Energy Levels of Quantum Periodic Systems and Quantum Chaos

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Abstract

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

1 The concepts of energy levels of quantum systems and distances between them

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

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi , \qquad (1)$$

where $\Psi = \Psi(q, t)$ is the wave function, namely a function of q for fixed t belonging to Hilbert space L^2 . Let $\Psi(q, t)$ be the solution of equation (1) for $t \ge t_0$ satisfying the initial condition $\psi(q) = \Psi(q, t_0) \in L^2$. We define the (Floquet) monodromy operator $U = U_{t_0} : \Psi(q, t_0) \to \Psi(q, t_0 + T)$. 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 of absolute value 1. First, we assume that the spectrum of the operator U is discrete and is represented by the sequence of eigenvalues λ_n such that $\lambda_n = e^{i\alpha_n}$ where $n \in \mathbb{Z}$ is an integer and α_n is a real number. Let $\psi_{\lambda_n}(q)$ be the eigenfunction corresponding to the eigenvalue λ_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 $E_n = \frac{\hbar \alpha_n}{T}$ introduced in [13] is called *quasienergy*. In this article we will call the value α_n the energy level.

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

$$U\psi_n(q) = e^{-i\mu_n(q)}\psi_n(q) .$$
⁽²⁾

In (2) $\mu_n(q)$ is a real function such that for any pair (n', n'') of integers, the function $\Delta_{n',n''}(q) \stackrel{\text{def}}{=} \mu_{n'}(q) - \mu_{n''}(q)$ takes only finitely or countably many different values. The functions $\Delta_{n',n''}(q)$ play the 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:

$$U\psi_n(q) = \lambda^{(n)}(q)\Psi_n(q) , \quad \lambda^{(n)}(q) = e^{-i(\mu(q) + \alpha_n)} .$$
 (3)

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 $\Delta_{n',n''}(q) = i\left(\ln \frac{\lambda^{(n')}(q)}{\lambda^{(0)}(q)} - \ln \frac{\lambda^{(n'')}(q)}{\lambda^{(0)}(q)}\right)$ 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 $[\mu_{n'}(q), \mu_{n''}(q)]$.

$$\min(\mu_{n'}(q), \mu_{n''}(q)) \le \mu_n(q) \le \max(\mu_{n'}(q), \mu_{n''}(q)) .$$
(4)

The Hilbert space L^2 is the space of 2π -periodic square integrable functions and assume that the energy levels are defined with respect to its orthogonal basis $\psi_n(q) = e^{inq} (n \in$ **Z**). We represent the energy level $\mu_n(q)$ as follows:

$$\mu_n(q) = 2\pi m_n(q) + 2\pi \beta_n(q) , \qquad (5)$$

where $m_n(q)$ is an integer and function $\beta_n(q)$ satisfies $0 \leq \beta_n(q) < 1$. It follows from (5) that $m_n(q) = \left[\frac{\mu_n(q)}{2\pi}\right]$ is the integer part of the number $\frac{\mu_n(q)}{2\pi}$ and $\beta_n(q) = \left\{\frac{\mu_n(q)}{2\pi}\right\} = \frac{\mu_n(q)}{2\pi} - \left[\frac{\mu_n(q)}{2\pi}\right]$ 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 the 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

$$\rho(\mu_{n'}(q), \mu_{n''}(q)) = \beta_{n''}(q) - \beta_{n'}(q) .$$
(6)

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. Ther 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 the quantum analogue of a classical strong nonintegrable system, the distribution law of distances is close to the distribution with the density $const \sigma$ 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 corresponding classical model. We consider a one-dimensional nonlinear oscillator associated to the 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 2π in q, period T > 0 in t, and is represented in the form

$$H_1(q,t) = F(q) \sum_{k=-\infty}^{\infty} \delta(t - kT) .$$
(7)

Here F(q) is a smooth 2π -periodic function, $\delta = \delta(t)$ is the Dirac measure, 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 nothing else than a "kicked rotator".

Getting onto the quantum model, we introduce the Hilbert space L^2 of complex 2π periodic in q square integrable 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 $\Psi = \Psi(q, t) \in L^2$ 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) after replacing the *delta*-function by a smooth function δ_{ϵ} with support on the interval $[0, \epsilon]$ with $\int_0^{\epsilon} \delta_{\epsilon} = 1$.

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 has been 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

$$\lambda_n(q) = \exp(-i\mu_n(q)), \mu_n(q) = \left(F(q) + T\sum_{s=0}^\infty a_s n^s\right)/\hbar .$$
(8)

The 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) = const, then the spectrum of U is discrete, $\psi_n(q)$ are the corresponding eigenfunctions, and the $\lambda_n(q)$'s are the corresponding eigenvalues.

Assume that the real function $G(x) = \frac{T}{2\pi\hbar} \sum_{s=0}^{\infty} a_s x^s$ of 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 σ_1 and σ_2 satisfying $0 < \sigma_{\nu} \leq 1$, $\nu = 1, 2$, the number $D_N(\sigma_1, \sigma_2)$ of two-dimensional vectors $\vec{\kappa}_n = (\{G(n)\}\{G(n+1)\})$ in the sequence $\vec{\kappa}_1, \ldots, \vec{\kappa}_N$ 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_ℓ 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 frequences $\frac{n}{2\pi}$ 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:

$$P^*(\sigma) \stackrel{\text{def}}{=} \lim_{N \to \infty} \frac{D_N^*(\sigma, q)}{N} = |\Pi^*| = \sigma - \frac{\sigma^2}{2} .$$
(9)

Here, Π^* stands for the set

 $\Pi^* = \{ y = (y_1, y_2) : 0 \le y_1 < 1, 0 \le y_2 < 1, 0 \le y_2 - y_1 < \sigma \}$

and $|\Pi^*|$ stands for the area of Π^* . 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 third order in σ , 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 general polynomial, this result has been obtained in [11] and [12] from pure mathematical point of view.

References

- Bellissard, J.: Non commutative methods in semiclassical analysis, Transition to chaos in classical and quantum mechanics (S. Graffi, ed.), Springer-Verlag, Berlin 1991, pp. 1–47.
- [2] Berry, M.V., and Tabor, M.: Level clustering in the regular spectrum, Proc. Roy. Soc. London A 356 (1977), 375–394.
- [3] Casati, G., and Guarneri, I.: Non-recurrent behaviour in quantum dynamics, Commun. Math. Phys. 95 (1984), 121–127.
- [4] Chirikov, B.V., Izrailev, F.M., and Shepelyansky, D.L.: Quantum chaos: localization vs. ergodicity, Physica D 33 (1988), 77–88.
- [5] Grempel, D.R., Prange, R.E., and Fishman, S.: Quantum dynamics of a nonintegrable system, Phys. Rev. A 29 (1984), 1639–1647.
- [6] Knauf, A., and Sinai, Ya.G.: Classical nonintegrability, quantum chaos, Birkhäuser, Basel 1997.
- [7] Kosygin, D.V., Minasov, A.A., and Sinai, Ya.G.: Statistical properties of the spectra of Laplace-Beltrami operators on Liouville surfaces, Uspekhi Mat. Nau 48:4 (1993), 3–130; English transl. in Russian Math. Surveys 48:4 (1993).
- [8] Pustyl'nikov, L.D.: Unbounded growth of an action variable in some physical models", Trudy Moskov. Mat. Obshch. 46 (1983), 187–200; English transl. in Trans. Moscow Math. Soc. 1984:2.
- [9] Pustyl'nikov, L.D.: The Quantum Chaos Conjecture, in "Proc. of NATO ASI on Computational Noncommutative Algebra and Applications" p. 421–422, Ed. J.S. Byrnes, Series II: Mathematics, Physics and Chemistry, Kluwer Academic Publishers, 2004.
- [10] Pustyl'nikov, L.D.: Probability laws in the distribution of the fractional parts of the values of polynomials, and evidence for the quantum chaos conjecture, Uspekhi Mat. Nauk 54:6 (1999), 173–174; English transl. in Russian Math. Surveys 54 (1999).

- [11] Pustyl'nikov, L.D.: A proof of the quantum chaos conjecture, and generalized continued fractions, Uspekhi Mat. Nauk 57:1 (2002), 161–162; English transl. in Russian Math. Surveys 57 (2002).
- [12] Pustyl'nikov, L.D.: The quantum chaos conjecture and generalized continued fractions, Sbornik: Mathematics (2003), 194:4, 575–587.
- [13] Zel'dovich, Ya. B.: The quasienergy of quantum-mechanical system subjected to a periodic action, Zh. Eksper. Teor. Fiz. 51 (1966), 1492–1495; English transl. in Soviet Physics JETP 24 (1967).