GREEN'S FUNCTION SEMICLASSICAL QUANTIZATION OF NON-CLOSED QUASIPERIODIC CLASSICAL TRAJECTORIES ‡

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A semiclassical quantization procedure is introduced within the Green's function formalism for non-closed quasiperiodic trajectories which have previously defied quantization with this formalism The results are interpreted in terms of the uncertainty principle and lead to conjectures concerning the semiclassical quantization of ergodic trajectories

1 Introduction

When applying quantum theory to complicated multidimensional chemical or physical systems, it is often necessary to determine the set of energy eigenvalues. One approach to the problem is provided by the stationary phase integral approximation, commonly known as WKB or semiclassical methods. Semiclassical quantization methods have been developed in a variety of different fashions for situations (and energies, etc) where the classical equations are integrable [1–6]. Considerable interest remains in the semiclassical quantization for cases where the classical trajectories are stochastic [5]

The majority of semiclassical quantization methods either utilize, or are closely related to, the Einstein formulation [7,8] which quantizes the action along a set of topologically inequivalent paths whose number equals the dimensionality of the system. These types of quantization methods leave unanswered the physically interesting question as to which classical paths actually contribute to generating the semiclassical wavefunctions [9] for multidimensional non-separable systems. Such questions require the retention of phase information, and Green's function semiclassical quantization methods can, in principle, attack this problem [5,6,9–11]. However, within the Green's function formalism, as described below, some of the simplest readily solvable classical systems have defied semiclassical quantization [12] Here we generalize these methods to enable them to apply to cases of quasiperiodic non-closed orbits. The quantization conditions involve a set of classical trajectories as allowed by the uncertainty principle. One important reason for pursuing the generalization of the Green's function method to integrable systems, which are quantizable by other means, is the fact that these semiclassical Green's function techniques do not appear to be limited to the domain of integrable classical trajectories. Indeed, this formalism permits us to make some conjectures concerning semiclassical quantization of ergodic classical trajectories.

A direct method for calculating the semiclassical eigenvalues is obtained by examining the density of states of the system. The poles generate the eigenvalues Gutzwiller [6], Berry and Tabor [12] and others [11] have developed methods of evaluating the density

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of states by a series of stationary phase integrals. Their somewhat differing methods all use only periodic classical orbits as a base for the quantization. The present paper, on the other hand, shows that in any quantization of multidimensional systems quasiperiodic trajectories have to be considered as well. This is illustrated by use of a simple example for which there are *no periodic classical orbits*

The starting point for obtaining the semiclassical approximation involves the propagator $G(q, q', t)$ with q the spatial position and t the time. According to the spirit of method, this propagator is calculated from a path integral using the stationary phase method The classical nature comes about through the stationary phase integration which selects out the classical trajectory of duration t connecting the end points q and q'. This trajectory is then used to evaluate the action of the propagator. At this point quantum features appear through the possibility of many different classical trajectories contributing to the propagator $G(q, q', t)$. This arises because, although the position of the end points and the transit time are fixed, the momenta at the end points are not. Therefore, there is the possibility of many contributions to the propagator [13] from classical trajectories with different momenta.

The second stage of approximation, following Gutzwiller [6], is to convert the propagator $G(q, q', t)$ to the energy Green's function $G(q, q', E)$ through a Fourier transform. In the semiclassical approximation this integral is approximated by the method of stationary phase, and the result is [6,14]

$$G(q, q', E) = (2\pi\hbar)^{-2} \sum_{\substack{\text{classical} \\ \text{paths}}} |D_S|^{1/2} \times \exp[i\hbar^{-1} W^*(q, q', E) - \text{phases}], \quad (1.1)$$

where

$$W^*(q, q', E) = \int_q^{q'} p \cdot dq,$$

$$D_S = \begin{vmatrix} \partial^2 W/\partial q \partial q' & \partial^2 W/\partial q \partial E \\ \partial^2 W/\partial E \partial q' & \partial^2 W/\partial E^2 \end{vmatrix} \quad (1.1a)$$

and the phases in (1.1) are discussed after (2.17) below.

Formula (1.1) is the starting point of Gutzwiller's method. Then he proceeds to calculate the density of states through

$$n(E) = \int dq\, G(q, q, E). \quad (1.2)$$

Thus q integral is also approximated by the stationary phase method, so only classical trajectories are found to contribute to the density of states in which the initial and final momenta are equal. This implies that only periodic orbitals can be considered. A pole in the density of states is found whenever the action of the periodic orbit is a multiple of $2\pi\hbar$ (apart from some constants arising from the phases in (1.1) which are discussed below) [15]. A similar conclusion is found in the work of Berry and Tabor [12] who utilize an action–angle variable formulation

Once this theory had been developed, it became apparent that systems without periodic orbits could not be quantized by these Green's function methods. The most obvious example is the two-dimensional harmonic oscillator whose frequencies have ratios which are irrational. Berry and Tabor recognized this problem in their paper [12].

The present paper, whose main motivation is a critical examination of the semiclassical Green's function, deals with the quasiperiodic classical orbits directly, showing that and how they contribute to semiclassical quantization. This significant conclusion expands the family of trajectories which can be quantized by this semiclassical method; it provides interesting physical insight into those classical trajectories which contribute to the wavefunction; and it enables us to provide conjectures on the quantization of ergodic trajectories.

2. The eigenvalues of the two-dimensional incommensurable harmonic oscillator

Because one-dimensional semiclassical methods for quantum analysis are so effective, it is surprising that so far multidimensional methods have not been. For example, the one-dimensional semiclassical theory of the harmonic oscillator matches almost exactly the full quantum mechanical theory [11]. On the other hand, the harmonic oscillator had not been quantized successfully in multidimensional Green's function theory. Using the incommensurable multidimensional harmonic oscillator as the example, therefore, the present section of this paper examines the reason why the

multidimensional theory has been difficult and how the proposed modifications clear up these previous difficulties

When the Green's function method is critically examined in the spirit of the semiclassical approximation, it would seem that it ought to have a certain degree of fuzziness in accord with the uncertainty principle, a fuzziness which is absent in previous calculations with strictly periodic orbits It is by incorporating this fuzziness of variables into the semiclassical Green's function method that the multidimensional quasiperiodic systems can be quantized

As discussed in section 1, the common method of identifying eigenvalues of a system within the Green's function formalism is to calculate the poles in the density of states function This requires the performance of three successive stationary phase approximations for the path integral (The methods of Gutzwiller [6] and of Berry and Tabor [12] differ in the orders of integration chosen) Instead of proceeding to calculate the density of states it is possible to obtain the eigenvalues one step earlier [9,10], starting from the energy Green's function,

$$G(q,q',E)=\sum_j \phi_j(q)\,\phi_j^*(q')/(E-E_j) \qquad (2\,1)$$

for the points q and q' The eigenvalues of the system can be identified as poles of $G(q,q',L)$, regardless of the end points q and q' This conclusion is important because any initial and final points and not only $q=q'$ have to reflect the full quantum nature of the system Methods based upon (2 1) retain phase information which is destroyed in the stationary phase approximation to the q integral in (1 2) Hence, the semiclassical wavefunctions $\phi_j(q)$ can in principle, be obtained as residues of (2 1) at the poles E_j [9]

In the spirit of the semiclassical approximation, our starting point for the Green's function is eq (1 1) The next step is to analyze how a pole can be built up in the semiclassical approximation Examining eq (1 1), it can be seen that a pole is possible whenever a constructive interference is accumulated by an infinite number of classical trajectories which have the same end points $q-q'$ and their actions in phase The main deviation from the previous theories is at this point In previous theories all trajectories have actions that contribute exactly in phase, here the actions contribute almost in phase (modulo $2\pi\hbar$) It is this slight change which opens a new family of classical trajectories to contributing to the quantization scheme In order to illustrate our ideas, we solve in detail the semiclassical quantization of the incommensurable two-dimensional harmonic oscillator

Consider a two-dimensional harmonic oscillator with frequencies ω_x and ω_y whose ratio is irrational We seek a pole at energy E As mentioned above, trajectories with almost the same action are required to constructively interfere to produce the pole Consider first the reference trajectory starting with x_0,y_0 at $t=0$ and ending at x_1,y_1 at time $t=t_1$ Since the energy and time are fixed, the values x_0,y_0,x_1,y_1 are enough to calculate the amplitude and phase of the two oscillations in the x and y directions from the well-known trajectories

$$x(t)=A_x\cos(\omega_x t+\phi_x),$$

$$y(t)=A_y\cos(\omega_y t+\phi_y) \qquad (2\,2)$$

Next, another trajectory is sought with the same initial and end points Of necessity, the new trajectory reaches the end point at a different time $t=t_{nm}$ The subscripts denote that the trajectory oscillates n more times in the x direction and m more times in the y direction than the first reference trajectory This trajectory is found by adjusting the amplitude and phases subject to conservation of the total energy which confines the amplitudes to

$$E=\alpha_x A_x^2+\alpha_y A_y^2, \qquad (2\,3)$$

where $\alpha_i=\frac{1}{2}m_i\omega_i^2$, and the matching of end points which relates the amplitudes to phases by

$$A_x=x_0/\cos\phi_x, \quad A_y=y_0/\cos\phi_y \qquad (2\,4)$$

Using (2 3) and (2 4) there is a relationship between the amplitude and phase of the two trajectories Denoting these phases by ϕ_x^0,ϕ_x^{nm}, etc , this gives

$$\frac{\cos(\phi_y^0+\omega_y t_1)}{\cos\phi_y^0}=\frac{\cos(\phi_y^{nm}+\omega_y t_{nm})}{\cos\phi_y^{nm}} \qquad (2\,5)$$

A time adjustment constant is defined by the relation,

$$t_{nm}=t_1+2\pi n/\omega_x+\delta_x \qquad (2\,6)$$

The constant δ_x measures the deviation from strict periodicity of the nm trajectory from the reference trajectory Define also a phase adjustment constant

$$\omega\phi_x = \phi_x^0 - \phi_x^{nm} \tag{2.7}$$

Next n and m are chosen in order to minimize the differences δ_x and δ_y. Therefore, by using (2.6) and (2.7) eq (2.5) can be expanded to the first order in δ and $\Delta\phi$ yielding

$$\Delta\phi_x \sin\phi_x \cos(\phi_x + \omega_x t_1)$$

$$= [\cos\phi_x \sin(\phi_x + \omega_x t_1)](\omega_x\delta_x + \Delta\phi_x), \tag{2.8}$$

or

$$\Delta\phi_x = \beta_x\delta_x,$$

where

$$\beta_x = \omega_x[1 - \tan\phi_x \cot(\phi_x + \omega_x t_1)]^{-1}$$

Similar relations are obtained for δ_y and $\Delta\phi_y$. Using the condition (2.3) of conservation of energy $\Delta\phi_x$ and $\Delta\phi_y$ can be related by

$$\xi_x\Delta\phi_x = -\xi_y\Delta\phi_y, \tag{2.9}$$

where

$$\xi_i = E_i \tan\phi_i \quad (i = x, y),$$

with

$$E_x = \alpha_x A_x^2, \text{ etc}$$

We now define the important constant ϵ,

$$\epsilon \equiv \delta_x - \delta_y = 2\pi\left(\frac{m}{\omega_y} - \frac{n}{\omega_x}\right) = \frac{2\pi m}{\omega_x}\left(\frac{\omega_x}{\omega_y} - \frac{n}{m}\right) \tag{2.10}$$

Examining eq (2.10) it can be seen that ϵ is proportional to the error in a rational approximation to the irrational number ω_x/ω_y. This approximation improves faster than $1/n^2$ for n large. Therefore for large n and m, ϵ can be made as small as we please. Using the relations between the adjustment constants, up to first order all remaining quantities can be expressed as functions of ϵ.

In order to sum the Green's function over classical trajectories, the following compares the action of the reference trajectory to the one which revolves n times on the x axis and m times on the y axis. The action of the reference trajectory

$$W_1^* = S^*(t_1) + Et_1, \tag{2.11}$$

with

$$S^*(t_1) = S_x(t_1) + S_y(t_1),$$

$$Et_1 = E_x t_1 + E_y t_1,$$

and

$$S_i(t_1) = [m_i\omega_i/2 \sin(\omega_i t_1)]$$

$$\times \{[(q_i^0)^2 + (q_i')^2] \cos(\omega_i t_1) - 2q_i^0 q_i'\},$$

is compared to the action of the nm trajectory,

$$W_{nm}^* = S_x(t_{nm}) + S_y(t_{nm}) + E_x^{nm} t_{nm} \quad {}^{nm}_{y} t_{nm} \tag{2.12}$$

Using the definition (2.6) of t_{nm} we get

$$W_{nm}^* = S_x(t_1 + \delta_x) + E_x^{nm}(t_1 + \delta_x) + S_y(t_1 + \delta_y)$$

$$+ E_y^{nm}(t_1 + \delta_y) + 2\pi m E_x^{nm}/\omega_x + 2\pi m E_y^{nm}/\omega_y \tag{2.13}$$

Next the action is expanded in powers of ϵ with the result

$$W_{nm}^* = W_1^* + \left(\frac{\partial S_x(t_1+\delta_x)}{\partial E_x}\frac{\partial E_x}{\partial\epsilon} + \frac{\partial S_y(t_1+\delta_y)}{\partial E_y}\frac{\partial E_y}{\partial\epsilon}\right)\epsilon$$

$$+ \frac{2\pi n}{\omega_x}E_x + \frac{2\pi m}{\omega_y}E_y + \left(\frac{2\pi m}{\omega_x}\frac{\partial E_x}{\partial\epsilon} + \frac{2\pi n}{\omega_y}\frac{\partial E_y}{\partial\epsilon}\right)\epsilon, \tag{2.14}$$

where the unprimed variables correspond to the reference trajectory. Now using eqs (2.3)–(2.10) the action becomes

$$W_{nm}^* = W_1^* + 2\pi n E_x/\omega_x + 2\pi m E_y/\omega_y$$

$$+ \epsilon^2 \frac{\xi_y\beta_y\xi_x\beta_y}{\xi_y\beta_x + \xi_x\beta_y}(1\ 1) + O(\epsilon^3) \tag{2.15}$$

Eq (2.14) demonstrates that the action of the reference trajectory and the nm trajectory differ by the periodic factor

$$2\pi n E_x/\omega_x + 2\pi m E_y/\omega_y, \tag{2.16}$$

plus higher-order terms in the parameter ϵ. As discussed above, when n and m grow large, the difference in action between the reference trajectory and the nm trajectory [except for the periodic factor (2.15)] can be made small much faster than the growth in the period indices m or n. This means that for each preselected difference in action from the reference trajectory [excluding the periodic factor (2.15)] there are infinitely many *different* classical trajectories with the same spatial end points and actions within this range

Using the above results for the action, we can derive the pre-exponentials (1.1a). Using the relation (2.15) between the actions, we conclude that the pre-exponentials also differ by high-order terms in ϵ.

The next step in the semiclassical calculation of $G(q, q', E)$ is to add up the propagators for each contributing path in order to look for conditions for producing a pole. The contribution to the propagators from the reference trajectory is

$$G_1 = (i\hbar)^{-1} |D_S|^{1/2} \exp[(i\hbar)^{-1} W_1^*], \tag{2.17}$$

while for the nm trajectory it is necessary to add $\pi/4$ for each passage through a classical turning point [6,8],

$$G_{nm} = (i\hbar)^{-1} |D_S|^{1/2} \times \exp\{(i\hbar)^{-1} W_1^* + 2\pi[(E_x/\hbar\omega_x - \tfrac{1}{2})n + (E_y/\hbar\omega_y - \tfrac{1}{2})m] + O(\epsilon^3)\} \tag{2.18}$$

In order to have a pole, an infinite number of trajectories must contribute in phase. Examining (2.17), we find that n and m can be chosen of such large magnitude that the difference between (2.17) and (2.18) is small enough such that infinitely many trajectories add up provided the quantization conditions

$$E_x/\hbar\omega_x = l + \tfrac{1}{2}, \quad E_y/\hbar\omega_y = k + \tfrac{1}{2}, \quad l, k \text{ integers}, \tag{2.19}$$

are fulfilled. These are the well-known quantization conditions in the x and y directions. Because the system is separable, this result could have been guessed from combining the two one-dimensional oscillator quantization conditions.

Summarizing, it has been found that a pole can be constructed provided infinitely many trajectories add up in phase. The overwhelming majority of contributing trajectories are the ones with very long lifetimes. For this group the differences in action can be made as small as desired, so that all the trajectories constructively interfere. These contributing trajectories have a simple physical interpretation in terms of the (nonrigorous) time–energy uncertainty principle. Trajectories nm have energies which depart slightly from (2.19) for the x and y directions. (Of course, $E = E_x + E_y$ is fixed.) However, this deviation ΔE_x is allowed because of the finite transit time t_{nm} and $\Delta E_x t_{nm} < \hbar$. As nm grow large ΔE_x becomes smaller, and this is possible because ϵ of (2.10) is becoming small even faster.

3. Action–angle variables

Additional understanding of the problem can be gained by a transformation to action–angle variables to consider $G(\boldsymbol{\theta}, \boldsymbol{\theta}', E)$ with $\boldsymbol{\theta}$ the angle variables. For the harmonic oscillator, this change is trivial, and the classical orbits are of the form of eq. (2.2) with the angle variable appearing as argument while the amplitude consists of the action. The energy Green's function is again to be constructed as a sum of contributions from classical trajectories using the appropriate semiclassical formula. It is found, however, that only one classical trajectory connects the initial $\boldsymbol{\theta}$ and end $\boldsymbol{\theta}'$ angles. This can readily be seen from the classical trajectories (2.2). Let θ_x, θ_y be the starting points, and θ'_x, θ'_y be the final point. The reference trajectory has a transit time of t_1. We assume there exists a second trajectory with t_{nm}. Thus, we have for the reference orbit

$$\theta'_x = \theta_x + \omega_x t_1, \quad \theta'_y = \theta_y + \omega_y t_1, \tag{3.1}$$

while in the case of the nm trajectory it is necessary to note that the angles are defined only modulo 2π. Hence, this trajectory yields

$$\theta'_x = \theta_x + \omega_x t_{nm} + 2\pi k, \quad \theta'_y = \theta_y + \omega_y t_{nm} + 2\pi l, \tag{3.2}$$

where k and l are arbitrary integers (positive or negative). Equating $\theta'_x - \theta_x$ and $\theta'_y - \theta_y$ between the two trajectories gives

$$\omega_x(t_1 - t_{nm}) = 2\pi k, \quad \omega_y(t_1 - t_{nm}) = 2\pi l. \tag{3.3}$$

Dividing these two equations yields the contradiction $\omega_x/\omega_y = k/l$. Hence, only one trajectory exists going from $\boldsymbol{\theta}$ to $\boldsymbol{\theta}'$ (modulo 2π) for the incommensurable harmonic oscillator. This means that no poles can be developed in the semiclassical $G(\boldsymbol{\theta}, \boldsymbol{\theta}', E)$.

Obviously the system has quantum states, and the problem with the semiclassical quantization can arise for a variety of reasons. In the first place it may stem from the difficulty of employing action–angle type variables as canonical quantum mechanical variables. However, it is possible to consider $G(q, q', E)$ with q and q' defined by the classical canonical transforma-

tion from action–angle variables $\boldsymbol{\theta}$ and $\boldsymbol{\theta}'$, whereupon the semiclassical quantization becomes identical to that of section 2. Hence, the culprit again appears to be the stationary phase integrations converting the semiclassical $G(E)$ from q to $\boldsymbol{\theta}$ representations [‡]. Nevertheless, it should be possible to find a means for semiclassically quantizing $G(\boldsymbol{\theta}, \boldsymbol{\theta}', E)$ directly.

A way to overcome this deficiency is to allow a small degree of fuzziness in the angles $\boldsymbol{\theta}$ and $\boldsymbol{\theta}'$. This can be accomplished by extending the summation in the action–angle analog of eq. (1.1) to include all trajectories whose end angles are within a distance ϵ from $\boldsymbol{\theta}$ and $\boldsymbol{\theta}'$ (modulo 2π). Once this has been done, the situation returns to the one analyzed in section 2, and the correct quantization conditions are obtained. The rationale for this blurring procedure, of course, lies in the uncertainty principle. This fuzzied end-point construction is in accord with the observations of Heller [15] that constructive phase interference over small spatial regions occurs for semiclassical quantization.

Classically, once the angles have been specified, then their conjugate variable, the actions, also can be completely specified, leaving no room for uncertainty. Therefore, a certain degree of fuzziness has to be added to keep with the uncertainty principle. In the limit where $h \to 0$, the semiclassical limit, the degree of fuzziness ϵ (a function of h) has to disappear. Even for ϵ arbitrarily small there are infinitely many classical trajectories which can be added up in phase to produce a pole in $G(\boldsymbol{\theta}\boldsymbol{\theta}', E)$.

An important conclusion can be derived upon close examination of the above results. This is, that a pole can be found in the Green's function provided the difference in action between two trajectories with the same end points decreases faster than the number of revolutions (nm above) or than the time needed to reach the final position in the limit of large nm or long-time trajectories. As a conjecture, it can be concluded that if the difference in action between the reference trajectory and the multiperiodic one (modulo 2π), increases less than linearly in time, a pole can be produced. On the other hand, consider an unstable stochastic trajectory which begins initially very close to the reference trajectory. With each orbit the difference in action between trajectories grows exponentially in time. Therefore, they cannot add up to build a pole, unless some special conditions prevail in which this randomness does not appear modulo $2\pi\hbar$ on a scale of $2\pi\hbar$.

[‡] Marinov [11] explains that the original path integral cannot be written in action–angle variables because only linear canonical transformations are permitted.

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