

Semiclassical quantization of separatrix maps

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Quantization of energy balance equations, which describe a separatrixlike motion is presented. The method is based on an exact canonical transformation of the energy-time pair to the action-angle canonical pair, $(E, t) \rightarrow (I, \theta)$. Quantum mechanical dynamics can be studied in the framework of the new Hamiltonian. This transformation also establishes a relation between a wide class of the energy balance equations and dynamical localization of classical diffusion by quantum interference, that was studied in the field of quantum chaos. An exact solution for a simple system is presented as well.

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I. INTRODUCTION

It is known for many applications [1–4] that classical dynamics near hyperbolic points can be described by a map \hat{T} in the energy-time (E, t) canonical variables $\hat{T}(E, t) \rightarrow (E, t)$. This map is known as the separatrix map, and defines a motion in the vicinity of a separatrix, where a period of the unperturbed (twist) map is an arbitrary function of energy $T(E)$. Its explicit form is defined by $n+2$ turning points as follows [2]:

$$T(E) \sim \begin{cases} \log \frac{1}{|E|} & \text{if } n=1 \\ E^{-(n-1)/2} & \text{if } n>1, \end{cases} \quad (1.1)$$

where the energy of the separatrix without loss of generality is taken to be zero and it is assumed that $|E| \ll 1$. A perturbation which is a periodic function of time, for instance, $\epsilon \sin \nu t$, which is relevant for a variety of applications, may be considered. In this case, \hat{T} is an energy balance equation that describes the energy change over the period $T(E)$:

$$\begin{aligned} E_{n+1} &= E_n + \epsilon \sin \nu t_n, \\ t_{n+1} &= t_n + T(E_{n+1}), \end{aligned} \quad (1.2)$$

where ν is the frequency of the perturbation of the strength ϵ , and it is assumed that $E_n = E(t_n - 0)$. The period of the unperturbed nonlinear motion $T(E_n)$ describes a wide class of nonlinear systems with variety of applications, including the celestial mechanics of the perturbed Kepler system [5,6], charge particles in a field of a wave packet [2] leading to a separatrix mesh phenomenon in non-KAM (Kolmogorov-Arnold-Moser) systems [7] (with possible applications for atom cooling traps [8]), and of electron dynamics in superconducting Josephson junctions [9]. Maps such as Eq. (1.2) are also related to a description of Rydberg atoms in a microwave field by the Kepler map [10,11]. Also Bloch electrons in external fields are described by a separatrix map [12–16] and similar systems. Rigorous consideration of the separatrix map was considered in Refs. [17–20].

The map (1.2) can be derived from the Hamiltonian

$$H = H_0(E) + \tilde{V}(t, \tau) = H_0(E) + (\epsilon/\nu) \cos(\nu t) \delta_{2\pi}(\tau), \quad (1.3)$$

where the unperturbed Hamiltonian

$$H_0(E) = \frac{1}{2\pi} \int^E T(E') dE' \quad (1.4)$$

depends only on the energy E that is conjugate to time t , while τ is the formal time parameter, and $\delta_{2\pi}(\tau) \equiv \sum_{n=-\infty}^{\infty} \delta(\tau - 2\pi n)$ is the periodic δ function with period 2π . Quantization of the Hamiltonian (1.3) in the framework of the energy-time (E, t) canonical pair has been presented in previous studies (see, for instance, [9–11,21]). The main deficiency of quantization of the Hamiltonian (1.3) is an appearance of the unphysical time for a wave function and this fact has been pointed out earlier, in Refs. [10,11]. Classically it is always possible to establish a link between the formal time parameter τ and the real time t for any individual trajectory by the solution $t = t(\tau)$ (or by canonical transformation). In quantum mechanics (for a wave function), it is no longer possible. Therefore, this approach of quantization in the framework of (E, t) variables was used to study time independent characteristics, such as localization [9–11]. On the other hand, the properties that are explicitly time dependent, such as dynamical correlation functions or dynamical fluctuations, cannot be studied by this approach. Moreover, there is no rigorous proof of the validity of these asymptotic solutions. It is also believed that the main deficiency is related to the semiclassically approximate definition of the energy operator as $\hat{E} = -i\hbar \partial/\partial t$, where \hbar is the effective Planck's constant. There is no physical justification of this semiclassical definition. Therefore, to overcome these shortcomings of the quantum description, it is reasonable to rewrite the system in such a form, where the time parameter appears as the physical time. It is convenient to rewrite the system (1.2) and (1.3) in terms of the action-angle variables (I, θ) , related by a canonical transformation $H(E, t, \tau) \rightarrow \mathcal{H}(I, \theta, t)$, where t is the real time. This canonical transformation must be such that under this variable change one

transforms $H_0(E) \rightarrow \mathcal{H}_0(I)$ and $\tilde{V}(t, \tau) \rightarrow V(\theta, t)$. It should be stressed that for kicked systems this change of variables has some specific properties, namely, the new potential $V(\theta, t)$ must be independent of I and it must be a function only of phase θ and time t . Otherwise a shift in action at a kick is an ambiguous procedure due to the discontinuity of the action $I(t=t_n)$ at the n th kick.

In what follows, for the semiclassical quantization, the map (1.2) will be rewritten in the action-angle variables. In this case the semiclassical quantization procedure is standard [14,16]. Semiclassical quantization of area-preserving maps was subject of earlier studies. In particular, quantization of monotonic twist maps [22], with interpolating flows [23] was considered. We show first, in Sec. II, that the map (1.2) can be rewritten in terms of action-angle variables. Semiclassical quantization and an exactly solvable problem are presented in Sec. III. The results are summarized in Sec. IV.

II. EXACT CANONICAL TRANSFORMATION $(E, t) \rightarrow (I, \theta)$

Hamiltonian equations of motion that produce the map (1.2) have the following formal form:

$$dE/d\theta = -\partial H/\partial t = \epsilon \sin \nu t \sum_{n=-\infty}^{\infty} \delta(\theta - 2\pi n), \quad (2.1a)$$

$$dt/d\theta = \partial H/\partial E = T(E)/2\pi, \quad (2.1b)$$

where H is given by Eq. (1.3) and $d/d\theta$ is the formal time derivative ($\tau \equiv \theta$). Integration over θ in the limits $(2\pi n - 0, 2\pi n + 2\pi - 0)$ gives Eq. (1.2). We obtain from Eqs. (2.1a) and (2.1b) the Hamiltonian equations for the action-angle variables (I, θ) and the real time parameter t . Let us start from Eq. (2.1b). Inverting this equation, one obtains

$$\frac{d\theta}{dt} = [T(E)/2\pi]^{-1} = \Omega(I), \quad (2.2)$$

where it is supposed that $T(E) \neq 0$, that means that t is a single valued function of θ . The frequency $\Omega(I)$ corresponds to some parametric variable change $E = E(I)$ along a trajectory, such that

$$dE/dI = \Omega(I). \quad (2.3)$$

In this case the energy $E = \mathcal{H}_0(I)$ is an unperturbed Hamiltonian with the new action variable I , which is defined in Eq. (2.3). From Eqs. (2.1a)–(2.3) we perform the following chain of parametric changes:

$$\frac{dE}{d\theta} = \frac{dt}{d\theta} \frac{dE}{dt} = \frac{dt}{d\theta} \frac{dE}{dI} \frac{dI}{dt} = \dot{I}. \quad (2.4)$$

It follows from Eqs. (2.1a) and (2.4) that

$$\dot{I} = \epsilon \sin \nu t \sum_{n=-\infty}^{\infty} \delta(\theta - 2\pi n) = \epsilon \sin \nu t \frac{\partial}{\partial \theta} \Theta(\theta), \quad (2.5)$$

where $\Theta(\theta)$ is a step function of the following form:

$$\Theta(\theta) = \frac{\theta}{2\pi} + \frac{1}{\pi} \sum_{l=1}^{\infty} \frac{1}{l} \sin l\theta, \quad (2.6)$$

and it is a result of integration of the periodic δ function written in the form

$$\sum_{n=-\infty}^{\infty} \delta(\theta - 2\pi n) = \frac{1}{2\pi} + \frac{1}{\pi} \sum_{l=1}^{\infty} \cos l\theta. \quad (2.7)$$

Equations (2.2) and (2.5) are the Hamilton equations generated by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0(I) - 2\epsilon' \sin \nu t \left[\theta + \sum_{l=1}^{\infty} \frac{1}{l} \sin l\theta \right], \quad (2.8)$$

where $\epsilon' = \epsilon/2\pi$.

To restore periodicity of the Hamiltonian in θ , the following gauge-like transformation is carried out:

$$J = I + \frac{\epsilon'}{\nu} \cos \nu t. \quad (2.9)$$

The corresponding Hamiltonian is

$$\mathcal{H} = \mathcal{H}_0 \left(J - \frac{\epsilon'}{\nu} \cos \nu t \right) - 2\epsilon' \sin \nu t \sum_{l=1}^{\infty} \frac{1}{l} \sin l\theta \equiv \mathcal{H}_0 + V. \quad (2.10)$$

The equations of motion (2.2) and (2.5) take the form

$$\begin{aligned} \dot{J} &= 2\epsilon' \sin \nu t \sum_{l=1}^{\infty} \cos l\theta, \\ \dot{\theta} &= \Omega \left(J - \frac{\epsilon'}{\nu} \cos \nu t \right). \end{aligned} \quad (2.11)$$

In this form, the equations were derived from the Hamiltonian \mathcal{H} ; therefore, the transformation from H to \mathcal{H} , which is presented here, is a canonical transformation.

III. SEMICLASSICAL QUANTIZATION

A. Floquet operator

Equations (2.11) and (2.10) can be simply quantized semiclassically with

$$J \rightarrow \hat{J} = -i\tilde{\hbar} \partial / \partial \theta = \tilde{\hbar} \hat{n},$$

where $\tilde{\hbar}$, in our dimensionless units, is a dimensionless parameter, that plays the role of Planck's constant, while \hat{n} is a quantum number operator. In what follows $\tilde{\hbar}$ will be used for the semiclassical quantization. Since the Hamiltonian (2.10) is periodic both in time and in angle θ , the Floquet theory can be used for the analysis. Therefore, a solution of the Schrödinger equation

$$i\tilde{\hbar} \frac{\partial}{\partial t} \psi(\theta, t) = \hat{\mathcal{H}}(\hat{n}, \theta, t) \psi(\theta, t) \quad (3.1)$$

can be considered due to the Floquet theorem in the following form:

$$\psi(\theta, t) = e^{-i\lambda t} e^{i\kappa\theta} \psi_{\lambda, \kappa}(\theta, t), \quad (3.2)$$

where periodicity of $\hat{\mathcal{H}}$ in both θ and t is taken into account, and the functions

$$\psi_{\lambda, \kappa} \equiv \psi_{\lambda, \kappa}(\theta, t) = \psi_{\lambda, \kappa}(\theta + 2\pi, t + 2\pi/\nu) \quad (3.3)$$

are periodic in time with the periods of the perturbation $2\pi/\nu$ and periodic in θ with the period 2π , while $0 \leq \kappa < 1$ and λ are a ‘‘quasimomentum’’ and a quasienergy, respectively. Taking into account that commutation of the Hamiltonian with the exponential $e^{i\kappa\theta}$ leads to the shift on \hat{n} ,

$$\hat{\mathcal{H}}(\hat{n}, \theta, t) e^{i\kappa\theta} \psi_{\lambda, \kappa}(\theta, t) = e^{i\kappa\theta} \hat{\mathcal{H}}(\hat{n} + \kappa, \theta, t) \psi_{\lambda, \kappa}(\theta, t), \quad (3.4)$$

we can rewrite the Schrödinger equation (3.1) in the following form:

$$\hat{F}(\kappa) \psi_{\lambda, \kappa} = \tilde{h} \lambda \psi_{\lambda, \kappa}, \quad (3.5)$$

where $F \equiv F(\kappa)$ is the so-called Floquet operator

$$\hat{F}(\kappa) = -i\tilde{h} \frac{\partial}{\partial t} + \hat{\mathcal{H}}(\hat{n} + \kappa, \theta, t), \quad (3.6)$$

with λ and $\psi_{\lambda, \kappa}$ as the eigenvalues and eigenfunctions correspondingly. The solution is cast in the form of the Fourier expansion

$$|\psi_{\lambda, \kappa}\rangle = \sum_{n, j} \phi_{n, j} |n\rangle |j\rangle. \quad (3.7)$$

Moreover, the Fourier harmonics

$$|n, j\rangle \equiv |n\rangle |j\rangle = \frac{\sqrt{\nu}}{2\pi} e^{in\theta} e^{-ij\nu t} \quad (3.8)$$

are the eigenfunctions of the unperturbed system with $\epsilon = 0$, and $\phi_{n, j} = \langle j | \langle n | \psi_{\lambda, \kappa} \rangle$ are the coefficients, of the expansion. Matrix elements of the Floquet operator

$$F_{n, n'}^{j, j'} = \langle j | \langle n | \hat{F} | n' \rangle | j' \rangle \quad (3.9)$$

specify the equations for the coefficients $\phi_{n, j}$. First, we calculate the matrix elements for $\hat{\mathcal{H}}_0$. For this purpose we rewrite it formally as

$$\hat{\mathcal{H}}_0 \left(\hat{J} + \kappa - \frac{\epsilon'}{\nu} \cos \nu t \right) = e^{i(\epsilon'/\nu) \cos \nu t (i\partial_\kappa)} \hat{\mathcal{H}}_0(\hat{J} + \kappa), \quad (3.10)$$

where $\partial_\kappa \equiv \partial/\partial\kappa$ and it is assumed that \mathcal{H}_0 does not operate on functions of κ . Calculation of the matrix elements (3.9) yields, for Eq. (3.10),

$$\begin{aligned} \mathcal{H}_{0, n, n'}^{j, j'} &= \langle j | e^{i(\epsilon'/\nu) \cos \nu t (i\partial_\kappa)} | j' \rangle \langle n | \hat{\mathcal{H}}_0(\hat{J} + \kappa) | n' \rangle \\ &= \sum_m i^m J_m \left(i \frac{\epsilon'}{\nu} \partial_\kappa \right) \delta_{j', j+m} \mathcal{H}_0(n' + \kappa) \delta_{n', n}, \end{aligned} \quad (3.11)$$

where $J_m(x)$ is the Bessel function. Correspondingly, the matrix elements for the additive part of the perturbation in Eq. (2.10) are

$$V_{n, n'}^{j, j'} = \begin{cases} \frac{1}{2} \frac{\epsilon'}{n-n'} [\delta_{j', j+1} - \delta_{j', j-1}], & n \neq n' \\ 0, & n = n'. \end{cases} \quad (3.12)$$

These matrix elements of Eqs. (3.11) and (3.12) lead to the following equation for the expansion coefficients:

$$\begin{aligned} \sum_m i^m J_m \left(i \frac{\epsilon'}{\nu} \partial_\kappa \right) \mathcal{H}_0(n + \kappa) \phi_{n, j+m} \\ + \frac{\epsilon'}{2} \sum_{n' \neq n} \frac{1}{n-n'} [\phi_{n', j+1} - \phi_{n', j-1}] = \tilde{h}(\lambda + \nu j) \phi_{n, j}. \end{aligned} \quad (3.13)$$

It is similar to a quasi-one-dimensional Anderson-like chain for the cases when $\mathcal{H}_0(n + \kappa)$ corresponds to a random potential. It is also the generalization of a specific application in Ref. [24]. The classical motion is chaotic in many types of $T(E)$ in Eq. (1.2). Therefore, the obtained equation establishes a relation between a wide class of energy balance equations of the forms (1.2), (1.3), and dynamical localization of the classical chaotic diffusion [25]. In the general case this equation is useful for numerical studies. It is analytically tractable in perturbation theory for the parameter $\epsilon'/\nu \ll 1$. Some examples related to approximate treatments are considered in [13, 14, 26, 27]. Here, in the framework of the rigorous consideration, it is instructive to present an exactly solvable example, where Eq. (1.4) is linear, with a constant period $T(E) = 2\pi/\omega$. In this case a solution can be obtained in an explicit form analytically.

B. An exact model

An exact solution can be obtained for the harmonic oscillator $\mathcal{H}_0(I) = \omega I$ with constant frequency $\Omega(I) = \omega$. The linear driven system described by the Hamiltonian $\mathcal{H}(I, \theta, t)$ is integrable. Equation (3.13) takes the following simple form:

$$\begin{aligned} \tilde{h}[\omega n - \nu j - \lambda + \omega \kappa] \phi_{n, j} - \frac{\epsilon' \omega}{2\nu} [\phi_{n, j+1} + \phi_{n, j-1}] \\ + \frac{\epsilon'}{2} \sum_{n' \neq n} \frac{1}{n-n'} [\phi_{n', j+1} - \phi_{n', j-1}] = 0. \end{aligned} \quad (3.14)$$

For the specific case of the harmonic oscillator $\kappa = 0$. For other linear models, for example, models of an appropriate

band structure in solids, κ does not have to vanish. A solution of Eq. (3.14) is cast in the form of a sinc function by the following substitution:

$$\phi_{n,j} = Z_j \operatorname{sinc}[\pi(n - \lambda/\omega + \kappa)], \quad (3.15)$$

where the sinc function is $\operatorname{sinc}x = (\sin x)/x$ and Z_j has to be determined. In this case the quasienergy spectrum turns out to be

$$\lambda = \omega\kappa + \omega n. \quad (3.16)$$

Inserting Eq. (3.6) in Eq. (3.14) and taking into account that

$$\sum_{n' \neq n} \frac{1}{n - n'} \operatorname{sinc} \pi(n' - n) = 0, \quad (3.17)$$

since $\sin \pi(n' - n) = 0$, one obtains from Eq. (3.14) the following relation for Z_j :

$$2jZ_j + z[Z_{j+1} + Z_{j-1}] = 0, \quad (3.18)$$

where $z = \epsilon' \omega / \hbar \nu^2$. The solution is [28]

$$Z_j \equiv Z_j(z) = (-1)^j J_j(z). \quad (3.19)$$

The result, Eqs. (3.16) and (3.19), is only a specific solution. The general solution is found by replacing in Eq. (3.14) j by $j - j_0$ and λ by $\lambda - \nu j_0$. The resulting solution of the eigenvalue problem is

$$\lambda_{j_0} = \nu j_0 + \omega\kappa + \omega n, \quad (3.20)$$

and the corresponding eigenfunction is

$$Z_j = (-1)^{j-j_0} J_{j-j_0}(z). \quad (3.21)$$

The Floquet theory implies that only λ_{j_0} in an interval of size ν , say, $[0, \nu)$ should be used [see Eq. (3.2)]. In particular, for the harmonic oscillator

$$\lambda_{j_0} = \nu j_0 + \omega n, \quad (3.22)$$

if it is in the interval $[0, \nu)$, as expected.

IV. SUMMARY

Quantization of energy balance equations, in the form of the map (1.2), is presented. This procedure of quantization consists of the two steps. The first one is a transformation of the Hamiltonian (1.3) to the form (2.10) by the canonical transformation $(E, t) \rightarrow (I, \theta)$. The second stage is the semiclassical quantization. The Hamiltonian formulation of the problem allows semiclassical quantization of action-angle variables in the framework of the standard procedure: $I \rightarrow \hat{I} = -i\hbar \partial / \partial \theta \equiv \hbar \hat{n}$, where \hbar is a dimensionless semiclassical parameter such that the classical limit is $\hbar \rightarrow 0$. It should be noted that the semiclassical approximation requires that the width of the potential V is larger than the de Broglie wavelength. Therefore, it is necessary to truncate the Fourier expansion in Eq. (2.6), corresponding to replacement of the δ function by a function of finite width. The results obtained in Sec. III B in the semiclassical approximation are correct only up to the leading correction in \hbar to the classical ones [14]. The advantage of the present analysis is that the transition from Eq. (1.2) to Eq. (2.10) is exact, and wave functions depend on physical time, while the main deficiency of straightforward quantization of Eq. (1.2) is an appearance of an unphysical time parameter [10,11].

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