Pustylnikov L. D.

Energy Levels of Quantum Periodic Systems and Quantum Chaos

L. D. Pustyl’nikov

Energy Levels of Quantum Periodic Systems
and Quantum Chaos

Москва — 2014
Лев Давидович Пустыльников

Уровни энергии квантовой периодической системы и квантовый хаос

Объясняется понятие уровней энергии квантовой системы, зависящей от времени периодически и имеющей дискретный или непрерывный спектры. Вводится естественным образом понятие смежных и эффективных уровней энергии, а также понятие расстояний между уровнями. Представленные результаты используются для объяснения гипотезы квантового хаоса для некоторого класса систем, включающих в виде частного случая модель «вibriрующего волчка».

Ключевые слова: квантовый хаос, модель «вibriрующего волчка»

L. D. Pustyl’nikov
Energy Levels of Quantum Periodic Systems and Quantum Chaos

The concept of energy levels of quantum systems periodically depending on time and having a discrete or a continuous spectrum is justified. A natural concept of adjacent and effective energy levels as well as distances between the levels are introduced. The results of the theory presented are applied to justification of the quantum chaos conjecture for a class of systems including, as a special case, the “kicked rotator” model.

Key words: quantum chaos, “kicked rotator” model

© Keldysh Institute of Applied Mathematics of RAS, Moscow, 2013
© L. D. Pustyl’nikov, 2014
1. The concepts of energy levels of quantum systems and distances between them

We consider a quantum system given by Hamiltonian operator $\hat{H} = \hat{H}(t)$ that depends periodically on time $t$, i.e., $\hat{H}(t) = \hat{H}(t + T)$, where $T > 0$ is the operator’s period. The Schrödinger equation for this operator is given by

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi,$$

where $\Psi = \Psi(q,t)$ is the wave function, that is a function of $q$ for fixed $t$ that belongs to Hilbert space $L^2$. Let $\Psi(q,t)$ be the solution of equation (1) for $t \geq t_0$ satisfying the initial condition $\psi(q) = \Psi(q,t_0) \in L^2$. We define the (Floquet) monodromy operator $U = U_{t_0} : \Psi(q,t_0) \rightarrow \Psi(q,t_0 + T)$. It is well-known that $U$ is a unitary operator and for distinct values of $t_0$ the corresponding operators $U_{t_0}$ are unitarily equivalent to each other [1]. Hence, its spectrum is a set of complex numbers with their absolute value 1. First, we assume that the spectrum of the operator $U$ is discrete and is represented by the sequence of eigenvalues $\lambda_n$ such that $\lambda_n = e^{i\alpha_n}$ where $n \in \mathbb{Z}$ is an integer and $\alpha_n$ is a real number. Let $\psi_{\lambda_n}(q)$ be the eigenfunction corresponding to the eigenvalue $\lambda_n$ such that $U\psi_{\lambda_n}(q) = \lambda_n\psi_{\lambda_n}(q)$. Then solution $\Psi_{\alpha_n}(q,n)$ of equation (1) with the initial condition $\Psi_{\alpha_n}(q,t_0) = \psi_{\lambda_n}(q)$ satisfies

$$\Psi_{\alpha_n}(q,t_0 + T) = e^{-i\alpha_n}\Psi_{\alpha_n}(q,t_0).$$

Such a solution $\Psi_{\alpha_n}(q,t)$ is called quasistationary, and the corresponding value $E_n = \frac{h\alpha_n}{2}$ introduced in paper [13] is called quasienergy. In this article we call the value $\alpha_n$ the energy level.

We assume now that the spectrum of operator $U$ is continuous (i.e., there are no eigenvalues) and operator $U$ has the following structure: Hilbert space $L^2$ has a basis $\psi_n(q)(n \in \mathbb{Z})$ satisfying, for each $n \in \mathbb{Z}$,

$$U\psi_n(q) = e^{-i\mu_n(q)}\psi_n(q).$$

In (2) $\mu_n(q)$ is a real function such that for any pair $(n',n''$) of integers, the function $\Delta_{n',n''}(q) \overset{\text{def}}{=} \mu_{n'}(q) - \mu_{n''}(q)$ takes only finitely or countably many different values. Functions $\Delta_{n',n''}(q)$ play role of distances between the energy levels $\mu_n(q)$ which exhibited in quantum mechanics over passing from one energy level to another. Thus, despite the fact that the set of the energy levels $\mu_n(q)$ is not discrete, the set of all possible values of the distances between them is discrete; this set treats the physical meaning of $\mu_n(q)$.

We consider a special important case for which operator $U = U_2 \cdot U_1$ is the composition of two unitary operators $U_1$ and $U_2$ such that operator $U_1$ is
represented by an infinite diagonal matrix with the diagonal entries $\lambda_n = e^{-i\alpha_n}$, and $U_2$ is the operator of multiplication by the function $\lambda(q) = e^{-\mu(q)}$, i.e., for any $n \in \mathbb{Z}$ the following equalities hold:

$$U \psi_n(q) = \lambda^{(n)}(q) \Psi_n(q), \quad \lambda^{(n)}(q) = e^{-i(\mu(q) + \alpha_n)}.$$  

In that latter case, the functions $\mu_n(q) = \mu(q) + \alpha_n$ are the energy levels, and the distances $\Delta_{n',n''}(q)$ do not depend on the basis $\psi_n(q)$. By (3), this statement is equivalent to the statement that the spectrum of operator $U_* = \frac{1}{\lambda^{(0)}(q)} U$ is discrete and is invariant. Consequently, the eigenvalue $\frac{\lambda^{(n)}(q)}{\lambda^{(0)}(q)}$ of operator $U_*$ and the distances $\Delta_{n',n''}(q) = i \left( \log \frac{\lambda^{(n')}(q)}{\lambda^{(0)}(q)} - \log \frac{\lambda^{(n'')}(q)}{\lambda^{(0)}(q)} \right)$ do not depend on the basis $\psi_n(q)$.

2. Adjacent, effective, and noneffective energy levels of quantum systems

Let $n'$ and $n''$ be two distinct integers. The energy levels $\mu_{n'}(q)$ and $\mu_{n''}(q)$ are called adjacent if for all $q$ does not exist on integer $n$, $n \neq n', n''$, such that $\mu_n(q)$ belongs to the closed interval with the ends $\mu_{n'}(q)$ and $\mu_{n''}(q)$:

$$\min(\mu_{n'}(q), \mu_{n''}(q)) \leq \mu_n(q) \leq \max(\mu_{n'}(q), \mu_{n''}(q)).$$

We set the Hilbert space $L^2$ to be the space of $2\pi$-periodic functions and assume that the energy levels are defined with respect to its orthogonal basis $\psi_n(q) = e^{i\pi q}(n \in \mathbb{Z})$. We represent the energy level $\mu_n(q)$ as follows:

$$\mu_n(q) = 2\pi m_n(q) + 2\pi \beta_n(q),$$

where $m_n(q)$ is an integer and function $\beta_n(q)$ satisfies $0 \leq \beta_n(q) < 1$. It follows from (5) that $m_n(q) = \left\lfloor \frac{\mu_n(q)}{2\pi} \right\rfloor$ is the integer part of the number $\frac{\mu_n(q)}{2\pi}$ and $\beta_n(q) = \left\{ \frac{\mu_n(q)}{2\pi} \right\} = \frac{\mu_n(q)}{2\pi} - \left\lfloor \frac{\mu_n(q)}{2\pi} \right\rfloor$ is its fractional part. From equalities (2) and (5) it follows that the first term $2\pi m_n(q)$ in (5) does not affect to the wave functions $\psi_n(q)$. Therefore, we call function $2\pi m_n(q)$ the noneffective energy level. On the contrast, we call the second term, $2\pi \beta_n(q)$, the effective energy level. For two energy levels, $\mu_{n'}(q)$ and $\mu_{n''}(q)$ with $\mu_{n'}(q) \leq \mu_{n''}(q)$, we define the distance $\rho(\mu_{n'}(q), \mu_{n''}(q))$ between them by

$$\rho(\mu_{n'}(q), \mu_{n''}(q)) = \beta_{n''}(q) - \beta_{n'}(q).$$
3. Justification of quantum chaos conjecture for some class of quantum systems

Quantum chaos theory studies the distribution of the distances between the adjacent energy levels of a quantum system. There are two main conjectures based on numerical simulations concerning distribution laws of these distances ([2],[6],[7],[9]). The first conjecture concerns quantum systems that are quantum analogues of classical integrable systems. The conjecture states that the distribution law of distances for such a system is close to the Poisson distribution with the density \( \exp(-\sigma) \) and coincides with it asymptotically as \( \sigma \to 0 \). The second conjecture states that for quantum analogue of a classical strong nonintegrable system, the distribution law of distances is close to the distribution with the density \( \text{const} \sigma \) as \( \sigma \to 0 \). In the present article, the quantum chaos conjecture is justified for a special class of quantum system. This class includes, as a special case, a “kicked rotator” model ([1], [3], [4], [5], [8], [9]).

To describe the quantum model, first we introduce the classical model of the system in question. We consider a one-dimensional nonlinear oscillator given by Hamiltonian function \( H = H(q, I, t) = H_0(I) + H_1(q, t) \), where \( I, q \) are the 'action-angle' variables, \( t \) is an independent variable, and function \( H_1(q, t) \) has period \( 2\pi \) in \( q \), period \( T > 0 \) in \( t \), and is represented in the form

\[
H_1(q, t) = F(q) \sum_{k=-\infty}^{\infty} \delta(t - kT).
\]

Here \( F(q) \) is a smooth \( 2\pi \)-periodic function, \( \delta = \delta(t) \) is the Dirac delta-function, and the summation is taken over all integers \( k \). The first rigorous results on behavior of the system’s solutions with the Hamiltonian function \( H = H_0(I) + H_1(q, t) \), where function \( H_0(I) \) is that of a general form, have been established in [8]. We assume here that \( H_0(I) = \sum_{s=0}^{\infty} b_s I^s \) is an entire function (in particular, a polynomial) with coefficients \( b_s = \frac{a_s}{\hbar} \), \( s = 0,1,\ldots \), where \( \hbar \) is Planck’s constant and \( a_s \) are real numbers. In a special case, when \( a_s = 0 \) for \( s \neq 2 \), \( F(q) = c \cos q \), \( c \) is a constant, this system is “kicked rotator”.

Getting onto the quantum model, we introduce the Hilbert space \( L^2 \) of complex \( 2\pi \)-periodic in \( q \) functions as the space of states of the quantum system and also introduce impulse operator \( \hat{I} = \frac{\hbar}{i} \frac{\partial}{\partial q} \). The wave function \( \Psi = \Psi(q, t) \in L^2 \) is satisfied the Schrödinger equation (1), where \( \hat{H} = \hat{H}(t) = \hat{H}_0 + \hat{H}_1(t) \), \( \hat{H}_0 = \sum_{s=0}^{\infty} b_s \hat{I}^s \) and operator \( \hat{H}_1(t) \) is the limit, as \( \epsilon \to 0 \) (\( \epsilon > 0 \)), of the operators of multiplication by function \( H_1(\epsilon) \) obtained from function \( H_1 \) in (7) in which the delta-function is replaced by a smooth function \( \delta_\epsilon \) concentrated on the interval \( [0, \epsilon] \) with the integral equals 1.

Let \( \Psi_+(q, nT) \) denote the solution of equation (1) immediately after the
instant $t = nT$ ($n \in \mathbb{Z}$). We define the monodromy operator $U : \Psi_+(q,nT) \to \Psi_+(q,(n+1)T)$ to be the limit as $\epsilon \to 0$, of the monodromy operators $U^{(\epsilon)}$ corresponding to equation (1) with operator $\hat{H}(t)$ on the right hand side replaced by operator $\hat{H}_0 + \hat{H}_1^{(\epsilon)}$, where $\hat{H}_1^{(\epsilon)}$ is the operator of multiplication by the function $H_1^{(\epsilon)}$. It is proven in [1], [5] and [12] that this limit exists and has the following form: $U = \exp \left(-i \frac{F}{\hbar}\right) \exp \left(-i \frac{T \hat{H}_0}{\hbar}\right)$.

Moreover, if $\psi(q) = \exp(inq)$, then $U\psi_n(q) = \lambda_n(q)\psi_n$, where

$$\lambda_n(q) = \exp(-i\mu_n(q)), \quad \mu_n(q) = \left(F(q) + T \sum_{s=0}^{\infty} a_s n^s\right)/\hbar.$$ 

Equalities (8) show that the functions $\mu_n(q)$ are the energy levels in the sense of the definition given in Section 1. In particular, if $F(q) = \text{const}$, then the spectrum of $U$ is discrete, $\psi_n(q)$ are its eigenfunctions, and the $\lambda_n(q)$’s are its corresponding eigenvalues.

Assume that the real function $G(x) = \frac{T}{2\pi\hbar} \sum_{s=0}^{\infty} a_s x^s$ of the real variable $x$ satisfies the following condition:

(i) all zeros of $G(x)$ (if they exist) lie in a bounded region of the real line;
(ii) $\lim_{n \to \infty} |G(n+1) - G(n)| = \infty$;
(iii) for any real numbers $\sigma_1$ and $\sigma_2$ satisfying $0 < \sigma_\nu \leq 1$, $\nu = 1,2$, the number $D_N(\sigma_1, \sigma_2)$ of two-dimensional vectors $\vec{r}_n = (\{G(n)\}\{G(n+1)\})$ in the sequence $\vec{r}_1, \ldots, \vec{r}_N$ that belong to rectangle $\Pi = \{y = (y_1, y_2) : 0 \leq y_1 < \sigma_1, 0 \leq y_2 < \sigma_2\}$ satisfies $\lim_{N \to \infty} \frac{D_N(\sigma_1, \sigma_2)}{N} = \sigma_1 \sigma_2$.

Condition (iii) means that the joint distribution of two adjacent fractional parts of function $G(x)$ is uniform. All the three conditions hold for polynomials $G(x) = \sum_{s=0}^{\ell} a_s x^s$ of degree $\ell \geq 2$, for which at least one of the coefficients $a_2, a_3, \ldots, a_\ell$ is an irrational number ([10]). By (8), if the conditions (i) and (ii) hold, then there is a number $n_0 \geq 0$ for which the energy levels $\mu_n(q)$ and $\mu_{n+1}(q)$ are adjacent whenever $n > n_0$. The adjacent energy levels correspond to the adjacent quantum states $\psi_n(q)$ and $\psi_{n+1}(q)$ with the adjacent frequencies $\frac{n}{2\pi}$ and $\frac{n+1}{2\pi}$. It follows from (iii) that for $0 < \sigma \leq 1$ and for the number $D_N^*(\sigma, q)$ of values $n, n \in \{1, \ldots, N\}$, for which $0 \leq \left\{\frac{\mu_{n+1}(q)}{2\pi}\right\} - \left\{\frac{\mu_n(q)}{2\pi}\right\} < \sigma$, the following holds:

$$P^*(\sigma) \overset{\text{def}}{=} \lim_{N \to \infty} \frac{D_N^*(\sigma, q)}{N} = Area(\Pi^*) = \sigma - \frac{\sigma^2}{2}.$$ 

Here, $\Pi^*$ stands for the set

$$\Pi^* = \{y = (y_1, y_2) : 0 \leq y_1 < 1, 0 \leq y_2 < 1, 0 \leq y_2 - y_1 < \sigma\}.$$
and $Area(\Pi^*)$ stands for the area of $\Pi^*$. In view of (6) and (9), the distribution function $P^*(\sigma)$ of the distances between the adjacent energy levels differs from the Poisson’s law distribution function $1 - \exp(-\sigma)$ with density $\exp(-\sigma)$ by terms of the third order of smallness in $\sigma$, as $\sigma \to 0$. Thus, the quantum chaos conjectures holds for the class of quantum systems in question. In the special case, when $H_0(I)$ is a polynomial of a general form, this result has been obtained in [11] and [12] from pure mathematical point of view.

**References**


