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Adiabatic invariants and the problem of quasiclassical quantization of many-dimensional systems

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A method for calculating spectra of complicated systems in the quasiclassical approximation is proposed, which is based on the adiabatic invariance of quantum numbers; this enables one to avoid the basic calculational difficulties involved in finding caustics and fixing initial data for the quantized classical trajectories. The validity of this method is verified with the example of a two-dimensional anharmonic oscillator. The results of the adiabatic calculation are identical with those obtained previously by an exact direct quasiclassical calculation for this case. Some general questions connected with the application of the method are discussed.

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1. INTRODUCTION

Much attention has been given to the development of the quasiclassical method for many-dimensional systems that do not permit separation of the variables (see, for example, Refs. 1–3 and references given there). Progress in this field is of great importance for the theoretical study of the spectra of such physically important objects as closed and open resonators, excitons, hydrogenlike atoms in strong magnetic fields, polyatomic molecules (vibrational spectra), and so on. Nevertheless we know of only two papers[2,3] devoted to the quasiclassically exact calculation of the discrete spectrum; the cases considered were the nondegenerate and the degenerate two-dimensional anharmonic oscillator. This situation is due to the lack of a practical recipe for finding the quantized classical trajectories. The only way at present is to choose initial data directly and then check the quantum conditions for the resulting trajectories. For systems with several degrees of freedom this method requires an excessive amount of computer time, mainly spent in rejecting unsuitable trajectories. Furthermore, the checking of the quantum conditions requires the calculation of caustics,[1)] which are integral characteristics of trajectories, so that it is hard to find an algorithm for them. These difficulties naturally arise in the case of many-dimensional systems that do not admit separation of variables. Precisely this sort of situation is discussed in what follows.

In the present paper an approach is proposed which is different in principle, and which allows the removal of the main obstacles in the path of the quasiclassical calculation of spectra—those of fixing the initial data of trajectories and finding caustics. This approach is based on the adiabatic invariance of the quantum numbers. According to the adiabatic principle, the contracted action calculated over a closed path is conserved during a slow change of the potential; i.e., it is an adiabatic invariant.[4] Consequently, in a slow change of the potential the Bohr-Sommerfeld quantization conditions are not violated and the trajectory of a particle will continue throughout to be a quantized one. The adiabatic principle can be used to calculate the spectrum of a Hamiltonian H in the quasiclassical approximation in the following obvious way: First one chooses a reference Hamiltonian H_0 for which the classical trajectories that satisfy the quantization conditions are known, and then calculates with the classical equations of motion the development in time of these quantized trajectories during a slow change of the interaction $V = H - H_0$. When the interaction has been fully turned on, one obtains the quantized trajectory for the Hamiltonian H and the corresponding eigenvalue of the energy. The more slowly the interaction is turned on, the

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more precisely the quantization conditions are satisfied for the trajectory found in this way.

There has not been much investigation of the necessary conditions for the validity of the adiabatic principle. It was originally formulated by Ehrenfest for one-dimensional systems.[5] In papers by Burgers and by Krutkov[6] the validity of the adiabatic principle was proved for many-dimensional systems that permit complete separation of the variables. There is no proof for the general case. Moreover, in papers devoted to the investigation of adiabatic invariance, the opinion has been variously expressed that the principle of adiabatic invariance is a consquence of the separation of variables and does not hold for systems that do not allow complete separation (see, for example, Refs. 4–9). However, no full justification has been given for this view. On the other hand, the absence of adiabatic invariance in the general case would mean a violation of the correspondence principle in the adiabatic approximation of quantum mechanics. In our opinion a sufficient condition for the validity of the adiabatic principle is that the caustics must vary continously during a slow change of the potential. This sort of restriction is essentially related to the applicability of the quasiclassical approximation. For example, in the case of the violation of adiabatic invariance when the energy level touches the top of a barrier (Ref. 7, p. 54) the ordinary quasiclassical method also becomes inapplicable for the stationary Schrödinger equation of the system; here it is necessary to use a more refined method involving comparison with the parabolic-cylinder equation.

In Secs. 2 and 3 the adiabatic principle is used to calculate in the quasiclassical approximation spectra of two-dimensional systems for which the variables cannot be separated. So far as we know, this is the first time such a calculation has been done; therefore systems are studied for which the results of direct quasiclassically exact calculations are available.[2,3] The results of the adiabatic calculations agree with those found in Refs. 2 and 3. This indicates that adiabatic invariance does not depend on the separation of the variables. As compared with the method used in Refs. 2 and 3, the adiabatic method of calculation of spectra is much simpler and does not require any considerable computer time. However, it can be applied only when one can find a reference Hamiltonian H_0 whose quantized trajectories are not qualitatively different from those of the Hamiltonian and violation of adiabatic invariance are considered in Secs. 3 and 4. Further possible applications of this method are also discussed in Sec. 4.

2. NONDEGENERATE TWO-DIMENSIONAL ANHARMONIC OSCILLATOR

Eastes and Marcus[2] have calculated the spectrum of the Hamiltonian

$$H(\lambda)=\frac{1}{2}(p_x^2+p_y^2+\omega_x^2x^2+\omega_y^2y^2)+\lambda x(y^2+\eta x^2) \qquad (1)$$

in the quasiclassical approximation for several values of the parameters ω_x, ω_y, λ, and η, with different values of ω_x and ω_y. The Hamiltonian (1) occurs in the study of triatomic molecule.

For the adiabatic calculation of the spectrum of the Hamiltonian (1) we chose $H(0)=H(\lambda)\big|_{\lambda=0}$ as the reference Hamiltonian. The quantized trajectories for this Hamiltonian are well known:

$$\begin{aligned} x_0(t)&=A_x\sin(\omega_x t+\varphi_x),\\ y_0(t)&=A_y\sin(\omega_y t+\varphi_y). \end{aligned} \qquad (2)$$

Here[2)]

$$A_x=[(2n_x+1)/\omega_x]^{1/2},\quad A_y=[(2n_y+1)/\omega_y]^{1/2},$$

n_x and n_y are the quantum numbers of the oscillators along the x and y axes, and φ_x and φ_y are arbitrary phases. If the frequencies ω_x and ω_y are incommensurable[3)] the trajectories will in the course of time completely fill a rectangle in the xy plane: $|x|<A_x$, $|y|<A_y$. The sides of the rectangle are the caustics. At each point inside the rectangle the particle can be in four states, which differ from each other in the signs of the x and y components of the momentum p. In other words, the solution of the Hamiltonian-Jacobi equation is four-valued. Each of these states, taken at an arbitrary point inside the rectangle, can be used as an initial condition for a trajectory which evolves, in the process of slowly turning on the interaction $V=H(\lambda)-H(0)$, into a quantized trajectory of the Hamiltonian (1). We shall describe the turning on with equations of motion corresponding to the Hamiltonian (1), in which the parameter λ is replaced by a linear function of the time $\Lambda(t)=\lambda vt$. For $t=0$ this Hamiltonian is identical with $H(0)$, and for $t=1/v$ it is the Hamiltonian (1) with which we are concerned. There are other possible ways of turning on the interaction.

During the numerical solution of the equations of motion the quantity $H(\Lambda(t))$ was calculated in parallel with the calculation of the trajectory. According to the adiabatic principle, as the rate v of turning on the interaction becomes smaller this quantity must approach the energy $E_{n_xn_y}(\Lambda)$ of the quantized trajectory. The quantity $E_{n_xn_y}(\Lambda)$ is an adiabatic term in the quasiclassical approximation. The calculation shows that the quantity $H(\Lambda(t))$ oscillates around the limiting value $E_{n_xn_y}(\Lambda)$ with an amplitude proportional to the rate v, a period of the order of the period of oscillation of the particle along the x axis, and an initial phase that depends on the choice of the initial conditions. These oscillations are due to the change of the potential in the region of positive values of x during the time when the particle was in the region of negative x, and vice versa. For the variable y the change of the potential is more uniform and produces less effect. These oscillations bear no relation to the adiabatic principle, which makes assertions about quantities averaged over time. The averaging can also be done by simultaneously calculating several trajectories which satisfy different initial conditions, and then calculating the average value

$$H_{av}(\Lambda(t))=\frac{1}{m}\sum_{i=1}^{m}H_i(\Lambda(t))$$

(i numbers the trajectories). A natural procedure is to choose the distribution of the initial conditions so that their density is proportional to the square of the quasiclassical wave function. The calculations show that this gives the result more rapidly than diminishing the value of v in calculations with one trajectory.

In Ref. 2 several of the lower energy levels of the Hamiltonian (1) were calculated to five significant figures for several values of the parameters ω_x and ω_y of the order of one, and λ and η of the order of one-tenth. The adiabatic calculation gives all five figures correctly, and also automatically provides, to the same accuracy, the values of the energy for all intermediate values of $\Lambda (0<\Lambda<\lambda)$. The calculation of an entire $E_{n_x n_y}(\Lambda)$ curve requires about two minutes on an M-222 computer (speed 27 thousand operations per second).

3. DEGENERATE TWO-DIMENSIONAL ANHARMONIC OSCILLATOR

In the paper of Noid and Marcus[3] the spectrum of the Hamiltonian (1) was calculated for the following values of the parameters: $\eta=-1/3$, $\lambda=(0.0125)^{1/2}\approx 0.112$, $\omega_x=\omega_y=1$. We calculate here the spectrum of this Hamiltonian by the method of adiabatic invariants. The reference Hamiltonian and the mode of turning on the interaction are the same as in Sec. 2. An essential difference is that for $\omega_x=\omega_y$ a quantum state of the reference Hamiltonian can correspond to an infinite number of different classical trajectories, and for the adiabatic calculation we must first select from among them the correct initial trajectory.

When ω_x and ω_y are equal the spectrum of the reference Hamiltonian $H(0)$ is degenerate; all the trajectories are ellipses, and a single trajectory is not sufficient to form a quasiclassical state, since it specifies the state of the particle only on a manifold of measure zero in configuration space. To obtain a quasiclassical state defined in a finite volume it is necessary to take an ensemble of trajectories of a given energy. The Bohr-Sommerfeld condition for an individual trajectory fixes only the energy of the particle $E=N+1$ ($N=0, 1, 2,\ldots$ is the principal quantum number). A second quantization condition appears in the formation of the ensemble are selected.

When a small perturbation is turned on the degeneracy is removed. The trajectory will now fill a finite volume in configuration space, with the formation of caustics, and it must now satisfy two quantization conditions. The shape of the caustics depends on the form of the perturbation. For example, when one of the frequencies is changed the trajectory fills a rectangle in the xy plane, but if the perturbation is spherically symmetric it fills a ring. According to the form of the perturbation the quantum conditions restrict the choice of the initial unperturbed motion which is the starting point for the calculation of the perturbed trajectory; in the first case the unperturbed trajectory must have half-integer values of the quantities

$$E_x=\frac{1}{2}(p_x^2+x^2),\quad E_y=\frac{1}{2}(p_y^2+y^2), \tag{3}$$

and in the second case the angular momentum L must be an integer. This situation is analogous to the quantum perturbation theory for the degenerate case: here also, before calculating the correction to the energy it is necessary to find the correct initial state, which is determined by the form of the perturbation.

Accordingly, to carry out the adiabatic calculation of the spectrum of the Hamiltonian $H(\lambda)$ it is necessary first to determine the parameters of the initial elliptical trajectory, so as to assure that when the anharmonic interaction is turned on it will develop into a trajectory that satisfies both quantization conditions. For this purpose we use the method of secular perturbations (see Ref. 9).[4] Under the action of the small perturbation the particle will move in an elliptical trajectory whose parameters will change slowly with time. To check the quantization conditions it is sufficient to find the parameters of the ellipse as functions of the time. As these parameters it is convenient to choose the quantities E_x and E_y given by Eq. (3) and the angular momentum L. The variation of the parameters with time is described by the equations

$$\frac{dE_x}{dt}=p_xf_x,\quad \frac{dE_y}{dt}=p_yf_y,\quad \frac{dL}{dt}=xf_y-yf_x, \tag{4}$$

where

$$f_x=-\frac{\partial W}{\partial x}=-\varkappa(y^2-x^2),\quad f_y=-\frac{\partial W}{\partial y}=-2\varkappa xy$$

are the projections of the perturbing force on the x and y axes, $W=H(\varkappa)-H(0)$, and $\varkappa$ is a small parameter. Then, according to the secular-perturbation method, we must replace the right-hand sides of Eqs. (4) with their averages over the unperturbed motion. But at $\eta=-1/3$ the averages of all of these right-hand sides are equal to zero. To obtain a nontrivial result one must use perturbation theory to a higher order. For this purpose we represent the radius vector of the particle in the form

$$\mathbf{r}(t)=\mathbf{r}_0(t)+\varkappa\mathbf{r}_1(t). \tag{5}$$

Here $\mathbf{r}_0(t)$ is the radius vector of the unperturbed motion of the particle along an ellipse with the components (2), and the components of the vector $\mathbf{r}_1(t)$ are to be determined from the equations of motion

$$\ddot{x}_1=x_0^2-y_0^2,\quad \ddot{y}_1=-2x_0y_0. \tag{6}$$

Solving the system of Eqs. (6) and then averaging the right-hand sides of Eqs. (4) over the trajectories $\mathbf{r}(t)$ given by Eq. (5), we get

$$\begin{aligned}\frac{dE_x}{dt}&=\frac{7}{3}\varkappa^2L(E_xE_y-L^2/4)^{1/2},\\ \frac{dE_y}{dt}&=-\frac{7}{3}\varkappa^2L(E_xE_y-L^2/4)^{1/2},\\ \frac{dL}{dt}&=0.\end{aligned} \tag{7}$$

The solution of the system (7) is

$$\begin{aligned}E_x&={}^1/_2[E+(E^2-L^2)^{1/2}\cos({}^7/_3\varkappa^2Lt)],\\ E_y&={}^1/_2[E-(E^2-L^2)^{1/2}\cos({}^7/_3\varkappa^2Lt)],\\ L&=\text{const}.\end{aligned} \tag{8}$$

It follows from (7) that the parameter $E=E_x+E_y$ (the energy of the particle in the unperturbed problem) is conserved; i.e., the ellipses among which the particle slowly wanders belong to a set of trajectories of the un-

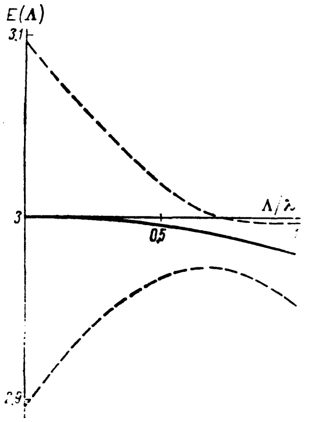

FIG. 1.

perturbed system. This is a natural result in perturbation theory. The character of the resulting trajectory is obvious if we choose as the parameters of an ellipse the quantities L, E, and θ. The angle θ, which gives the direction of the major axis of the ellipse, is expressed in terms of L, E_x, and E_y as follows:

$$\cos 2\theta = \frac{E_x - E_y}{(E^2 - L^2)^{1/2}}. \tag{9}$$

Substituting the solution (8) in Eq. (9), we get

$$\theta = {}^7/_6\varkappa^2 Lt,$$

i.e., the particle moves along an ellipse which keeps its shape (L = const, E = const) and rotates slowly and uniformly around the origin. Thus the trajectories fill a ring. This is the same sort of motion as is found for a spherically symmetric perturbation. It follows at once that the correct initial state will be one with integer L and E. The direction of the major axis is immaterial.

After finding out the kind of initial data that assures that we will get quantized trajectories when an infinitesimal perturbation is turned on, the further calculation is carried out precisely as in the case of different frequencies (Sec. 2). The results so obtained are identical with those of the direct calculations of Noid and Marcus,[3] who also gave the energy to five significant figures. As an example, Fig. 1 shows (solid curve) the energy as a function of Λ for the state with the quantum numbers (at $\Lambda = 0$) $L = \pm 2$, $N = 2$. This energy level is twofold degenerate.[3]

In the same figure we illustrate an important mechanism of breaking adiabatic invariance, which must be kept in mind in choosing a standard Hamiltonian. At first glance it would seem that the investigation by perturbation theory could be avoided as follows: start with an initial Hamiltonian with different frequencies, with no degeneracy, and then in parallel with the slow increase of Λ bring the frequencies to equality in such a way that when the interaction is fully turned on they are both equal to unity. In Fig. 1 the dashed lines show the results of such a calculation for two states whose quasiclassical terms should reach the same value, equal to that given by the solid curve, when the interaction has been fully turned on. The frequencies chosen in the initial Hamiltonian were as follows: $\omega_x^2 = 0.9$, $\omega_y^2 = 1.1$. We see from Fig. 1 that at first the two terms move toward the correct common value, but then they begin to move apart. The reason for the breaking of the adiabatic invariance is that the original state is four-valued and has only an outer caustic, but the final state, as was shown in Ref. 3, is two-valued and has both an outer and an inner caustic. If one chooses the origin of coordinates in configuration space at a point of formation of the inner caustic, and uses as the coordinates in the momentum space p_r (the radial component of the momentum) and p_φ (the angular component of the momentum), then for $t < t_0$ (t_0 is the time when the inner caustic forms) p_φ takes positive and negative values with equal probabilities, but for $t > t_0$ the particle moves in only one direction around the origin in configuration space and the quantity p_φ can no longer change sign. Thus at the instant t_0 there is a discontinuous (nonadiabatic) change of the caustic in the momentum space. At the same instant there is a change of the multiplicity of the solution of the Hamilton-Jacobi equation in configuration space.

4. CONCLUSIONS

The method of adiabatic invariance greatly simplifies the calculation of spectra of complicated systems and does not require large amounts of computer time. In a certain sense it is a generalization of the method of the reference equation to the case of many-dimensional systems. Precisely as in the method of the reference equation, the fundamental problem here is to find a reference Hamiltonian H_0 whose quasiclassical states do not differ qualitatively from the states of the Hamiltonian H. For the present case, however, unlike that of the reference equation, we do not have clear criteria for deciding whether or not a given function is a reference Hamiltonian for the Hamiltonian H. For many-dimensional systems a superficial similarity of the potentials is no longer sufficient, as is convincingly shown by the example of breaking of adiabatic invariance considered at the end of the previous section, in which outwardly similar Hamiltonians could not serve as the given and reference Hamiltonians. The point is that in the many-dimensional case, depending on the state of the particle, additional effective potentials appear, such as the centrifugal potential. This situation reflects the intrinsic complexity of the problem of calculating the spectra of many-dimensional systems.

Among the problems which can be investigated by the proposed method, we must first of all mention the calculation of the spectra of the helium atom and of the hydrogen atom in crossed fields. To calculate the helium spectrum it is natural to use an adiabatic turning-on of the interaction between the electrons. The reference Hamiltonian so obtained is degenerate. The classical perturbation theory for the interaction of the electrons in the helium atom, which is required for choosing the correct initial trajectory, was developed by Born, Heisenberg, and Kramers[10] (see also Ref. 9). The perturbation theory for hydrogen in crossed electric and magnetic fields is expounded in Ref. 9, and the initial elliptical trajectories of the electron which, when the fields are slowly switched on, will develop into trajectories satisfying the quantization conditions are known. One can check that the adiabatic principle holds either by selective verification of the quantization conditions or by varying the manner in which the interaction is turned on (if there is no violation of adiabatic invariance, the final result must obviously not depend on the way the interaction is turned on). At the present time it is evidently impossible to calculate the spectra of these systems in the quasiclassical approximation in any other way.

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[1)] Caustics are hypersurfaces in configuration space with separate regions in which a solution of the Hamilton-Jacobi equation has different multiplicities.

[2)] In this paper we use the atomic system of units $e=m=\hbar=1$.

[3)] Commensurability of frequencies cannot play any special role in the adiabatic method, since the Hamiltonian is nonstationary and resonance effects occur at a set of points of measure zero along the time axis.

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Radiative recombination and its application in experiments on electron cooling

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A simple closed expression is derived, in the dipole approximation, for the cross section for radiative recombination of an electron into an arbitrary level of a hydrogenlike atom. The effect of a magnetic field on this process is estimated. The possibility of using it in experiments on electron cooling of heavy charged particles is discussed.

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1. In connection with work now in progress on electron cooling[1] there is increasing interest on the process of recombination of electrons with protons. For example, detection of the resulting hydrogen atoms has been used directly in the NAP-M storage ring to bring the proton and electron beams into coincidence and to obtain a rough estimate of the temperature of the latter beam. As is shown in what follows, for values of the parameters corresponding to the experiment of Ref. 1 recombination is due to radiative transitions. For a formulation of the problem and a survey of the literature on this question, see Ref. 2. In the present paper an expression in closed analytic form for the cross section of radiative recombination to the level n of a hydrogenlike atom is obtained for the first time, by successfully performing the sum over all quantum numbers. An analysis of the experimental situation with electron cooling is also made, and in particular the influence of a magnetic field on the recombination rate is estimated.

Recombination can occur both through the involvement of three particles (ternary recombination) and owing to the emission of a photon (radiative recombination). The total number $\dot{N}$ of recombinations per unit time is given by

$$\dot{N}=\beta n_e N_p, \tag{1.1}$$

where n_e is the density of electrons, N_p is the total number of protons, and β is the recombination coefficient.

In ternary recombination there is a transfer of energy of the order of the mean kinetic energy from one electron to another. The characteristic length for this process is $\rho \sim e^2/T$ (the temperature T of the electron beam is in energy units), and its probability per unit time $\sim v_T \rho^2 n_e$ (v_T is the velocity corresponding to the temperature T). For recombination to occur, the electron that loses energy must be at a distance $\sim\rho$ from a proton. The number of such electrons per proton is