Manifestation of the Arnol’d Diffusion in Quantum Systems

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We study an analog of the classical Arnol’d diffusion in a quantum system of two coupled nonlinear oscillators, one of which is governed by an external periodic force with two frequencies. In the classical model this very weak diffusion happens in a narrow stochastic layer along the coupling resonance, and leads to an increase of total energy of the system. We show that the quantum dynamics of wave packets mimics, up to some extent, global properties of the classical Arnol’d diffusion. This specific diffusion represents a new type of quantum dynamics, and may be observed, for example, in 2D semiconductor structures (quantum billiards) perturbed by time-periodic external fields.

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As is known, the main mechanism for the onset of dynamical chaos in classical Hamiltonian systems is the destruction of separatrices of non-linear resonances due to perturbation terms. However, for a small enough perturbation in conservative systems with two degrees of freedom ($N = 2$), as well as for one-dimensional time-dependent Hamiltonians, chaotic regions are bounded in the phase space by the Kolmogorov-Arnol’d-Moser (KAM) surfaces \cite{1}. In this case the chaos is non-global since chaotic trajectories are located in restricted regions of the phase space of a system.

The situation changes drastically for many-dimensional systems ($N > 2$), where KAM surfaces no longer separate one stochastic region from another, and chaotic layers generically form a stochastic web \cite{2}. Thus, if trajectory starts in the vicinity of a specific non-linear resonance, it can diffuse along stochastic layers of many resonances that cover the whole phase space. This universal global instability known as the Arnol’d diffusion \cite{3}, for the first time was observed in numerical experiments \cite{4}, and then studied in detail in \cite{5,6} (see also review \cite{7} and the book \cite{8}).

It is very difficult to observe this specific diffusion since its rate is exponentially small, and it manifests itself only for initial conditions inside very narrow stochastic layers. However, it is believed that the Arnol’d diffusion may play an important role in different physical situations. For example, it is argued that this diffusion is crucial for the estimate of the stability of our Solar system, and is responsible for a loss of electrons in magnetic traps (see in \cite{9}). Also, the Arnol’d diffusion may have a strong influence for the dynamics of protons in high energy storage rings. Recently, the possibility of observation of the Arnol’d web for a Hydrogen atom in crossed electric and magnetic fields has been discussed in Ref. \cite{10}.

So far, all the studies of the Arnol’d diffusion refer to classical models. On the other hand, it is important to understand what is the fingerprint, if any, of this diffusion in quantum systems. This question is far from trivial since quantum effects are known to typically suppress classical effects of an exponentially weak diffusion \cite{11}. In this Letter we perform a detail study of the quantum Arnol’d diffusion in a simple model, and show what are peculiarities of quantum dynamics that are due to this phenomenon.

The system under consideration consists of two coupled quartic oscillators one of which is perturbed by a two-harmonic force. Following to Refs. \cite{5} where the corresponding classical model was studied both analytically and numerically, we write the Hamiltonian,

\begin{equation}
\hat{H} = \hat{H}_x^0 + \hat{H}_y^0 - \mu xy - f_0 x (\cos \Omega_1 t + \cos \Omega_2 t). \tag{1}
\end{equation}

Here

\begin{equation}
\hat{H}_x^0 = \frac{\hat{p}_x^2}{2} + \frac{x^4}{4}, \quad \hat{H}_y^0 = \frac{\hat{p}_y^2}{2} + \frac{y^4}{4}, \tag{2}
\end{equation}

and $\mu, f_0, \Omega_1, \Omega_2$ stand for the coupling constant, amplitude and two frequencies of an external force, respectively. For momentum and coordinate operators the standard commutation relations are assumed, $[\hat{p}_x, x] = -i\hbar_0$, $[\hat{p}_y, y] = -i\hbar_0$, with $\hbar_0$ as the dimensionless Plank constant.

In the classical model the separatrix of the main coupling resonance $\omega_x^0 \approx \omega_y^0$ (determined in the absence of perturbation, $f_0 = 0$) is destroyed and creates a very narrow stochastic layer. The Arnol’d diffusion is caused by two driving terms with commensurate frequencies $\Omega_1$ and $\Omega_2$, that “force” a chaotic trajectory diffuse along the resonance layer \cite{12}.

To consider the quantum model, first, one should find quantum eigenstates corresponding to this coupling resonance, for $f_0 = 0$. Then, by switching on the perturbation, the analysis can be performed by using the Floquet formalism, since the perturbation is periodic in time. In this way, one can construct the evolution operator that allows one to study the dynamics of the model.

In order to find stationary states corresponding to the coupling resonance, we write the wave function in the form,

\begin{equation}
\psi(x, y) = \sum_{n, m} c_{n, m} \psi_{n}^0(x) \psi_{m}^0(y). \tag{3}
\end{equation}
Here $\psi_n^0(x)$ and $\psi_m^0(y)$ are the eigenfunctions of $\hat{H}^0$ and $\hat{H}^0_y$ (calculated numerically), and coefficients $c_{n,m}$ satisfy to the stationary Schrödinger equation,

$$E c_{n,m} = (E_n + E_m) c_{n,m} - \mu \sum_{n',m'} x_{n,m,n'}^r y_{m,m',n'}^r c_{n',m'},$$

where $E_n$ and $E_m$ are the eigenvalues of the Hamiltonians $\hat{H}^0$ and $\hat{H}^0_y$.

Our interest is in the dynamics of the model in the vicinity of the main coupling resonance determined by the condition $\omega_m = \omega_m$. Here $\hbar \omega_m = E_{n_0}$, $\hbar \omega_m = E_{n_0}'$, and $n_0 = m_0$ defines the resonance centre. In this region one can expand $E_n$ and $E_m$ in the Tailor series, keeping second order terms. It is convenient to introduce the indexes $p = k + l$ and $k$, where $k = n - n_0$ and $l = m - m_0$. Then, one can write,

$$E_{ck,p} = \left[ \hbar \omega p + E_{n_0}' \left( k^2 - pk + \frac{p^2}{2} \right) \right] c_{k,p} - \mu \left( \cdots + \sum_{k'} x_{k,k'}^r y_{p-k,1-k'}^r c_{k',-1} + \sum_{k'} x_{k,k'}^r y_{p-k,-k'}^r c_{k',0} + \sum_{k'} x_{k,k'}^r y_{p-k,1-k'}^r c_{k',1} + \cdots \right),$$

with $\omega \equiv \omega_m$. Since matrix elements $x_{m,n}$ and $y_{m,n}$ of coordinates are equal to zero for transitions between states of the same parity, the solution of Eqs. (5) consists of two independent sets, for odd and even values of $p$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{energy_spectrum.png}
\caption{Energy spectrum of the system (6) in units of $\hbar \omega$. Five groups with 121 states in each group are shown for $\mu = 10^{-6}$, $\hbar \omega \approx 1.77 \cdot 10^{-5}$, and $n_0 = 446$.}
\end{figure}

Let us now consider the case of a small nonlinearity, when the condition $\hbar \omega p \gg E_{n_0}' \left( k^2 - pk + \frac{p^2}{2} \right)$ is satisfied. The corresponding numerical data for a fragment of the energy spectrum is shown in Fig.1. One can see that the spectrum consists of series of energy levels, that are shifted one from another by the value $\hbar \omega$. The structure of energy spectrum in each group is typical for a quantum nonlinear resonance [11]. Lowest levels are practically equidistant with the spacing equal to $\hbar \omega$, where $\omega$ is the classical frequency of small phase oscillations at coupling resonance. Accumulation points correspond to classical separatricies, and all energy levels inside separatricies are non-degenerate. The states slightly above separatricies are quasi-degenerate due to the symmetry of a rotation in opposite directions.

In accordance with the spectrum structure it is convenient to characterize the states at coupling resonance by two indexes, by the group number $q$ and by the index $s$ which stands for the levels inside groups. Then, the energy in each group can be written as $E_{q,s} = \hbar \omega q + E_{q,s}',$ where $E_{q,s}$ is the Mathieu-like spectrum of one group.

Now we analyze the dynamics of the model in the presence of the external force. For commensurate frequencies $\Omega_1$ and $\Omega_2$, the perturbation is periodic with the period $T = i T_1 = j T_2$, where $T_1 = 2\pi/\Omega_1$, $T_2 = 2\pi/\Omega_2$ and $i$, $j$ are integers. The initial conditions were taken for a system to be about half-way between the two driving resonances, $\omega = (\Omega_1 + \Omega_2)/2$.

Since the Hamiltonian (1) is periodic in time, the solution of the Schrödinger equation can be written as

$$\psi(x,y,t) = \exp \left( -i \varepsilon Q T \frac{\hbar}{\hbar_0} \right) u_Q(x,y,t).$$

Here $u_Q(x,y,t) = u_Q(x,y,t + T)$ and $\varepsilon Q$ are the quasienergy (QE) functions and quasienergies, respectively. They are determined by the evolution operator $\hat{U}$ describing the dynamics of our system in one period of the external field,

$$\hat{U} u_Q(x,y) = \exp \left( -i \varepsilon Q T \frac{\hbar}{\hbar_0} \right) u_Q(x,y).$$

Here the argument $t$ is omitted since we are interested in the wave function only for discrete times $NT$, with $N = 1, 2, \ldots$.

It is now naturally to represent the QE functions in the form $u_Q(x,y) = \sum_q A^Q_{q,s} \psi_{q,s}(x,y)$, where $\psi_{q,s}(x,y)$ are eigenstates of the unperturbed Hamiltonian $\hat{H}^0 = \hat{H}_x^0 + \hat{H}_y^0 - \mu x y$. The coefficients $A^Q_{q,s}$ are the eigenvectors of the operator $\hat{U}$ in the representation of two coupled nonlinear oscillators, that can be found by diagonalization of the corresponding matrix $U_{q,s,q',s'}$. This matrix can be numerically obtained in the following way. Let the evolution operator $\hat{U}$ act on the initial state $C_{(q_0,s_0)}^{(q_0,s_0)}(0) = \delta_{q_0,q_0} \delta_{s_0,s_0}$. Then the wave function $C_{(q_0,s_0)}^{(q,s)}(T)$ at time $T$ forms the column of the evolution operator matrix,

$$U_{q,s,q',s'}(T) C_{q',s'}^{(q_0,s_0)}(0) = U_{q,s,q_0,s_0}(T) C_{q,s}^{(q_0,s_0)}(T).$$

Repetition of this procedure for different initial states $C_{q,s}^{(q',s')} = \delta_{q,q'} \delta_{s,s'}$ determines the whole matrix.
$U_{q,s,q',s'}(T)$. As a result, the wave function $C_{q,s}^{(q_0,s_0)}(T)$ can be computed numerically by integration of the non-stationary Schrödinger equation,

$$i\hbar \dot{C}_{q,s} = \left( \hbar \omega q + E_{q,s}^M \right) C_{q,s} - f_0 \sum_{q',s'} x_{q,s;q',s'} \left( \cos \Omega_1 t + \cos \Omega_2 t \right) C_{q',s'}.$$

If we introduce slow amplitude $b_{q,s}(t)$ via the transformation

$$C_{q,s}(t) = b_{q,s}(t) \exp \left[ -i \left( q \omega + E_{q,s}^M / \hbar_0 \right) t \right],$$

then after some algebra one can obtain

$$i\hbar \dot{b}_{q,s} = -f_0 \cos \left( \frac{\delta \Omega}{2} \right) \times \sum_{q'} \left[ x_{q,s; q+1,s'} b_{q+1,s'} e^{-i \left( E_{q+1,s'}^M - E_{q,s}^M \right) t / \hbar_0} + x_{q,s; q-1,s'} b_{q-1,s'} e^{-i \left( E_{q-1,s'}^M - E_{q,s}^M \right) t / \hbar_0} \right],$$

where $\delta \Omega = \Omega_1 - \Omega_2$. Using the resonance approximation, we keep only the most important slowly oscillating terms with $q' = q \pm 1$.

The matrix elements $x_{q,s; q\pm 1, s'}$ in (11) define transition probabilities between the states $s$ and $s'$ from the neighbor groups. This matrix has a specific block structure shown in Fig. 2a.

![Fig. 2. (a) Matrix elements $|x_{q,s; q\pm 1, s'}|$ that define the transition probability along the coupling resonance, for the same parameters as in Fig. 1a. (b) Detailed structure of the "cross"-like broadening.](image)

Black and white regions correspond to big and small matrix elements, respectively. One fragment of this structure is shown in Fig. 2b in more details. The matrix elements in the center of Fig. 2 correspond to the transitions between lowest states (at the center of coupling resonance) of the groups with $q = 0$ and $q = 1$. Matrix elements at the corners of Fig. 2a, where $s, s' > 30$ or $s, s' < -30$, define transitions between the states above separatrix. All these elements quickly decrease with an increase of the difference $|s - s'|$. The "cross"-like broadening in Fig. 2b, where matrix elements are large, corresponds to the transitions between separatrix states. As a result, the transition probability between separatrix states of neighbor groups (along the coupling resonance) is much larger than the transition probability between other states. This phenomenon is analogous to the quantum diffusion inside a separatrix, which was investigated in a degenerate Hamiltonian system [13].

Solving numerically Eqs. (11), we obtain the matrix $U_{q,s,q',s'}(T)$ that determines the eigenvalues $\varepsilon_q$ and QE functions $A_{q,s}^Q$. Global properties of QE functions can be understood in terms of their "centers" $\bar{q} = \sum_q q \sum_s |A_{q,s}^Q|^2$, and dispersion $\sigma_q = \sum_q (q - \bar{q})^2 \sum_s |A_{q,s}^Q|^2$ in the unperturbed ($f_0 = 0$) basis, see Fig. 3. One can see that for a relatively small $\mu$ and $f_0$, the QE functions do not couple unperturbed states with different values of $q$. On the other hand, a stronger coupling results in a kind of "delocalization" that is characterized by the spread of QE functions over many groups of states with different $q$. This fact manifests a large probability for the transition between those states that are involved in the diffusion along the coupling resonance.

![Fig. 3. Plot of $\bar{q}$ versus $\sqrt{\sigma_q}$ for QE functions $A_{q,s}^Q$ in the regions $q = 0, \pm 1$ for different coupling constants: a) $\mu = 3 \cdot 10^{-5}$, b) $\mu = 10^{-4}$. Points correspond to different QE functions.](image)

Direct computation of the evolution of wave packets has confirmed the occurrence of a weak diffusion in energy space, that is analogous to the classical Arnold’tdiffusion. Numerical data have been obtained by computing the evolution matrix according to the relations,

$$U_{q,s,q',s'}(NT) = \sum_Q A_{q,s}^Q A_{q',s'}^Q \exp \left( -i \varepsilon_Q NT \right),$$

$$C_{q,s}(NT) = \sum_{q',s'} U_{q,s;q',s'}(NT) C_{q',s'}(0).$$

We have studied quantum dynamics and calculated diffusion coefficient for different initial states in the regime when the values of $\mu$ and $f_0$ are small enough and $f_0/\mu = 0.01$, so that the coupling and two driving resonances do not overlap.

Quantum dynamics for different initial conditions is illustrated in Fig. 4 where the energy dispersion $\Delta_q = (\Delta H)^2 / \hbar_0^2$ with $\Delta_q = \sum_q (q - \bar{q})^2 \sum_s |C_{q,s}|^2$ and
\( \bar{q} = \sum q^2 \sum \left| C_{q,s} \right|^2 \) is plotted versus the rescaled time \( N = t/T \). The figure clearly shows different character of the evolution for three initial states. For the states taken from below and above the separatrix, the energy width of packets oscillates, in contrast with a diffusion-like time-dependence for the case when the initial state corresponds to the classical separatrix.

We calculated quantum and classical diffusion coefficients and found that the diffusion in the quantum model is systematically weaker than the classical Arnol’d diffusion, see Fig. 4. However, the global dependence of the quantum diffusion coefficient on the control parameter \( 1/\sqrt{\mu} \) is similar to the classical one. The data in this figure are obtained for initial states corresponding to the centre of the stochastic layer, where the diffusion coefficient is maximal. For initial states corresponding to the border of the stochastic layer, the diffusion coefficient strongly fluctuates and can be several times smaller.

To count the number \( M_s \) of stationary states inside the classical separatrix layer, we calculated the width of the classical layer numerically, together with the number of energy levels in the corresponding energy interval. For \( \mu > 1.25 \cdot 10^{-4} \) the number \( M_s \) was found to be about 10. The right square in Fig. 5 for the lowest value of \( \mu \) corresponds to the Shuryak border \( [\big[ \big] \) ], the latter that only one quantum state is inside the classical stochastic layer. In this case, the classical chaos is completely suppressed by quantum effects. We have also found that for large times, \( t > 1000T \), the diffusion-like growth of the energy terminates, thus indicating the localization of the classical diffusion along stochastic layers.

In conclusion, we have shown that when the number \( M_s \) of stationary states inside classical chaotic separatrix layers is relatively large, one can observe weak quantum diffusion that is similar to the classical Arnol’d diffusion. In our model this diffusion occurs along the nonlinear coupling resonance, due to the influence of guiding resonances originated from the external time-dependent perturbation. Our results may find a confirmation in experiments on one-electron dynamics in 2D quantum billiards with time-periodic electric fields.

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