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ENERGY DIFFUSION IN STRONGLY DRIVEN QUANTUM CHAOTIC SYSTEMS

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The energy evolution of a quantum chaotic system under the perturbation that harmonically depends on time is studied in the case of a large perturbation, in which the transition rate calculated from the Fermi golden rule exceeds the frequency of the perturbation. It is shown that the energy evolution retains its diffusive character, with the diffusion coefficient that is asymptotically proportional to the magnitude of the perturbation and to the square root of the density of states. The results are supported by numerical calculation. Energy absorption by the system and quantum–classical correlations are discussed.

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1. INTRODUCTION

The problem of susceptibility of chaotic systems to perturbations has attracted much attention in the last decade [1–9]. This problem is fundamental because it includes the determination of the response of a material system to an imposed external electromagnetic field, the setup that is typical for many experiments. Due to the sensitivity of classical phase trajectories or quantum energy spectra and stationary wave functions of chaotic systems to small changes of their parameters, the problem is challengingly difficult. A consistent and noncontroversial picture covering (albeit qualitatively) all the essential cases of the response has not yet been drawn at present. From the standpoint of general theory, the problem is related to the applicability of the concept of quantum–classical correspondence to chaotic systems, which is a long-standing question in its own right [10, 11].

We study a one-particle system with the Hamiltonian of the form

$$\hat{H} = \hat{H}_0 - F\hat{x}\cos(\omega_0 t),$$

where $\hat{H}_0(\hat{\mathbf{p}}, \hat{\mathbf{r}})$ is the Hamiltonian of the unperturbed system; $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ are the operators of Cartesian components of the particle momentum and position. The classical system with the Hamiltonian function $H_0(\mathbf{p}, \mathbf{r})$ is assumed to be strongly chaotic, that is, nearly ergodic on the energy surfaces in a wide range of energy values, a system with $d \geq 2$ degrees of freedom. In the perturbation operator

$$\hat{V}(t) = -F\hat{x}\cos(\omega_0 t),$$

the active variable $\hat{x}$ is one of the Cartesian coordinates of the particle, coupled to the external uniform force field. The amplitude F is called the field in what follows. We consider the semiclassical case, where the Planck constant $\hbar$ is small in comparison with the action scale of the system H_0.

Under the influence of the perturbation, the energy value

$$E(t) \equiv H_0(t)$$

varies in a quasirandom way. These variations can frequently be described as the process of energy diffusion [12, 13], when for the ensemble with the microcanonical initial energy distribution $H_0(0) = E$, the energy dispersion increases linearly with time,

$$\langle \Delta E^2(t) \rangle = 2Dt,$$

where $D(E, F, \omega_0)$ is the energy diffusion coefficient.

If the external field F is sufficiently small in comparison with the appropriately averaged values of the forces acting on a particle in the unperturbed system, then the energy diffusion coefficient D in the classical model can be expressed through the characteristics of

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the unperturbed chaotic motion of the active coordinate as

$$D = \frac{\pi}{2}\omega_0^2 F^2 S_x(E,\omega_0), \tag{1}$$

where $S_x(E,\omega_0)$ is the power spectrum of the active coordinate (the Fourier transform of its autocorrelation function) for the motion over the surface with the constant energy value E [9]. The same expression (1) in the case of a weak perturbation can be obtained in the classical limit from the quantum model. The evolution of the quantum system can be treated as a sequence of one-photon transitions between stationary states $|n\rangle \to |k\rangle$ of the unperturbed system, accompanied by the absorption or emission of the quanta $\hbar\omega_0$. For small $\hbar$, the energy spectrum of $\hat{H}_0$ is quasicontinuous, and hence the transition rates are given by the Fermi golden rule (FGR)

$$\dot{W}_F = \frac{\pi}{2\hbar}F^2|x_{nk}|^2\rho(E_k), \tag{2}$$

where x_{nk} is the matrix element of the active coordinate and $\rho(E_k)$ is the density of states near the final state of the transition. Although the matrix elements x_{nk} in quantum chaotic systems fluctuate wildly with the variation of k [10, 11], the averaged squared quantity $\overline{|x_{nk}|^2}$ in the limit as $\hbar \to 0$ is smooth; it is proportional to the power spectrum $S_x(E,\omega_0)$ of the coordinate [14, 15],

$$\overline{|x_{nk}|^2} \approx \frac{S_x(E,\omega_0)}{\hbar\rho(E)}\,. \tag{3}$$

From Eqs. (2) and (3), we have the transition rate

$$\dot{W}_F = \frac{\pi}{2\hbar^2}\,F^2 S_x(E,\omega). \tag{4}$$

Then for the energy dispersion for small t, we have

$$\langle \Delta E^2\rangle = 2(\hbar\omega_0)^2\dot{W}_F t,$$

which brings us back to Eq. (1) for the energy diffusion coefficient. It can be shown that the same expression for D also holds for large t [9].

The energy absorption in chaotic systems occurs as an epiphenomenon of the energy diffusion [4]. With the dependence of the power spectrum $S_x(E,\omega)$ and the density of states $\rho(E)$ on energy taken into account, the diffusion becomes biased, and the energy absorption rate Q is given by the formula [2, 4]

$$Q = \frac{1}{\rho}\,\frac{d}{dE}\,(\rho D). \tag{5}$$

Although D does not depend on the Planck constant $\hbar$ for weak fields, the applicability condition for Eq. (2) does. The FGR is, after all, only a formula of the first-order perturbation theory. It is based on the assumption that the transition process has a resonant character, i.e., that the width Δ of the energy distribution of states populated from the original one, given by the Weisskopf–Wigner formula [16]

$$\Delta = \hbar\dot{W},$$

is small in comparison with the energy quanta $\hbar\omega_0$. From Eq. (4), it is evident that in the classical limit $\hbar \to 0$, this applicability condition is violated.

By analogy with other models, beyond the limits of the applicability of the perturbation theory, one can expect a slow-down of the growth of the energy diffusion coefficient D and of the energy absorption rate Q. For example, for a two-level system with relaxation, the perturbative quadratic dependence of the absorption rate $Q \propto F^2$ turns into a field-independent value Q_0 in the domain $\Omega^2 \gg \Gamma_1\Gamma_2$, where Ω is the Rabi frequency and Γ_1 and Γ_2 are longitudinal and transverse relaxation rates respectively [17]. The rate of transitions from the discrete to continuous energy spectrum (which are basically covariant with the energy absorption rate Q), studied in the context of the theory of photoionization, first slows its growth with the transfer from the multiphoton to the tunneling regime and then can even decrease with the further increase of F — the effect that is known as atom stabilization by a strong field [18].

In what follows, we use the border value of the field F_b, defined by the condition

$$\dot{W}_F(F_b) = \omega_0.$$

For the weak field, $F \ll F_b$, the FGR is applicable, whereas the domain of the strong field, $F \gg F_b$, must be treated differently. The slow-down of the energy diffusion in quantum chaotic systems in strong harmonic fields was first demonstrated by Cohen and Kottos [5]. However, their analytic estimates and data of numerical experiments are in quantitative disagreement with the results in the present paper.

It must be noted that the strong field regime is easily attainable in experiments. For example, for the excitation of multiatomic molecules with infrared laser radiation, the border field corresponds to the intensity value $I \sim 10^9$ W $\cdot$ cm^{-2}, which has been reached in experiments long time ago [19].

2. THEORY

For the system with the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}\cos(\omega_0 t),$$

we take the wave function in the form of the expansion in the basis of stationary states $\{\varphi_m\}$ of $\hat{H}_0$,

$$\Psi(t) = \sum_m a_m \varphi_m(\mathbf{r}) e^{-i\omega_m t}. \quad (6)$$

For the amplitudes $\{a_m(t)\}$, we then obtain the system of equations

$$i\frac{da_k}{dt} = \sum_k \Omega_{km} \cos(\omega_0 t) e^{i\omega_{km} t} a_m, \quad (7)$$

where the quantities

$$\Omega_{kn} = \hbar^{-1} F x_{kn}$$

are the Rabi frequencies of transitions. We use the initial conditions $a_m(0) = \delta_{mn}$: at the initial time instant, only one of the stationary states, φ_n, is populated. Following Refs. [14, 15], we assume that x_{nk} are independent random Gaussian variables with zero mean and the dispersion given by Eq. (3). System of equations (7) is treated as a member of the corresponding statistical ensemble.

We concentrate on the process of energy diffusion. Then in the zeroth approximation, we can restrict ourselves by consideration of the probability density evolution in a narrow energy range around the initial state and use the power spectrum and the density of states values at this energy,

$$S_x(\omega) \equiv S_x(E_n, \omega)$$

and

$$\rho \equiv \rho(E_n).$$

For the calculation of the absorption coefficient, the global dependence on energy must be restored.

The power spectrum $S_x(\omega)$ has the symmetry property

$$S_x(-\omega) = S_x(\omega).$$

The dependence $S_x(\omega)$ in the domain $\omega > 0$ in typical strongly chaotic systems, such as nonlinear oscillators [20] and billiards [21, 22], has the form of an asymmetric peak. We define the peak value of the Rabi frequency simply as Ω, the frequency of the maximum as $\tilde{\omega}$, and the characteristic width of the peak as Γ. Typically, the ratio $\tilde{\omega}/\Gamma$ is about few units.

Immediately after switching the perturbation on, all amplitudes (except that of the initially populated state) grow in absolute value linearly in time. At this ballistic stage, the energy dispersion grows quadratically in time,

$$\langle \Delta E^2 \rangle \approx K_1 \hbar^3 \tilde{\omega}^2 \Omega^2 \Gamma \rho t^2, \quad (8)$$

where K_1 is a numerical constant. This stage is limited by the depletion of the initial population and lasts until the depletion time

$$t_d \sim \Omega^{-1} (\hbar \Gamma \rho)^{-1/2}.$$

At this time instant, considerably populated levels are spread over the energy range $\Delta E \sim \hbar\tilde{\omega}$ that contains many levels (because $\rho \propto \hbar^{-d}$ with $d \geq 2$). We expect that at the next stage, the ensemble-averaged probability density is a smooth function with a characteristic scale $\Delta E \gg \hbar\tilde{\omega}$.

It is convenient to write the indices in Eq. (7) as arguments of functions. We use the frequency distance from the initial level as a basic independent variable ω, and thus a_k is denoted as $a(\varepsilon)$, where

$$\varepsilon = \frac{E_k - E_n}{\hbar}.$$

Dummy variables η and η' have the same meaning. By formal integration of Eq. (7) and subsequent recursive substitution, we obtain the equation for the rate of change of the local probability density $w(\varepsilon) = |a(\varepsilon)|^2$:

$$\frac{dw(\varepsilon)}{dt} = \sum_{\eta,\eta'} \Omega(\varepsilon,\eta) \exp\left(i(\varepsilon-\eta)t\right) \cos(\omega_0 t) a(\eta,t) \times \\ \times \int^t dt' \Omega(\varepsilon,\eta') \exp\left(-i(\varepsilon-\eta')t'\right) \times \\ \times \cos(\omega_0 t') a^*(\eta',t') + \text{c.c.} \quad (9)$$

Summation in this formula goes over discrete values of η and η', and this equation is still exact.

We now assume that the amplitudes $a(\eta,t)$ are random processes that are not correlated for different states:

$$\langle a(\eta,t) a^*(\eta',t') \rangle \propto \delta_{\eta\eta'}.$$

Then for the averaged probability density, we can retain only diagonal terms in Eq. (9):

$$\frac{d\langle w(\varepsilon)\rangle}{dt} = \sum_\eta \langle \Omega^2(\varepsilon,\eta)\rangle \cos(\omega_0 t) \times \\ \times \int^t dt' \exp\left(i(\varepsilon-\eta)(t-t')\right) \times \\ \times \cos(\omega_0 t') \langle a(\eta,t) a^*(\eta,t')\rangle + \text{c.c.} \quad (10)$$

Under the assumption that the averaged $\langle w(\varepsilon,t)\rangle$ is a smooth function of ε and a slowly varying function of t, we can rewrite the product of amplitudes as

$$\langle a(\eta,t) a^*(\eta,t')\rangle + \text{c.c.} = 2\langle w(\eta,t)\rangle B(t-t'), \quad (11)$$

where $B(\tau)$ is the normalized ($B(0) = 1$) autocorrelation function of the probability amplitudes.

By replacing the averaged square of the Rabi frequency by its value from Eq. (3) (which depends only on the difference $\varepsilon - \eta$), substituting the summation over the states by the integration weighted with the density of states, and averaging over the time intervals that are much larger than the field period, we obtain the equation

$$\frac{dw(\varepsilon)}{dt} = \int d\eta\, \Omega^2(\varepsilon - \eta)\rho(\eta) \times \\ \times \int_0^\infty d\tau\, \cos(\varepsilon - \eta)\tau \cos(\omega_0 \tau) B(\tau) w(\eta). \quad (12)$$

Henceforth, we drop the angular brackets and deal only with ensemble-averaged quantities. If the rate of variations of $w(\eta, t)$ is small in comparison with the decay of correlations of the amplitudes given by $B(\tau)$, we can treat Eq. (12) as a summation over the probability flow that comes from the different parts of the frequency range with a constant rate,

$$\dot{W}(\eta \to \varepsilon) = \Omega^2(\varepsilon - \eta) \times \\ \times \int_0^\infty d\tau\, \cos(\varepsilon - \eta)\tau \cos(\omega_0 \tau) B(\tau). \quad (13)$$

This approximate expression to some extent replaces the Fermi golden rule for strong perturbations.

To construct the kinetic equation, we must take both incoming and outgoing probability flows into account. By taking the total probability flow into account and expanding $w(\varepsilon)$ in the Taylor series, we obtain a diffusion equation with the probability diffusion coefficient in the energy scale

$$D \approx \int_{-\infty}^\infty d\eta\, \hbar^3 \eta^2 \Omega^2(\eta) \rho J(\eta, \omega_0), \quad (14)$$

where

$$J(\eta, \omega_0) = \int_0^\infty d\tau\, \cos(\eta\tau) \cos(\omega_0 \tau) B(\tau). \quad (15)$$

The problem now reduces to the calculation of the integral $J(\eta, \omega_0)$. For sufficiently long times, the average probability density, which is governed by the diffusion equation, varies slowly, and we can treat the system in Eq. (7) as a set of equations in which all $a_m(t)$ are noncorrelated random processes with the same statistical properties. Then by averaging the equation for the squared time derivative of amplitudes, we obtain the expression for the mean squared frequency of these processes, which also gives an estimate for the square of the correlation decay rate γ,

$$\langle \omega^2 \rangle = \frac{1}{2} \int \Omega^2(\eta) \hbar \rho\, d\eta \equiv \gamma^2. \quad (16)$$

From Eq. (16) for the decay correlation rate, we have the estimate

$$\gamma \approx K_2 \Omega \sqrt{\Gamma \hbar \rho}, \quad (17)$$

where K_2 is a numerical constant. In the strong-field domain, the autocorrelation function is the fastest component in the integrand in Eq. (15). We then have

$$J \sim \gamma^{-1} \approx \left(K_2 \Omega \sqrt{\Gamma \hbar \rho} \right)^{-1}.$$

Substituting this expression in Eq. (14), we obtain the estimate of the energy diffusion coefficient

$$D \approx K_3 \hbar^2 \tilde{\omega}^2 \Omega \sqrt{\Gamma \hbar \rho}, \quad (18)$$

where K_3 is a numerical constant. We must recall that Eq. (18) is valid only for nearly resonant perturbation frequencies $|\omega_0 - \tilde{\omega}| \le \Gamma$. Here, we do not analyze the dependence of D on the perturbation frequency ω_0 in a wider domain, postponing it until further studies.

3. NUMERICAL EXPERIMENT

To check the analytic results in the preceding section, we integrated the system of equations in (7) numerically. The number of equations varied from $N = 300$ to $N = 1200$ with the purpose to suppress the effect of the boundary. The envelope of the Rabi frequencies was taken in the double-Lorentzian form

$$\Omega_{m,n} = \Omega \left[\frac{\Gamma^2}{(\omega_m - \omega_n + \tilde{\omega})^2 + \Gamma^2} + \right. \\ \left. + \frac{\Gamma^2}{(\omega_m - \omega_n - \tilde{\omega})^2 + \Gamma^2} \right]. \quad (19)$$

All calculations were performed for the «resonant» perturbation frequency $\omega_0 = \tilde{\omega}$ and the peak width $\Gamma = 0.3\tilde{\omega}$.

Figure 1 shows the distribution of the probability as a function of the dimensionless frequency $\varepsilon' = \varepsilon/\tilde{\omega}$ for different time instants. It is clearly seen that even for relatively short time

$$t = 5\tilde{\omega}^{-1} = 2.2 t_d,$$

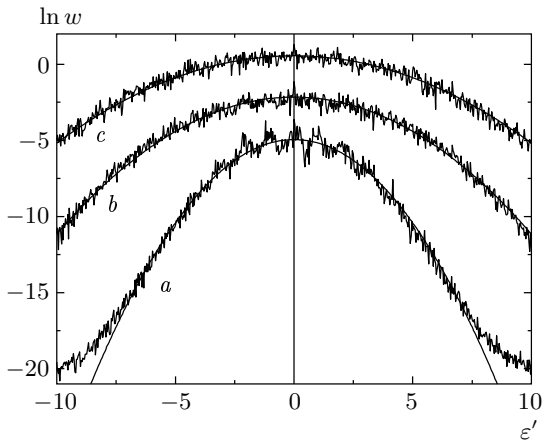

Fig. 1. The dependence of the logarithm of the probability density w on the dimensionless frequency $\varepsilon' = \varepsilon/\tilde{\omega}$ for the time values $t = 5\tilde{\omega}^{-1}$ (a), $10\tilde{\omega}^{-1}$ (b), and $15\tilde{\omega}^{-1}$ (c). The grassy lines are the values of $\ln w(\varepsilon')$ averaged over 10 different sets of matrix elements, solid lines are fitted parabolas. To avoid the overlap of graphs, the plots in cases (b) and (c) are shifted upwards by 3 and 6 units respectively

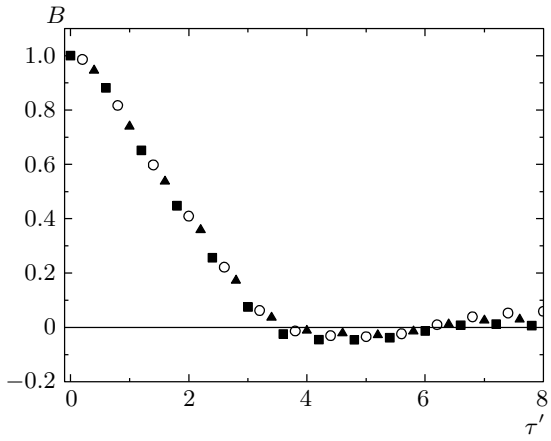

Fig. 2. Dependence of the autocorrelation function B of the probability amplitudes on the dimensionless time shift $\tau' = \tau\tilde{\omega}$ for three different sets of parameters with $\tilde{\omega}\hbar\rho = 30$ (black squares), $\tilde{\omega}\hbar\rho = 60$ (open circles), and $\tilde{\omega}\hbar\rho = 120$ (black triangles) and the same value of $\Omega\sqrt{\Gamma\hbar\rho} = 0.618\tilde{\omega}$. The statistical errors are about the size of the data symbols

the distribution has a very accurate Gaussian form, with deviations noticeable only for $|\varepsilon'| \geq 7.5$. Therefore, we quantitatively support our conclusion about the diffusive character of the energy evolution.

Figure 2 depicts the form of the normalized autocorrelation function of the probability amplitudes. The

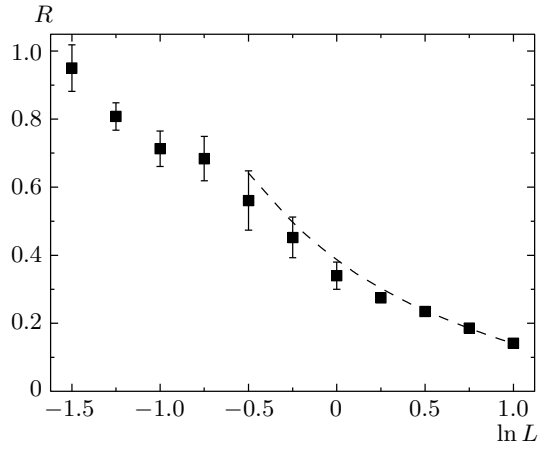

Fig. 3. The dependence of the ratio $R = D/2\dot{W}_F$ of the energy diffusion constant D to the doubled Fermi transition rate $\dot{W}_F = (\pi/2)\Omega^2\hbar\rho$ on the logarithm of the ratio of the Rabi frequency to its boundary value $L = \Omega/\Omega_b$, $\Omega_b = (2\tilde{\omega}/\pi\hbar\rho)^{1/2}$. The dashed line represents the curve $R = A\exp(-L)$ that corresponds to the theoretical dependence in Eq. (18); it is fitted to the last three points

values of $B(\tau)$ have been calculated numerically for three sets of parameters with different values of ρ but with the same value of the product $\Omega\sqrt{\hbar\Gamma\rho}$. It is clearly seen that $B(\tau)$ for these sets are nearly identical, as expected. The decay rate γ taken from the equation

$$B(\gamma^{-1}) = \exp(-1)$$

is

$$\gamma = 0.77\Omega\sqrt{\hbar\Gamma\rho};$$

this supports the estimate in Eq. (17).

Figure 3 represents the dependence of the ratio $R = D/2\dot{W}_F$ of the energy diffusion constant D to the doubled Fermi transition rate $\dot{W}_F = (\pi/2)\Omega^2\hbar\rho$ on the logarithm of the ratio of the Rabi frequency to its boundary value $L = \Omega/\Omega_b$, $\Omega_b = (2\tilde{\omega}/\pi\hbar\rho)^{1/2}$. It is seen that for the weak field, this ratio comes close to the asymptotic limit (unity), decreases in the vicinity of the boundary, and decays as F^{-1} for sufficiently strong fields. The agreement with the theoretical estimates is quite convincing.

4. CONCLUSION

From the comparison of the numerical data with the theoretical estimates, we can conclude that the approach in Sec. 2 gives a reasonably accurate description of the energy evolution process in strong fields, in spite of numerous simplifying approximations used in the calculation.

To improve the accuracy and to derive the equation for the correlation function $B(\tau)$ from first principles, the model of the random process must be improved. We used the model of the stationary process, whereas we can conclude from Eq. (7) that the model of periodic random process would be more appropriate.

The main conclusion of our calculation is a qualitative one: by substituting Eq. (3) in Eq. (14), we obtain

$$D \approx K_3 \hbar \tilde{\omega}^2 F \left[S_x(\omega_0)\Gamma\right]^{1/2}.$$

This quantity in the classical limit $h \to 0$ vanishes along with the energy absorption rate Q (see Eq. (5)). This means a violation of the quantum–classical correspondence for the absorption and, more generally, of the linear susceptibility of chaotic systems to harmonic external fields.

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