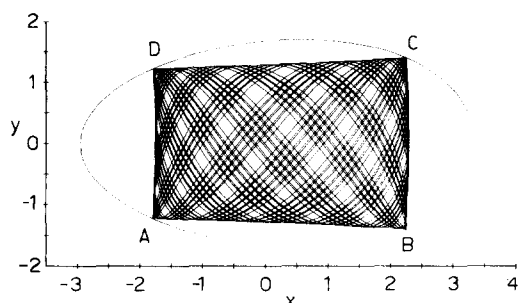


FIG. 1. A typical quasiperiodic trajectory for the systems in Table I.

emerges on this (x, p_x) phase plane (Fig. 3). The different "ellipses" arise from different trajectories. Similar remarks apply to the crossing of the $x=0$ plane by the trajectory, giving rise to a figure on the (y, p_y) phase plane at $x=0$ (Fig. 4). These two planes are surfaces of section and the patterns of points on them have been used in the celestial mechanics and stellar dynamics literature to investigate whether or not the classical motion appears to be largely quasiperiodic or largely ergodic.¹³ In the largely ergodic case, a shotgun pattern emerges on the phase plane rather than some relatively simple pattern. Fundamental nonperturbative discussions of the fact that some systems are largely quasiperiodic have been given.¹⁴

II. SEMICLASSICAL QUANTUM CONDITIONS

The Hamiltonian for the system to be studied in this paper is given by^{2,13}

$$H = \frac{1}{2} (\dot{p}_x^2 + \dot{p}_y^2 + \omega_x^2 x^2 + \omega_y^2 y^2) + \lambda x(y^2 + \eta x^2), \quad (2.1)$$

where x and y are coordinates and \dot{p}_x and \dot{p}_y are the conjugate momenta; ω_x , ω_y , λ , and η are constants. This Hamiltonian represents a system of harmonic oscillators of unit masses with frequencies ω_x and ω_y , coupled by a cubic potential. λ and η determine the degree of anharmonicity.

It has been shown by Kolmogorov, Arnold, and Moser¹⁴ that a many-dimensional coupled system may possess quasiperiodic trajectories, and we shall consider systems with this property. Such trajectories (at least simple ones) produce simple patterns on the surfaces of section.

A quasiperiodic trajectory is one in which p 's and q 's can be represented as a function of time by a convergent Fourier series which has at most N -independent fundamental frequencies for a system of N degrees of freedom:

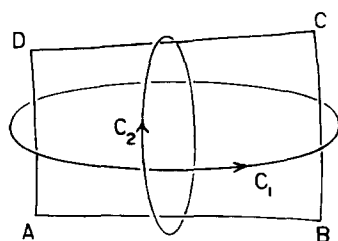


FIG. 2. Independent closed paths for the phase integrals in Eq. (2.3).

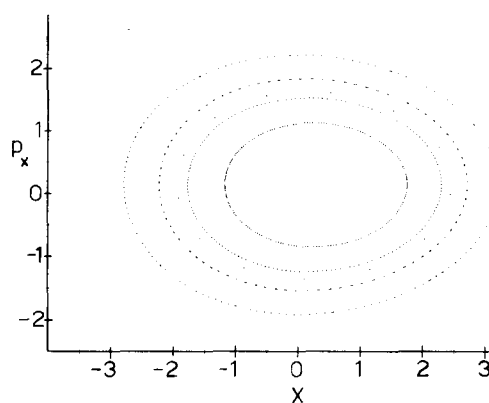


FIG. 3. Example of a surface of section at $y=0$ for five trajectories, all with the same E but different f_x 's.

$$p_k(t) = \sum_{m_1, \dots, m_N} A_{m_1, \dots, m_N}^k \exp[2\pi i(m_1 \nu_1 t + \dots + m_N \nu_N t)], \quad (2.2)$$

$$q_k(t) = \sum_{m_1, \dots, m_N} B_{m_1, \dots, m_N}^k \exp[2\pi i(m_1 \nu_1 t + \dots + m_N \nu_N t)].$$

The m 's are integers which range from $-\infty$ to ∞ and the coefficients A and B decrease sufficiently rapidly with increasing $\sum_{i=1}^N |m_i|$.¹⁴

A typical quasiperiodic trajectory for a system treated later in Table I is shown in Fig. 1. One property of such a trajectory is that it does not cover the entire area energetically accessible to it. The potential energy contour for the case that the potential energy equals the total energy is also shown. The trajectory is seen to be reflected from the envelope curves, the "caustics." The quantum conditions^{9,10} are, using the topologically independent paths C_1 and C_2 in Fig. 2, given by (2.3), in units of $\hbar = 1$:

$$2\pi(n_1 + \frac{1}{2}) = \oint_{C_1} (p_x dx + p_y dy), \quad (2.3)$$

$$2\pi(n_2 + \frac{1}{2}) = \oint_{C_2} (p_x dx + p_y dy).$$

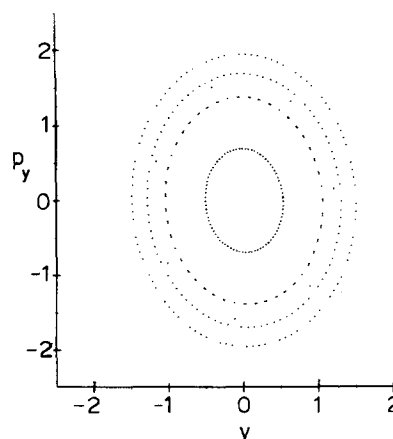


FIG. 4. Example of a surface of section at $x=0$ for the five trajectories in Fig. 3. The innermost one here corresponds to the outermost one in Fig. 3, etc.

TABLE I. Comparison of the semiclassical and quantum energy levels for various systems.

| System* ω_x^2, ω_y^2 λ, η | Quantum numbers (n_x, n_y) | Semiclassical | | | Uncoupled $\lambda=0$ |
|--|-----------------------------------|---------------|---------------------|--------|--------------------------|
| | | Quantum | Present | Ref. 2 | |
| 0.29375, 2.12581, -0.1116, 0.08414 | 0, 0 | 0.9916 | 0.9922 | 0.9920 | 1.0000 |
| | 1, 0 | 1.5159 | 1.5164 | 1.5164 | 1.5420 |
| | 2, 0 | 2.0308 | 2.0313 ^b | 2.0313 | 2.0840 |
| | 0, 1 | 2.4188 | 2.4198 | 2.4196 | 2.4580 |
| 0.36, 1.96 -0.1, 0.1 | 0, 0 | 0.9939 | 0.9942 | 0.9942 | 1.0000 |
| | 1, 0 | 1.5809 | 1.5812 | 1.5813 | 1.6000 |
| | 2, 0 | 2.1612 | 2.1616 | 2.1615 | 2.2000 |
| 0.49, 1.69 -0.1, 0.1 | 0, 0 | 0.9955 | 0.9954 | 0.9955 | 1.0000 |
| | 1, 0 | 1.6870 | 1.6870 | 1.6870 | 1.7000 |
| | 0, 1 | 2.2781 | 2.2785 | 2.2780 | 2.3000 |
| | 2, 0 | 2.3750 | 2.3751 | 2.3750 | 2.4000 |
| | 1, 1 | 2.9583 | 2.9588 | 2.9584 | 3.0000 |
| 0.81, 1.21 -0.08, 0.1 | 0, 0 | 0.9980 | 0.9978 | 0.9978 | 1.0000 |
| | 1, 0 | 1.8944 | 1.8944 | 1.8941 | 1.9000 |
| | 0, 1 | 2.0890 | 2.0889 | 2.0897 | 2.1000 |
| | 2, 0 | 2.7899 | 2.7900 | 2.7895 | 2.8000 |

*The four parameters are those of Eq. (2.1).

^bEquation (3.5) was used.

^cThis trajectory could not be treated in Ref. 2 (see present text).

The n_1 and n_2 are integers when the energy is an eigenvalue.

Along the caustics in Fig. 1 or 2, these equations became²

$$2\pi(n_1 + \frac{1}{2}) = 2 \int_A^B (p_x dx + p_y dy), \quad (2.4)$$

$$2\pi(n_2 + \frac{1}{2}) = 2 \int_A^D (p_x dx + p_y dy).$$

Two surfaces of section (one at $x=0$ and the other at $y=0$) generated by the trajectory in Fig. 1 are shown by the curves second from the inside in Fig. 3 and second from the outside in Fig. 4. On each surface of section in these figures it is seen that this quasiperiodic trajectory generates a set of points which form an "invariant curve" rather than forming a shotgun pattern. Different trajectories, starting with the same energy but with suitably different initial conditions, generate different invariant curves, also shown in Figs. 3 and 4, and these curves are seen to be "nested." One of the five "curves" (the middle one) is actually a set of 13 points in Fig. 3 and seven points in Fig. 4. A longer time trajectory does not change the number of points in this middle "curve." The latter arises from a periodic trajectory. The latter is given in Fig. 5, which also gives the potential energy contour for which the potential energy equals the total energy.

The curves on the surfaces of section $x=0$ and $y=0$ are topologically equivalent to paths C_2 and C_1 in Fig. 2, respectively, and so to the C_2 and C_1 in Eq. (2.3). The latter equation thus yields

$$2\pi(n_1 + \frac{1}{2}) = \oint p_x dx, \quad (y=0) \quad (2.5)$$

$$2\pi(n_2 + \frac{1}{2}) = \oint p_y dy, \quad (x=0).$$

Equation (2.5) is applied in the next section.

III. THE CALCULATION

Hamilton's equations of motion,

$$\dot{q}_i = \partial H / \partial p_i, \quad \dot{p}_i = -\partial H / \partial q_i, \quad (q_i \equiv x, y) \quad (3.1)$$

were integrated numerically, using the Hamiltonian (2.1). As initial conditions, we set $x(0) = y(0) = 0$ at $t=0$ and chose various initial values of positive p_x , $p_x(0)$.

The initial value of p_y , $p_y(0)$, was chosen to be positive, and was determined from the other initial values of x , y , and p_x by energy conservation, namely setting (2.1) equal to E and solving the resulting equation for p_y .

These initial conditions were characterized by a quantity f_x , defined by

$$f_x = p_x^2(0) / [p_x^2(0) + p_y^2(0)]. \quad (3.2)$$

Roughly speaking, f_x denotes the fraction of energy in the "x oscillator."

To obtain each point on a surface of section from the trajectory data, a linear interpolation of two points along the trajectory, one on either side of the surface, was used. The phase integral along the invariant curve for $y=0$ (Fig. 3) and the one for $x=0$ (Fig. 4) were calculated. A Simpson's Rule integration was developed for nonequally spaced points to obtain the phase integral $\int p_x dx$ on a closed path consisting of points on the section $y=0$. The $\int p_y dy$ phase integral over the closed path on the $x=0$ section was similarly evaluated.

The above procedure yields the quantities n_1 and n_2 to any desired degree of accuracy, provided a sufficient number of points on the surfaces of section is used so as to generate an almost continuous curve on each of the two surfaces. Tests show that the accuracy of the method is quite adequate¹⁵ for the present calculations. Only for certain energies (eigenvalues) are n_1 and n_2 integers.

All the integrations of (3.1) and (2.5) were performed with an IBM 360-75 computer, using FORTRAN programs.

The initial choice of f_x and of E in an iterative procedure to find each eigenvalue was (as in Ref. 2) based on the appropriate values of f_x and E of the uncoupled systems, for the given quantum numbers. This initial choice was convenient in that it reduced the number of

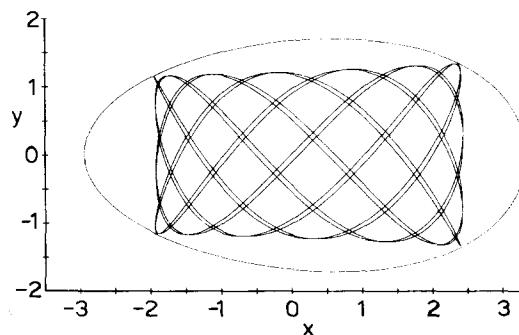


FIG. 5. Example of the periodic trajectory giving rise to the middle "curve" (13 points) in Fig. 3 and to the middle "curve" (7 points) in Fig. 4.

trajectories ultimately needed, but wasn't essential. If instead, the starting E 's were far from the values for the eigenvalues of the uncoupled problem, the same final results for the eigenvalues were obtained for the coupled problem.

Given the above initial choice of E and f_x , each eigenvalue was then found from an interpolation using the procedure described in the previous paper of this series²: n_1 and n_2 are nearly linear functions of f_x and E . Values of n_1 and n_2 were fitted with expressions of the form

$$\begin{aligned} n_1 &= a_1 E + b_1 f_x + c_1, \\ n_2 &= a_2 E + b_2 f_x + c_2 \end{aligned} \quad (3.3)$$

for the small interval of interpolation needed. The constants a_1 , b_1 , and c_1 were obtained from the values of n_1 for three trajectories, and a_2 , b_2 , and c_2 were obtained from the n_2 values also obtained from these three trajectories. With these constants, an estimate of the value of f_x and E needed to yield integer values for n_1 and n_2 was made from (3.3). Using one or two further trajectories near this f_x and E , the eigenvalue was obtained and is given later in Table I.¹⁶

In the rare case that the correct trajectory determined as above was nearly a periodic one, the points on the surfaces of section were too widely spaced to be able to evaluate the integrals in (2.5) with the accuracy given in Table I.¹⁷ In this case, we first found, as before by use of the above interpolation (3.3), the estimated trajectory for which both n_1 and n_2 would be integers. Then, at this given E and f_x a phase integral ϕ was calculated by integrating the equation

$$\frac{d\phi}{dt} = p_x(t)\dot{x}(t) + p_y(t)\dot{y}(t) \quad (3.4)$$

along the trajectory, simultaneously with integrating Hamilton's equations of motion (3.1). The number of cycles was chosen so that the trajectory returned to a point A_f on the surface of section, within a distance $(\Delta x^2 + \Delta p_x^2)^{1/2}$ of about $\sqrt{2} \times 10^{-3}$, in present units, from its initial position A_i on that surface. The integral of (3.4) then provided the value of $\phi(A_f) - \phi(A_i)$ evaluated along the trajectory. This path could then be closed by a simple interpolation,¹⁸ the correction to $\phi(A_f) - \phi(A_i)$ being denoted by Δ .¹⁸ We now have

$$\phi(A_f) - \phi(A_i) + \Delta = 2\pi N_x(n_1 + \frac{1}{2}) + 2\pi N_y(n_2 + \frac{1}{2}), \quad (3.5)$$

where N_x and N_y are the number of completed cycles of the trajectory along the x and y directions. Equation (3.5) arises since this closed path is topologically equivalent to the integral over N_x curves of the C_1 type plus N_y curves of the C_2 type. To determine the eigenvalue in this case the energy E was varied at the given f_x until the value of $N_x n_1 + N_y n_2$ determined from (3.5) was an integer to the desired accuracy. The result obtained by this second method of evaluating a phase integral is given in Table I by the entry labelled b.

The Δ in (3.5) was negligible, giving rise to a correction to the n_i only of the order of 2×10^{-5} in the cited case, and so did not even appear in the significant figures of the relevant eigenvalue in Table I. The number

of cycles N_x and N_y in (3.5) were readily found, for systems of the type indicated in Fig. 1, from the number of times that p_x and p_y underwent sign changes, respectively, being one-half of those respective numbers.

IV. RESULTS OBTAINED USING ONLY PERIODIC TRAJECTORIES

In an analysis based on a use of the Feynman propagator, it has been argued that to obtain eigenvalues semiclassically one should find periodic trajectories and then compute the phase integral $\Delta\phi$ along a periodic trajectory³⁻⁵:

$$\Delta\phi = \int_0^\tau dt \sum_{i=1}^N p_i(t)\dot{q}_i(t), \quad (4.1)$$

where τ is the time required for the system to return to its starting point. If l is the number of turning points along the trajectory, then the quantum condition was

$$\Delta\phi = 2\pi N + l\pi/2, \quad (4.2)$$

where N is an integer.

Against this idea, in nondegenerate systems, are the theoretical arguments given in Refs. 8-10. To describe one of these we show how one might attempt to derive (4.2) using a wavefunction approach. Let us write the semiclassical wavefunction as

$$\psi(q) \sim \left| \frac{\partial^2 \phi}{\partial q \partial n} \right|^{1/2} \exp(i\phi), \quad (4.3)$$

and use a periodic trajectory to evaluate the ϕ using (4.1). The phase of the preexponential factor decreases by $\pi/2$ at each turning point.⁹ Thus if l is the number of turning points along the trajectory, the phase of ψ over the time τ changes by $\Delta\phi - (l\pi/2)$. Single-valuedness of ψ requires that the net phase change of ψ be $2\pi N$, where N is an integer. Thus

$$\Delta\phi - (l\pi/2) = 2\pi N. \quad (4.4)$$

This equation is identical with (4.2). However, (4.4) and hence (4.2) miss the requirement that the wavefunction is characterized not only by a single-valuedness but also by an exponential decrease of $\psi(q)$ outside the region occupied by the caustics. This latter event, and the semiclassical connection formulas at the caustics, led to the requirement of N conditions (1.1) in the nondegenerate case.¹⁰

Nevertheless, it is interesting to examine the results based on (4.1)-(4.2) by finding the periodic trajectories. To find them, we made use of the Poincaré surface of section. The concept of a rotation number,¹³ defined below, is helpful in this connection in explaining their origin.

For a system which is largely quasiperiodic, the invariant curves are nested, as in Figs. 3 and 4, each curve in the present case corresponding to a different value of f_x for any given E . The rotation number is the mean angle between two successive vectors, each vector leading from the center of the nested curves to a point on the surface of section. (Successive vectors are vectors drawn from this center to two successive points on this surface of section.)

Usually this rotation number is irrational, since rational numbers are of zero measure in the space of real numbers, and then the trajectory is quasiperiodic. When the rotation number is rational the trajectory is periodic. The rotation numbers have been found to vary continuously between certain limits when a quantity such as f_x is varied.¹⁹ (The rotation number is a measure of the relative frequencies for motions in the x and y directions, and would be independent of f_x if the motions were harmonic. The anharmonicity causes the ratio to vary somewhat with f_x .) By varying f_x , an effort was made to find periodic trajectories of various rotation numbers. Periodic trajectories are relatively rare, and many trajectories were needed to find one giving an integer N in Eq. (4.2). Typically 10 to 12 were used, and in one case as many as 24. The search involved first varying the f_x until the $A_i - A_j$ distance $\sqrt{(x_i - x_j)^2 + (p_{x_i} - p_{x_j})^2}$ referred to in Sec. III was $\sim\sqrt{2} \times 10^{-3}$. Then, variation of both E and f_x was made until both the N in Eq. (4.2) was an integer and simultaneously the $A_i - A_j$ distance was $\sim\sqrt{2} \times 10^{-3}$. To calculate N , Hamilton's equations were integrated together with Eq. (3.4) for ϕ .²⁰

When the initial choice of f_x was ~ 0.47 , results obtained for the "eigenvalues" using the periodic trajectories method are given in Table II. Additional "eigenvalues" corresponding to the missing values of N (last column) could also have been obtained. We made no effort to do so, since the results obtained were sufficient to demonstrate that numerous wrong eigenvalues are obtained.

Other values of f_x lead to still other eigenvalues. A

TABLE II. Comparison of quantum energy levels with values from periodic trajectories.^a

| Quantum | Eq. (4.2) | Uncoupled ($\lambda = 0$) | f_x | N |
|---------|-----------|-----------------------------|--------|-----|
| 0.9955 | 0.9955 | 1.0000 | 0.4700 | 0 |
| | 1.0945 | | 0.4700 | 1 |
| | 1.1936 | | 0.4700 | 2 |
| | 1.2923 | | 0.4700 | 3 |
| | 1.3910 | | 0.4700 | 4 |
| | 1.4890 | | 0.4700 | 5 |
| | 1.5882 | | 0.4700 | 6 |
| | 1.6867 | | 0.4700 | 7 |
| 1.6870 | 1.9815 | 1.7000 | 0.4690 | 10 |
| | 2.2755 | | 0.4675 | 13 |
| 2.2781 | 2.3732 | 2.3000 | 0.4675 | 14 |
| | 2.3750 | | 0.4665 | 17 |
| 2.3750 | 2.7632 | 2.4000 | 0.4665 | 18 |
| | 2.9576 | | 0.4655 | 20 |
| | 2.9583 | | 0.4645 | 23 |
| 2.9583 | 3.2484 | 3.0000 | 0.4640 | 24 |
| | 3.3452 | | 0.4635 | 26 |
| | 3.5385 | | 0.4635 | 26 |
| 3.5479 | | 3.6000 | | |

^aParameters (ω_x^2 , ω_y^2 , λ , η) for the system studied are (0.49, 1.69, -0.1, 0.1).

TABLE III. Comparison of initial energies with values from periodic trajectories.^a

| Initial E | f_x | Eq. (4.2) | N |
|-------------|---------------------|-----------|-----|
| 0.9955 | 0.4700 | 0.9955 | 0 |
| 0.9955 | 0.8720 | 0.9942 | 0 |
| 0.9955 | 0.1058 ^b | 0.9953 | 0 |
| 1.6870 | 0.0149 ^b | 1.6606 | 30 |
| 1.6870 | 0.4700 | 1.6867 | 7 |
| 1.6870 | 0.6985 | 1.6869 | 20 |
| 2.2781 | 0.9999 | 2.2581 | 11 |
| 2.2781 | 0.4675 | 2.2755 | 13 |
| 2.2781 | 0.0335 | 2.1927 | 14 |
| 2.3750 | 0.9900 | 2.3730 | 12 |
| 2.3750 | 0.4675 | 2.3732 | 14 |
| 2.3750 | 0.0675 ^b | 2.3631 | 16 |
| 2.9583 | 0.8750 | 2.9452 | 17 |
| 2.9583 | 0.4655 | 2.9576 | 20 |
| 2.9583 | 0.0254 | 2.9542 | 49 |
| 3.5479 | 0.4635 | 3.5385 | 26 |
| 3.5479 | 0.7965 | 3.5138 | 22 |

^aParameters are the same as those in Table II.

^bThis f_x is the mean of the f_x 's of the two trajectories used in the interpolation, as in Ref. 21.

few examples are given in Table III. For the results in Table III, the initial E 's chosen for the iterative procedure were close to the exact E 's, and so the final iterated eigenvalues were also typically close to them. The table shows how the resulting "eigenvalues" vary with f_x .

V. DISCUSSION

From Table I, one sees that the present results are in excellent agreement with those obtained in the previous paper, based on the same concepts but a different method. The agreement with the exact results is also excellent. The absolute magnitude of the difference in energy of the exact and semiclassical eigenvalues is, on the average, ~ 0.0003 . In the series in Table I ($\omega_x^2 = 0.49$, etc.) that was used later in Table II, the mean difference is also 0.0003. The present method could be used in the case of the more "uneven" caustics where the method in Ref. 2 could not (entry labelled c in Table I). It can also be modified, as could the method in Ref. 2, and used easily when the correct trajectory is nearly periodic (entry labelled b in Table I).

Results are given in Table II for the eigenvalues obtained from Eqs. (4.1) and (4.2) using only periodic trajectories. The third series in Table I was the one selected for this latter study. It is seen that this "eigenvalue" depends on the initial E used in the iteration. When the latter was not close to an exact eigenvalue, neither was the "eigenvalue" close to an exact eigenvalue. In contrast, the method described in the present paper yields results always close to the exact eigenvalues (Table I), regardless of whether the initial E was close to or far from an eigenvalue for the uncoupled problem. Again, this latter method yielded results independent of the initial f_x , unlike the periodic

trajectories method. (Results with the latter are given in Table III.)

In summary, Eqs. (4.1) and (4.2) are not correct for the purpose of determining the individual eigenvalues of nondegenerate systems. One needs $N-r$ equations (1.1) when there is an r -fold degeneracy, and so two equations for a nondegenerate system with $N=2$. Certain periodic trajectories have been successfully used, however, for determining bunching of eigenvalues, i. e., density of eigenvalues.⁷ This problem is quite a different one from that of determining individual eigenvalues.²²

The invariant curves for the systems described in Table I are quite simple (Figs. 3 and 4). Other Hamiltonians or nearly degenerate systems can give more complex patterns than those in these figures and we hope to consider some in a later paper.

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¹For example, D. R. Bates, *Quantum Theory* (Academic, New York, 1961), Vol. I; pp. 321-329.

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³M. C. Gutzwiller, *J. Math. Phys.* **12**, 343 (1971).

⁴W. H. Miller, *J. Chem. Phys.* **56**, 38 (1972).

⁵Compare with M. C. Gutzwiller, *J. Math. Phys.* **8**, 1979 (1967); **10**, 1004 (1969).

⁶M. C. Gutzwiller, *J. Math. Phys.* **11**, 1791 (1970).

⁷R. Balian and C. Bloch, *Ann. Phys.* **69**, 76 (1972).

⁸A. Einstein, *Verh. Dtsch. Phys. Ges.* **19**, 82 (1917).

⁹J. B. Keller, *Ann. Phys. (N.Y.)* **4**, 180 (1958).

¹⁰R. A. Marcus, *Chem. Soc. Faraday Discuss.* **55**, 34 (1973).

¹¹For example, see the δ_i 's in Eq. (3.4) of R. A. Marcus, *J. Chem. Phys.* **54**, 3965 (1971).

¹²H. Poincaré, *New Methods of Celestial Mechanics*, Vol. 3 (1897) (Transl. NASA, Washington, D.C., 1967, Document N67-27279), Chap. 27, where the theory of the surface of section is called the theory of consequents.

¹³For example, M. Henon and C. Heiles, *Astron. J.* **69**, 73 (1964); G. Contopoulos and M. Moutsoulas, *Astron. J.* **70**, 817 (1965); W. H. Jeffreys, *ibid.* **71**, 306 (1965); B. Barbanis, *ibid.* **71**, 415 (1966); G. H. Walker and J. Ford, *Phys. Rev.* **188**, 416 (1969).

¹⁴For a review, see J. Moser, *Stable and Random Motions in Dynamical Systems*, Annals of Mathematics Studies, No. 77 (Princeton University, Princeton, 1973); C. L. Siegel and J. K. Moser, *Lectures on Celestial Mechanics* (Springer-Verlag, Berlin, 1971).

¹⁵For example, to test accuracy of the integration method itself on the surface of section, tests were made for arbitrary E 's and f_x 's, with the uncoupled equations ($\lambda=\eta=0$) whose solution is known analytically, and hence exactly. Trajectories were performed with $\omega_x^2=0.48$ and $\omega_y^2=1.69$. For $E=0.9954$ and $f_x=0.3458$, the calculated values and, in brackets, the exact

values of $2\pi(n_x+\frac{1}{2})$ and $2\pi(n_y+\frac{1}{2})$ were 3.1217 [3.1216] and 3.1473 [3.1473]. When $E=3.548$ and $f_x=0.0800$, the corresponding values were 2.5742 [2.5741] and 15.776 [15.776]. For $\omega_x^2=0.29375$, $\omega_y^2=2.12581$, $E=0.992$, and $f_x=0.26$, the values were 2.9900 [2.9900] and 3.1635 [3.1634].

¹⁶To obtain the new interpolated value of E and f_x , three trajectories were used consisting of either two or one of the originals (depending on how many were close to the interpolated value for the eigenvalue) and the one or two further trajectories. The convergence of this procedure for calculating E and f_x was tested using these same trajectories, integrated for a longer time, i. e., having more points on the two surfaces of section. To obtain the data in Table I, a trajectory which typically provided ~ 60 points in the $y=0$ plane and ~ 120 points in the $x=0$ plane was used. Use of a larger number of points did not change the values of the eigenvalues for the systems in Table I by more than 0.0003 on the average. The eigenvalue for the last but one line in Table I required ~ 110 ($y=0$ plane) and ~ 140 points ($x=0$ plane) for convergence.

¹⁷The occurrence of this case was made evident by the factor that the procedure stated in the first sentence in Footnote 16 did not converge. Namely, the interpolated eigenvalue was sensitive to the three trajectories used even though all three were close to the interpolated value.

¹⁸If A_f was chosen to lie on the $y=0$ surface of section, the points A_f and A_l were joined by a straight line. The resulting value for Δ in (3.5) is $\frac{1}{2}(p_{x_f}+p_{x_l})(x_f-x_l)$, where x_l and p_{x_l} are the coordinates of A_l on this surface of section.

¹⁹G. Contopoulos, *Bull. Astron.* **2**, 223 (1967).

²⁰The only turning points we found, obtained by examining intersections of successive cycles of a nearby nearly periodic trajectory, were those which occurred on the "box-like" caustic boundaries, similar to those in Fig. 1 or 5.

²¹The f_x at 0.1058 in Table II denotes the mean of an $f_x=0.1055$ at $E=0.9950$ and of an $f_x=0.1060$ at $E=0.9960$. The f_x at 0.0149 denotes the mean of $f_x=0.0150$ at $E=1.6610$ and $f_x=0.0147$ at $E=1.6600$. The f_x at 0.0678 denotes the mean of $f_x=0.0680$ at $E=2.3640$ and $f_x=0.0675$ at $E=2.3630$.

²²Numerical values for the density of eigenvalues of a particle-in-a-sphere system are given in Ref. 7. Since this system permits a separation of variables, it was possible to delineate clearly the difference between the problem of determining a density of eigenvalues and that of determining individual eigenvalues. To determine the former, the authors used certain periodic trajectories (those of low p and t , in the notation of Ref. 7), but to determine the individual eigenvalues the authors used, as usual, a separation of variables and evaluated the requisite number of phase integrals. (The latter were *not* evaluated from periodic trajectories in the system as a whole.) The contrast in the two problems is clearly seen by comparing Eq. (13.16) for the spacing of the eigenvalue bunches, an equation which involves certain periodic trajectories, with Eqs. (13.8) and (13.9) for the individual eigenvalues, equations which do not involve periodic trajectories. An illuminating discussion of the relation between the two sets of equations is given in pp. 149-152 of Ref. 7. The fact that there is not a one-to-one correspondence between periodic trajectories and individual eigenvalues was further pointed out in R. Balian and C. Bloch, *Ann. Phys. N.Y.* **85**, 514 (1974).