Semiclassical quantization of nonseparable systems: A new look at periodic orbit theory*

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(Received 27 March 1975)

A modified version of Gutzwiller's periodic orbit theory of semiclassical eigenvalues is presented which eliminates some of the principal shortcomings of the original result. In particular, for a nonseparable system with N degrees of freedom the new quantum condition characterizes the eigenvalues by N quantum numbers (rather than just one), and it also reduces to the correct result in the limit that the system is a separable set of harmonic oscillators (whereas the original quantum condition does not). This new periodic orbit quantum condition is seen to bear an interesting relation to Marcus' recent theory of semiclassical eigenvalues which involves manifolds of quasiperiodic trajectories.

I. INTRODUCTION

The possibility of generalizing the WKB, or Bohr–Sommerfeld quantum condition[1] for one-dimensional potential wells,

$$\hbar^{-1}\oint dx\, p(x,E) = 2\pi(n+\tfrac{1}{2}) ,$$
$$p(x,E) = \sqrt{2m[E-V(x)]} , \tag{1.1}$$

to multidimensionable nonseparable systems has intrigued theorists for many years. Einstein[2] was the first to make significant progress on the problem, and important contributions have also been made by Keller[3] and Maslov.[4]

More recently, Gutzwiller,[5] using an analysis based on the semiclassical approximation to the quantum propagator, made an important advance by showing that the semiclassical quantum condition is intimately related to the periodic classical trajectories, or periodic orbits of the system. The connection between periodic classical trajectories and quantum mechanical eigenvalues is appealing on physically intuitive grounds, but the specific quantum condition obtained by Gutzwiller has a number of deficiencies, not the least of which is that it does not give the correct result in the limit that the system becomes separable. This and other shortcomings have been discussed by Pechukas[6] in his approach to constructing a more satisfactory quantum condition. Marcus[7] has also recently made important advances, and his theory, based on phase space manifolds generated by quasiperiodic trajectories, is most closely related to the present work; Sec. IV discusses this relation in more detail.

This paper pursues the periodic orbit theory of Gutzwiller,[5] but introduces an important modification of the analysis leading to the quantum condition itself. This modification, though simple and fairly obvious (in retrospect), leads to a significantly different semiclassical quantum condition which eliminates some of the flagrant deficiencies of the original result. For a system of N degrees of freedom, for example, the new quantum condition labels the energy levels with N quantum numbers, whereas the original result provided only one quantum number. The new quantum condition, too, gives the correct result in the limit that the system is a set of separable harmonic oscillators.

II. BASIC THEORY

There is no need to redo most of Gutzwiller's derivation,[5] but it is worthwhile to recall the way in which periodic orbits arise. The density of states per unit energy, $\rho(E)$, is defined by

$$\rho(E) = \mathrm{Tr}[\delta(E-H)] , \tag{2.1}$$

and it is clear that this is given quantum mechanically by

$$\rho(E) = \sum_n \delta(E-E_n) , \tag{2.2}$$

where $\{E_n\}$ are the eigenvalues of the Hamiltonian; $\rho(E)$, therefore, has delta function singularities when E is equal to an eigenvalue. Since

$$\delta(E-H) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{iEt/\hbar}\, e^{-iHt/\hbar} , \tag{2.3}$$

Eq. (2.1) is equivalent to

$$\rho(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{iEt/\hbar}\,\mathrm{Tr}(e^{-iHt/\hbar})$$
$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{iEt/\hbar}\int d\mathbf{q}\,\langle \mathbf{q}|e^{-iHt/\hbar}|\mathbf{q}\rangle . \tag{2.4}$$

One now introduces the semiclassical approximation for matrix elements of the propagator,[8]

$$\langle \mathbf{q}_2|e^{-iHt/\hbar}|\mathbf{q}_1\rangle \sim e^{i\phi(\mathbf{q}_2,\mathbf{q}_1)/\hbar} , \tag{2.5}$$

where $\phi(\mathbf{q}_2,\mathbf{q}_1)$ is the action integral along the classical trajectory connecting $\mathbf{q}_1$ and $\mathbf{q}_2$ in time interval $(0,t)$, and the integral over $\mathbf{q}$ in Eq. (2.4) is evaluated by the stationary phase approximation[9]; since[10]

$$\frac{\partial\phi(\mathbf{q}_2,\mathbf{q}_1)}{\partial\mathbf{q}_2} = \mathbf{p}_2 , \tag{2.6a}$$

$$\frac{\partial\phi(\mathbf{q}_2,\mathbf{q}_1)}{\partial\mathbf{q}_1} = -\mathbf{p}_1 , \tag{2.6b}$$

where $\mathbf{p}_2$ and $\mathbf{p}_1$ are the values of the classical momenta at time t and time 0, respectively, the stationary phase condition for the integral over coordinates in Eq. (2.4) is

$$0 = \frac{\partial}{\partial\mathbf{q}}\phi(\mathbf{q},\mathbf{q}) = \left[\frac{\partial\phi(\mathbf{q}_2,\mathbf{q}_1)}{\partial\mathbf{q}_2} + \frac{\partial\phi(\mathbf{q}_2,\mathbf{q}_1)}{\partial\mathbf{q}_1}\right]_{\mathbf{q}_1=\mathbf{q}_2=\mathbf{q}} = \mathbf{p}_2 - \mathbf{p}_1 ; \tag{2.7}$$

i.e., $\mathbf{q}(0)=\mathbf{q}(t)$ and $\mathbf{p}(0)=\mathbf{p}(t)$, so that the values of $\mathbf{q}$ which contribute in a stationary phase sense to the integral in Eq. (2.4) must lie on a periodic trajectory. Periodic orbits arise, therefore, because the stationary phase approximation is used to carry out the trace of the propagator.

Carrying out this stationary phase integration over $\mathbf{q}$, and also over t, gives the equivalent of Gutzwiller's Eq. (36),

$$\rho(E)=\mathrm{Re}\frac{T}{\pi\hbar}\sum_{n=1}^{\infty}\frac{\exp\{in[\Phi-\lambda(\pi/2)]\}}{2i\sin(nv/2)}, \tag{2.8}$$

where $\Phi\equiv\Phi(E)$ is the action integral, in units of $\hbar$,

$$\Phi=\hbar^{-1}\int_0^T dt\,\mathbf{p}\cdot\dot{\mathbf{q}}, \tag{2.9}$$

along the periodic trajectory with energy E; $T=T(E)$ is the period of this trajectory; and $v=v(E)$ is its stability parameter. Equation (2.8) is written explicitly for the case of two degrees of freedom; the extension to N degrees of freedom is trivial and will be discussed below. λ in Eq. (2.8) is the number of turning points encountered along the periodic trajectory; Gutzwiller assumes $\lambda=0$, but we shall see in Sec. III that this need not be the case. [Gutzwiller's Eq. (36) actually gives the trace of the Green's function

$$\mathrm{Tr}[G(E)]=-\frac{T}{\hbar}\sum_{n=1}^{\infty}\frac{\exp\{in[\Phi-\lambda(\pi/2)]\}}{2\sin(nv/2)}, \tag{2.10}$$

but since

$$\mathrm{Im}G(E)=-\pi\delta(E-H), \tag{2.11}$$

Eq. (2.8) follows directly from Eq. (2.10).] Since

$$\mathrm{Re}\frac{\exp\{in[\Phi-(\lambda\pi/2)]\}}{2i\sin(nv/2)}=\frac{\sin\{n[\Phi-(\lambda\pi/2)]\}}{2\sin(nv/2)},$$

and since the period $T(E)$ is related to the energy derivative of the classical action,

$$T(E)=\hbar\Phi'(E), \tag{2.12}$$

Eq. (2.8) is equivalent to

$$\rho(E)=\frac{\Phi'(E)}{2\pi}\mathrm{Re}\sum_{n=-\infty}^{\infty}\frac{\exp\{in[\Phi(E)-(\lambda\pi/2)]\}}{2i\sin[\frac{1}{2}n\hbar\omega(E)\Phi'(E)]}, \tag{2.13}$$

where the stability *frequency* $\omega(E)$ is defined by

$$\omega(E)=v(E)/T(E)=\frac{v(E)}{\hbar\Phi'(E)}.$$

Equation (2.13) is essentially Gutzwiller's[5] Eq. (36), and it is obtained with no approximation other than use of the semiclassical limit of the propagator and the stationary phase approximation for evaluating the integrals in Eq. (2.4); as has been emphasized in other contexts,[10] the stationary phase approximation is the fundamental semiclassical approximation, and in the classical limit, $\hbar\to 0$, it becomes exact. The sum over n in Eq. (2.13) is a sum over the infinite number of multiple passes about the periodic orbit, and it is the interference of these amplitudes which leads to quantization.

It is now that the essential departure from Gutzwiller's[5] analysis is made. Gutzwiller introduces an approximation to the denominator of the summand in Eq. (2.13), but this is not necessary and actually causes the loss of certain important features. More accurately, one notes that

$$\frac{1}{2i\sin(x/2)}=\frac{e^{-ix/2}}{1-e^{-ix}}=\sum_{m=0}^{\infty}e^{-i(m+1/2)x}, \tag{2.14}$$

so that Eq. (2.13) becomes

$$\rho(E)=\frac{\Phi'(E)}{2\pi}\mathrm{Re}\sum_{m=0}^{\infty}\sum_{n=-\infty}^{\infty}\exp\left\{in\left[\Phi(E)-\frac{\lambda\pi}{2}-\left(m+\frac{1}{2}\right)\hbar\omega(E)\Phi'(E)\right]\right\}. \tag{2.15}$$

The Poisson sum formula,[11]

$$\sum_{n=-\infty}^{\infty}e^{inx}=2\pi\sum_{n=-\infty}^{\infty}\delta(x-2\pi n), \tag{2.16}$$

then converts Eq. (2.15) into

$$\rho(E)=\Phi'(E)\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\delta\left[\Phi(E)-\frac{\lambda\pi}{2}-\left(m+\frac{1}{2}\right)\hbar\omega(E)\Phi'(E)-2\pi n\right]. \tag{2.17}$$

Upon comparing Eq. (2.17) with Eq. (2.2), one identifies the quantum condition as

$$\Phi(E)-(m+\tfrac{1}{2})\hbar\omega(E)\Phi'(E)=2\pi(n+\tfrac{1}{4}\lambda),\quad n \text{ and } m=0,1,2,\cdots. \tag{2.18}$$

If one sets $\lambda=0$ and $m=0$ and recalls that $\hbar\omega(E)\Phi'(E)=v(E)$, the stability parameter, then Eq. (2.18) is identical to Gutzwiller's[5] quantum condition, his Eq. (39).

The approximation introduced by Gutzwiller[5] to obtain the quantum condition from Eq. (2.13) thus misses the possibility of a nonzero value of the quantum number m in Eq. (2.18). The above, more correct, procedure thus obtains a quantum condition characterized by two quantum numbers; i.e., the eigenvalue $E_{n,m}$ is determined implicitly by Eq. (2.18) in terms of the quantum numbers n and m.

Equations (2.13)–(2.19) are generalized in a rather obvious way to the case of N degrees of freedom. Equation (2.13) is modified by the replacement

$$2i\sin[\tfrac{1}{2}n\hbar\omega(E)\Phi'(E)]\to\prod_{i=1}^{N-1}2i\sin[\tfrac{1}{2}n\hbar\omega_i(E)\Phi'(E)], \tag{2.19}$$

where $\{\omega_i(E)\}$ are the $N-1$ stability frequencies which are defined in terms of the stability parameters $\{v_i(E)\}$ by

$$\omega_i(E)=v_i(E)/T(E)=\frac{v_i(E)}{\hbar\Phi'(E)}. \tag{2.20}$$

An expansion like Eq. (2.14) is made for each of the $N-1$ sine functions in Eq. (2.19), and the generalization of Eq. (2.15) is

$$\rho(E)=\frac{\Phi'(E)}{2\pi}\,\mathrm{Re}\sum_{\mathbf{m}=0}^{\infty}\sum_{n=-\infty}^{\infty}\exp\left\{in\left[\Phi(E)-\frac{\lambda\pi}{2}-\sum_{i=1}^{N-1}\left(m_i+\frac{1}{2}\right)\hbar\omega_i(E)\Phi'(E)\right]\right\}, \tag{2.21}$$

where

$$\sum_{\mathbf{m}=0}^{\infty}\equiv\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\cdots\sum_{m_{N-1}=0}^{\infty}.$$

Use of the Poisson sum formula Eq. (2.16) in the same manner then leads to the following quantum condition:

$$\Phi(E)-\sum_{i=1}^{N-1}\left(m_i+\frac{1}{2}\right)\hbar\omega_i(E)\Phi'(E)=2\pi\left(n+\frac{\lambda}{4}\right), \tag{2.22}$$

which determines E implicitly in terms of the N quantum numbers $\{m_i\}$, $i=1, 2, \ldots, N-1$, and n. Equation (2.18) is clearly the two-dimensional version of Eq. (2.22).

In concluding this section, it is interesting to consider a modification of Eq. (2.22) analogous to one that has been found useful in an application[12] of a similar analysis to the semiclassical limit of quantum mechanical transition state theory.[13] One recognizes that the left hand side of Eq. (2.22) looks like the first two terms of a Taylor series expansion

$$\Phi(E-\epsilon)=\Phi(E)-\epsilon\Phi'(E)+\cdots,$$

where one identifies

$$\epsilon=\sum_{i=1}^{N-1}\left(m_i+\frac{1}{2}\right)\hbar\omega_i(E).$$

Since ϵ is proportional to $\hbar$, it is clear that to lowest order in $\hbar$ Eq. (2.22) is also equivalent to

$$\Phi\left(E-\sum_{i=1}^{N-1}\left(m_i+\frac{1}{2}\right)\hbar\omega_i(E)\right)=2\pi\left(n+\frac{\lambda}{4}\right). \tag{2.23}$$

If $\Phi^{-1}[\cdots]$ is the inverse function of $\Phi(E)$, then Eq. (2.23) can be written as

$$E=\Phi^{-1}\left[2\pi\left(n+\frac{\lambda}{4}\right)\right]+\sum_{i=1}^{N-1}\left(m_i+\frac{1}{2}\right)\hbar\omega_i(E), \tag{2.24}$$

which we refer to as the *modified* periodic orbit quantum condition. Equation (2.24) is still not an explicit expression for the eigenvalues $E_{n,m_1\cdots m_{N-1}}$, however, because the stability frequencies are functions of energy; it would thus be necessary to solve Eq. (2.24) iteratively.

The modified quantum condition, Eq. (2.24), has a strikingly simple form. As has been discussed before,[13] the stability frequencies $\{\omega_i\}$ are the dynamical generalization of normal mode frequencies; they are the normal mode frequencies for harmonic perturbations about the periodic orbit. The total energy E, therefore, is a sum of contributions: The first term in Eq. (2.24) is the energy of n quanta in motion *along* the periodic orbit, and the ith term in the sum of $N-1$ terms is the energy of m_i quanta in the ith normal mode of deviation about the periodic orbit.

III. SEPARABLE LIMIT

It is easy to show that the quantum condition obtained in Sec. II is correct in the separable limit if the separate potential functions are harmonic. For simplicity, consider the case of two degrees of freedom: The potential function is

$$V(x,y)=\tfrac{1}{2}\mu\omega_1^2x^2+\tfrac{1}{2}\mu\omega_2^2y^2,$$

where μ is the mass, and ω_1 and ω_2 are the two harmonic frequencies. The question of whether or not ω_1 and ω_2 are commensurable, i.e., whether or not ω_1/ω_2 is a rational number, does not enter in the treatment below.

The relevant periodic trajectory is the one with all the energy E in the x mode, say, and thus no energy in the y mode; it is clear that λ, the number of turning points along the periodic trajectory, is then 2. It is easy to show that in this case the action integral $\Phi(E)$ is

$$\Phi(E)=\frac{2\pi E}{\hbar\omega_1}. \tag{3.1}$$

It is also easy to show[13] that the stability frequency $\omega(E)$ is simply the frequency of the y mode; i.e.,

$$\omega(E)=\omega_2. \tag{3.2}$$

With Eqs. (3.1) and (3.2), and $\lambda=2$, the periodic orbit quantum condition, Eq. (2.18), gives

$$E=(m+\tfrac{1}{2})\hbar\omega_2+(n+\tfrac{1}{2})\hbar\omega_1, \tag{3.3}$$

the correct result. Since $\Phi(E)$ in Eq. (3.1) is a linear function of E, the modified quantum condition, Eq. (2.24), also leads to Eq. (3.3). It is also clear that one obtains the same result by considering the periodic trajectory with all the energy in the y mode.

Unfortunately, however, one can see that Eq. (2.18) will *not* give the correct eigenvalues for the separable case if the two one-dimensional potential functions are not harmonic. The modified quantum condition, Eq. (2.24), gives the correct result if only one of the potential functions in anharmonic and the periodic orbit is with all energy along this direction, but it also fails if both periodic functions are anharmonic.

IV. CONCLUDING REMARKS

The analysis presented in Sec. II eliminates some of the most glaring deficiencies of the periodic orbit approach to semiclassical quantization of nonseparable systems. In particular, the new quantum condition characterizes the energy levels of an N-dimensional system by N quantum numbers, and it reduces to the correct result in the limit that the system is N independent harmonic oscillators.

The new quantum condition, however, is not entirely satisfactory. The correct separable limit is not obtained if the potential functions for coordinates orthogonal to the periodic orbit are not harmonic. This shortcoming stems directly from the stationary phase approximation for evaluating the integral over coordinates in Eq. (2.4); in this approximation, only small quadratic deviations about the periodic orbit are considered in computing the trace of the propagator, and thus only a harmonic approximation is obtained for the modes describing displacements away from the periodic orbit. Because the stationary phase approximation is such a fundamental element of semiclassical mechanics, it is not clear how one can remedy this defect within the present formalism.

In conclusion, it is interesting to note the resemblance of the present version of periodic orbit theory to Marcus'[7] recent work involving manifolds of quasiperiodic trajectories. A periodic orbit plus all harmonic deviations about it is clearly an approximate representation of a quasiperiodic manifold; i.e., a slightly perturbed periodic trajectory, which is stable, will be quasiperiodic, its stability frequencies being the normal mode of oscillation about the periodic orbit. Because of the stationary phase approximation, however, periodic orbit theory is only able to include deviations about the periodic trajectory within a harmonic approximation, whereas Marcus' approach is not limited in this way. For the case of a separable or a near separable system, therefore, it seems clear that the present version of periodic orbit theory is an approximation to Marcus's quasiperiodic theory. Whether this is also true for strongly coupled systems is difficult to say, since the nature, or even the existence, or periodic orbits and quasiperiodic manifolds is not well understood in such cases.

*Supported in part by the U. S. Energy Research and Development Administration, and by the National Science Foundation under Grant GP-41509X.

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