Resonant phenomena in classical dynamics of three-body Coulomb systems

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We consider dynamics of a planar three-body Coulomb system similar to a hydrogen molecular ion (heavy-light-heavy particles). The system has three degrees of freedom. In the limit of infinitely heavy nuclei the system is reduced to the famous two-center problem which is integrable. When masses of heavy particles are finite, one degree of freedom in the Hamiltonian system corresponds to slow nuclei motion, while other two degrees of freedom correspond to fast electron motion. The averaging method predicts that actions of ''fast'' motions of the system with frozen nuclei are approximate integrals of the full system (adiabatic invariants). However, during slow evolution of the ''heavy'' subsystem certain resonance conditions can be satisfied. We study the phenomena of capture into resonances and scattering on resonances which can lead to destruction of adiabatic invariance in the system.

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I. INTRODUCTION

A famous dynamical problem known as the ''problem of three bodies'' [1] has been investigated for more than 240 years [2] because of its importance in celestial mechanics [3], as well as in one-electron molecular ions [4–7], doubly excited states in atoms [8], and exotic molecular systems [9]. A huge number of papers dealing with nonintegrable classical motion of three gravitating bodies has been published. On the other hand, only in a limited number of papers has the classical three-body Coulomb (TBC) problem been investigated analytically (see Refs. [7–15] and references therein). A systematic investigation of the classical dynamics of TBC problem is desirable because, beside being of fundamental interest, it may provide useful information for modern semiclassical methods dealing with quantum mechanics of atomic and molecular systems [3]. In both gravitational three-body systems and TBC systems the masses of the particles involved usually differ by orders of magnitude. The main difference between TBC problems and gravitational three-body problems is that in the latter interparticle interactions depend on the particle masses, whereas in the former they depend on charges (which usually are of the same order of magnitude). As a result, perturbative treatment of a TBC system such as a hydrogen molecular ion is quite different from that of gravitational systems in celestial mechanics. In the present paper, we consider dynamics of a planar TBC system similar to hydrogen molecular ion [two heavy (mass M) and one light (mass m) charged particles]. We consider the problem for different mass ratios (not restricting ourself to the hydrogen molecular ion). In the limiting case of fixed nuclei (i.e., $M/m=\infty$) the system becomes separable (in classical mechanics, separation of Hamilton-Jacobi equation for the two-fixed center three-body problem has been known already to Euler and Jacobi). Then the mass ratio is finite, the problem is nonintegrable, but the presence of slow and fast motions in the system enables one to use averaging methods. However, the averaging technique in the system is not straightforward because of resonant phenomena, which complicate the analysis. We use a scheme of analysis of resonant phenomena in Hamiltonian systems possessing slow and fast variables [16]; this scheme is a Hamiltonian version of a more general scheme [17,18] (see also Refs. [19–21]).

II. HAMILTONIAN EQUATIONS OF MOTION

Consider three particles with masses m_i and charges Z_i moving in a plane (x,y). The Hamiltonian of the system is

$$H=\sum_{i=1}^{3}\left(\frac{p_{x_i}^2+p_{y_i}^2}{2m_i}\right)+\frac{Z_1Z_2}{r_{12}}+\frac{Z_2Z_3}{r_{23}}+\frac{Z_1Z_3}{r_{13}}, \qquad (1)$$

where r_{ij} are interparticle distances

$$r_{ij}=[(x_i-x_j)^2+(y_i-y_j)^2]^{1/2}. \qquad (2)$$

We assume $m_{1,2}=M$, $m_3=m$, $M\gg m$, $Z_{1,2}=1$, $Z_3=-1$. Before applying canonical perturbation theory to the system (1), let us perform some transformations. By means of simple canonical transformation with generating function $W_1=\tilde{p}_{x_1}(x_1-x_3)+\tilde{p}_{y_1}(y_1-y_3)+\tilde{p}_{x_2}(x_2-x_3)+\tilde{p}_{y_2}(y_2-y_3)+\tilde{p}_{x_3}x_3+\tilde{p}_{y_3}y_3$ the Hamiltonian is reduced from six to four degrees of freedom [15]:

$$H=\frac{\tilde{p}_{x_1}^2+\tilde{p}_{y_1}^2+\tilde{p}_{x_2}^2+\tilde{p}_{y_2}^2}{2\mu}+\frac{\tilde{p}_{x_1}\tilde{p}_{x_2}+\tilde{p}_{y_1}\tilde{p}_{y_2}}{m}-\frac{1}{\sqrt{\tilde{x}_1^2+\tilde{y}_1^2}}$$
$$-\frac{1}{\sqrt{\tilde{x}_2^2+\tilde{y}_2^2}}+\frac{1}{\sqrt{(\tilde{x}_1-\tilde{x}_2)^2+(\tilde{y}_1-\tilde{y}_2)^2}}, \qquad (3)$$

where μ is the reduced mass, $\mu=mM/(m+M)$. Then, we change to variables $(P_x,x,P_y,y,P_R,R,P_\Theta,\Theta)$ by means of a generating function

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$$W_2=\tilde{p}_{x_2}(\tfrac{1}{2}R\cos\Theta+x\cos\Theta-y\sin\Theta)$$
$$+\tilde{p}_{y_2}(\tfrac{1}{2}R\sin\Theta+x\sin\Theta+y\cos\Theta)$$
$$-\tilde{p}_{x_1}(\tfrac{1}{2}R\cos\Theta-x\cos\Theta+y\sin\Theta)$$
$$-\tilde{p}_{y_1}(\tfrac{1}{2}R\sin\Theta-x\sin\Theta-y\cos\Theta).$$

New coordinates are determined by the following relations:

$$\tilde{x}_2=-\frac{1}{2}R\cos\Theta-x\cos\Theta+y\sin\Theta,$$
$$\tilde{y}_2=-\frac{1}{2}R\sin\Theta-x\sin\Theta-y\cos\Theta,$$
$$\tilde{x}_1=\frac{1}{2}R\cos\Theta-x\cos\Theta+y\sin\Theta,$$
$$\tilde{y}_1=\frac{1}{2}R\sin\Theta-x\sin\Theta-y\cos\Theta. \tag{4}$$

The resulting Hamiltonian $H(P_x,x,P_y,y,P_R,R,P_\Theta)$ does not depend on Θ, therefore, $P_\Theta=\text{const}$ and we get the system with three degrees of freedom. It is easy to calculate that P_Θ is equal to the total angular momentum L : $P_\Theta=L$. Let us introduce a small parameter $\epsilon=\sqrt{m/M}$ and new momenta $P'_R=\epsilon P_R$ (we are interested in motions where typical values of P_R are high, so that $P'_R\gg\epsilon$). Denote also $P'_\Theta=\epsilon P_\Theta$. Substituting P'_R in the Hamiltonian, we get the Hamiltonian $H(P_x,x,P_y,y,P'_R,R,P'_\Theta)$ with canonically conjugated variables $(\epsilon^{-1}P'_R,R)$, (P_x,x), (P_y,y) which contains P'_Θ as a parameter. The next step is to introduce variables $(P_u,u,P_v,v,\tilde{P}_R,\tilde{R})$ by means of a generating function $W_3(P_x,P_y,P_R,u,v,\tilde{R})=(\tilde{R}/2)(P_x\cosh v\cos u-P_y\sin u\sinh v)-\epsilon^{-1}\tilde{R}P_R+Et$, where E is the value of the Hamiltonian (3) (see also Refs. [7,22]). New coordinates are determined by the following relations:

$$x=-\frac{R}{2}\cosh v\cos u,\quad y=\frac{R}{2}\sinh v\sin u,\quad \tilde{R}=R. \tag{5}$$

The resulting Hamiltonian is (omitting tildes and primes)

$$H=\frac{1}{m}\left(P_R^2+\frac{P_\Theta^2}{R^2}\right)+\frac{1}{R}+\frac{2}{mR^2}\,\frac{P_v^2+P_u^2}{\cosh^2v-\cos^2u} \tag{6}$$
$$-\frac{4\cosh v}{R(\cosh^2v-\cos^2u)}-E$$
$$+\frac{\epsilon P_\Theta}{mR^2}\,\frac{P_u\sinh 2v+P_v\sin 2u}{\cosh^2v-\cos^2u}$$
$$+\frac{\epsilon P_R}{mR}\,\frac{P_u\sin 2u-P_v\sinh 2v}{\cosh^2v-\cos^2u}$$
$$+\frac{\epsilon^2}{mR^2}(P_v^2+P_u^2)\frac{\cosh^2v+\cos^2u}{\cosh^2v-\cos^2u}=0.$$

In order to regularize the Hamiltonian let us introduce a new time variable t' satisfying $dt/dt'=(\cosh^2v-\cos^2u)m/2$ [22]. The resulting Hamiltonian is (omitting tildes)

$$\mathcal{H}=\frac{1}{4}\left(P_R^2+\frac{P_\Theta^2}{R^2}+\frac{m}{R}-mE\right)(\cosh 2v-\cos 2u)+\frac{P_v^2+P_u^2}{R^2}$$
$$-\frac{2m}{R}\cosh v+\epsilon\frac{P_R}{2R}(P_u\sin 2u-P_v\sinh 2v)$$
$$+\epsilon\frac{P_\Theta}{2R^2}(P_u\sinh 2v+P_v\sin 2u)+\frac{\epsilon^2}{4R^2}(P_v^2+P_u^2)$$
$$\times(2+\cosh 2v+\cos 2u)=\mathcal{F}_0+\epsilon\mathcal{F}_1+O(\epsilon^2)\equiv 0. \tag{7}$$

Variables $\epsilon^{-1}P_R$ and R (where R is still the internuclei distance) are canonically conjugated

$$\dot{P}_R=\epsilon\frac{\partial\mathcal{H}}{\partial R},\quad \dot{R}=\epsilon\frac{\partial\mathcal{H}}{\partial P_R}, \tag{8}$$

so that this pair of variables is ''slow,'' whereas other two pairs are ''fast.'' If one froze R,P_R and neglect terms $O(\epsilon)$ in Eq. (7), one will get the problem of two fixed Coulomb centers (two-center problem) which is integrable. Therefore, the Hamiltonian system (7) can be investigated using the technique developed in Refs. [16,18] and employed recently in Refs. [23–26]. So, consider first the Hamiltonian $\mathcal{F}_0$ of the system (7) with frozen P_R,R and with terms $O(\epsilon)$ omitted

$$\mathcal{F}_0=\frac{P_v^2}{R^2}+\frac{P_u^2}{R^2}-(\cosh 2v-\cos 2u)E_{el}-\frac{2m}{R}\cosh v, \tag{9}$$

where $E_{el}=(m/4)(E-P_R^2/m-P_\Theta^2/mR^2-1/R)$. Hamiltonian $\mathcal{F}_0$ in addition to conserved energy has a second constant of motion Ω:

$$P_u^2+\mathcal{E}_{el}\cos 2u=\Omega,$$
$$P_v^2-\mathcal{E}_{el}\cosh 2v-2mR\cosh v=-\Omega, \tag{10}$$

where $\mathcal{E}_{el}=R^2E_{el}$. The system is separated into two decoupled oscillators whose phase portraits are shown in Fig. 1. Since the Hamiltonian $\mathcal{F}_0$ is integrable, one can define action-angle variables I_u,ϕ_u,I_v,ϕ_v in the domain of its phase space filled up by two-dimensional invariant tori.

We define the action variables in the following (''natural'') way. For a phase point in Fig. 1(a) moving in the oscillation domain of the phase portrait (''inside'' the separatrix) I_u is the area encircled by its trajectory (i.e., the line of constant $\mathcal{E}_{el}$ and Ω), divided by 2π. For a phase point in Fig. 1(a) moving in the domain of rotation, I_u is the area between the two lines of constant $\mathcal{E}_{el}$, Ω (one of which passes through the point) and lines $u=0$, $u=2\pi$, divided by 4π (so that we avoid a geometric jump in the action by a

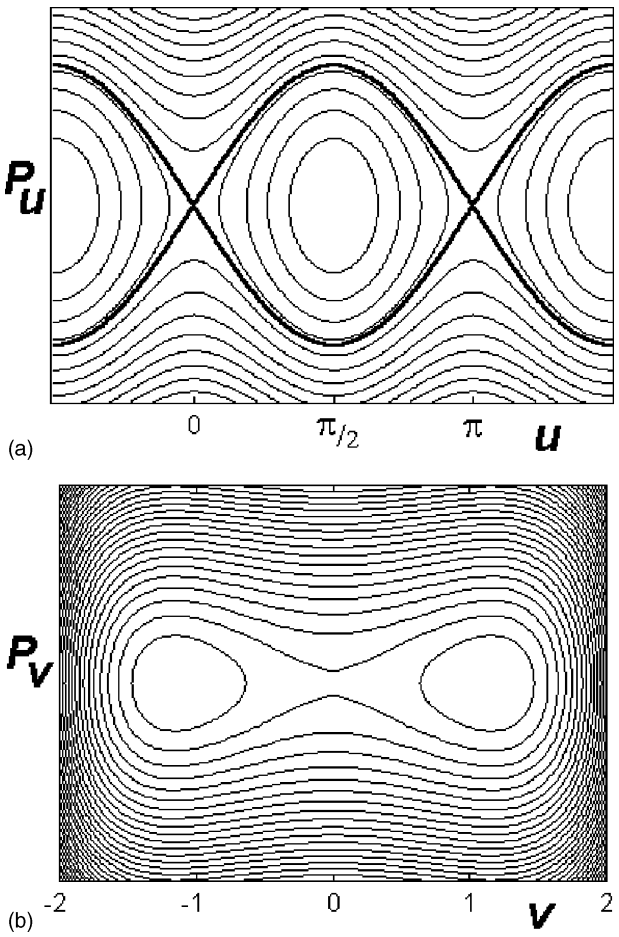

FIG. 1. Phase portraits of the subsystems (10). (a) (P_u,u) plane (b) (P_v,v) plane.

factor of 2 at the separatrix). In the same way the action I_v is introduced. For a phase point in Fig. 1(b) moving in one of the potential wells (inside the separatrix), I_v is the area encircled by its trajectory, divided by 2π. For a phase point in Fig. 1(b) moving around both of the two stable equilibria (''outside'' the separatrix), I_v is the area encircled by its trajectory, divided by 4π. For simplicity actions of the system can be written in the following form:

$$I_u=\frac{1}{2\pi}\oint\sqrt{\Omega-\mathcal{E}_{el}\cos 2u}\,du,$$

$$I_v=\frac{1}{2\pi}\oint\sqrt{-\Omega+\mathcal{E}_{el}\cosh 2v+2mR\cosh v}\,dv, \quad (11)$$

where the symbol ''$\oint$'' takes into account the geometric factor 2 in the different domains of the phase space as described above. The transformation $(P_u,u,P_v,v)\rightarrow(I_u,\phi_u,I_v,\phi_v)$ is canonical and can be performed using a generating function $S(u,v,I_u,I_v,R,P_R,E)$ that contains R,P_R,E as parameters. In the new variables the Hamiltonian $\mathcal{F}_0$ transforms to $\mathcal{H}_0=\mathcal{H}_0(I_u,I_v,P_R,R,E)$. The function S has the form

$$S=\int_{v_0}^{v}\sqrt{-\Omega+\mathcal{E}_{el}\cosh 2x+2mR\cosh x}\,dx+\int_{u_0}^{u}\sqrt{\Omega-\mathcal{E}_{el}\cos 2y}\,dy, \quad (12)$$

where in the first part of right-hand side of Eq. (12) Ω is considered as a function of I_v, whereas in the second part it is considered as a function of I_u [see Eq. (11)]. Initial coordinates u_0 and v_0 are functions of I_u and I_v correspondingly; one can define v_0 as the root of the integrand of I_v, and u_0 as either $\pi/2$ or $3\pi/2$ depending on the domain of motion in Fig. 1(a). Frequencies of the system have the form

$$\omega_v=\frac{\partial\mathcal{H}_0}{\partial I_v}=-\frac{1}{\dfrac{\partial I_v}{\partial\Omega}}=4\pi\left\{\oint\frac{1}{\sqrt{-\Omega+\mathcal{E}_{el}\cosh 2v+2mR\cosh v}}dv\right\}^{-1},$$

$$\omega_u=\frac{\partial\mathcal{H}_0}{\partial I_u}=\frac{1}{\dfrac{\partial I_u}{\partial\Omega}}=4\pi\left\{\oint\frac{1}{\sqrt{\Omega-\mathcal{E}_{el}\cos 2u}}du\right\}^{-1}.$$

Now, following Ref. [16], let us make in the system with Hamiltonian (7) the canonical transformation of the variables

$$(P_u,u,P_v,v,P_R,R)\rightarrow(\bar{I}_u,\bar{\phi}_u,\bar{I}_v,\bar{\phi}_v,\bar{P}_R,\bar{R}) \quad (13)$$

determined by the generating function

$$\frac{1}{\epsilon}\bar{P}_R R+S(u,v,\bar{I}_u,\bar{I}_v,R,\bar{P}_R,E), \quad (14)$$

which contains E as a parameter. The canonically conjugated pairs of new variables are $(\bar{I}_u,\bar{\phi}_u)$, $(\bar{I}_v,\bar{\phi}_v)$, $(\epsilon^{-1}\bar{P}_R,\bar{R})$. Formulas for the transformation of the variables have the form

$$\phi_\alpha=\frac{\partial S}{\partial\bar{I}_\alpha},\quad P_\alpha=\frac{\partial S}{\partial\alpha},\quad \alpha=u,v,$$

$$\bar{R}=R+\epsilon\frac{\partial S}{\partial\bar{P}_R},\quad P_R=\bar{P}_R+\epsilon\frac{\partial S}{\partial R}. \quad (15)$$

Hamiltonian (7) in the new variables has the form [16]

$$\mathcal{H}=\mathcal{H}_0(\bar{I}_u,\bar{I}_v,\bar{P}_R,\bar{R},E)+\epsilon\mathcal{H}_1(\bar{I}_u,\bar{\phi}_u,\bar{I}_v,\bar{\phi}_v,\bar{P}_R,\bar{R},E)+O(\epsilon^2),$$

$$\mathcal{H}_1=\mathcal{F}_1+\frac{\partial\mathcal{F}_0}{\partial P_R}\frac{\partial S}{\partial R}-\frac{\partial\mathcal{H}_0}{\partial R}\frac{\partial S}{\partial\bar{P}_R}. \quad (16)$$

The variables $(\overline{I_u},\overline{\phi_u},\overline{I_v},\overline{\phi_v},\overline{P_R},\overline{R})$ are $O(\epsilon)$- close to the variables $(I_u,\phi_u,I_v,\phi_v,P_R,R)$. Henceforth, the bars over the new variables are omitted and the new Hamiltonian is

$$\mathcal{H}=\mathcal{H}_0(I_u,I_v,P_R,R,E)+\epsilon\mathcal{H}_1(I_u,\phi_u,I_v,\phi_v,P_R,R,E)+O(\epsilon^2). \tag{17}$$

The differential equations of the motion have the form

$$\dot{I}_\alpha=-\epsilon\frac{\partial\mathcal{H}_1}{\partial\phi_\alpha}+O(\epsilon^2),$$

$$\dot{\phi}_\alpha=\omega_\alpha(I_u,I_v,P_R,R,E)+\epsilon\frac{\partial\mathcal{H}_1}{\partial I_\alpha}+O(\epsilon^2),\quad \alpha=u,v,$$

$$\dot{P}_R=-\epsilon\frac{\partial\mathcal{H}_0}{\partial R}-\epsilon^2\frac{\partial\mathcal{H}_1}{\partial R}+O(\epsilon^3),$$

$$\dot{R}=\epsilon\frac{\partial\mathcal{H}_0}{\partial P_R}+\epsilon^2\frac{\partial\mathcal{H}_1}{\partial P_R}+O(\epsilon^3). \tag{18}$$

Averaging of the right-hand sides of Eq. (18) over ϕ_α and discarding terms $O(\epsilon^2)$ gives an averaged system

$$\dot{I}_\alpha=0,\quad \dot{P}_R=-\epsilon\frac{\partial\mathcal{H}_0}{\partial R},\quad \dot{R}=\epsilon\frac{\partial\mathcal{H}_0}{\partial P_R}. \tag{19}$$

Approximation (19) is called an adiabatic approximation [16,18]. Trajectories of the system (19) are called adiabatic trajectories. In the adiabatic approximation $I_{u,v}=$ const. The adiabatic approximation breaks down in a vicinity of resonant surfaces which are defined by a resonance condition $k_u\omega_u+k_v\omega_v=0$ (k_u,k_v are integers) and near separatrices where either ω_u or ω_v equals to zero. In the full (nonaveraged) system variables I_α are approximate adiabatic invariants, i.e., they are well conserved in a large area of phase space (far from resonant surfaces and separatrices). Although resonant surfaces are dense in the phase space of our three-dimensional Hamiltonian system, for small ϵ only finite number of low-order resonances are important (the order of an resonance is the value of $k=|k_u|+|k_v|$) [16]. If an adiabatic trajectory crosses an resonant surface in the averaged system, it cross the surface at the same point periodically in time (because the averaged system is a one-dimensional Hamiltonian system for P_R,R and therefore is integrable). Note that in Eq. (7) $P_\Theta=\epsilon L$, so the terms containing P_Θ are important only in case of very high L (fast rotation). If $L\sim 1$, the perturbation $\mathcal{F}_1$ is separated in (u,v): the Hamiltonian (7) with frozen P_R,R and with terms $O(\epsilon^2)$ omitted is integrable. That enables one to introduce ''improved'' adiabatic invariants $I_u^{(1)},I_v^{(1)}$ as the actions of the Hamiltonian $\mathcal{F}_0+\epsilon(P_R/2R)(P_u\sin 2u-P_v\sinh 2v)$ [see Eq. (7)]. Formulas for them have the form

$$I_u^{(1)}=\frac{1}{\pi}\int_{u_{min}}^{u_{max}}\sqrt{\Omega^{(1)}-\mathcal{E}_{el}\cos 2u+\frac{\epsilon^2}{16}P_R^2R^2\sin^2 2u}\,du,$$

$$I_v^{(1)}=\frac{1}{\pi}\int_{v_{min}}^{v_{max}}\sqrt{-\Omega^{(1)}+\mathcal{E}_{el}\cosh 2v+2mR\cosh v+\frac{\epsilon^2}{16}P_R^2R^2\sinh^2 2v}\,dv, \tag{20}$$

where

$$P_u^2+\mathcal{E}_{el}\cos 2u+\frac{\epsilon}{2}P_RRP_u\sin 2u=\Omega^{(1)},$$

$$P_v^2-\mathcal{E}_{el}\cosh 2v-2mR\cosh v-\frac{\epsilon}{2}P_RRP_v\sinh 2v=-\Omega^{(1)}. \tag{21}$$

The variables I_α [Eq. (11)], $I_\alpha^{(1)}$, and $\overline{I_\alpha}(\alpha=u,v)$ are $O(\epsilon)$-close to each other. Variations of $I_\alpha^{(1)}$ far from low-order resonant surfaces are of order of ϵ, nevertheless, they are sufficiently smaller than those of I_α because the perturbation is partly included into the unperturbed Hamiltonian.

The phenomena of scattering on a resonance and capture into a resonance being described below lead to changes in $\overline{I_\alpha}$, which scale as $O(\sqrt{\epsilon})$ and $O(1)$ correspondingly. So that for numerical investigations of these resonant phenomena either of variables $I_\alpha,I_\alpha^{(1)},\overline{I_\alpha}$ could be used, but the variables $I_\alpha^{(1)}$ are more convenient and in the figures below dynamics of $I_\alpha^{(1)}$ is demonstrated [with indexes (1) being omitted]. At the same time, in the analytical expressions in the text below the variables $\overline{I_\alpha}$ are investigated, and bars in the formulas are omitted.

III. DYNAMICS IN A VICINITY OF RESONANCES

Consider dynamics of the system in a resonance region following Ref. [16]. Near a resonant surface of a given resonance the system (18) can be transformed into standard ''perturbed pendulumlike system'' form. This transformation is carried out in a $O(\sqrt{\epsilon})$- neighborhood of the resonant surface. For a given pair of resonance indexes (k_u,k_v) there exist integers l_u,l_v such that $k_ul_v-k_vl_u=1$. Let us make a

canonical transformation of the variables $(I_u, I_v, \phi_u, \phi_v) \rightarrow (K, J, \gamma, \psi)$ using formulas

$$\gamma = k_u \phi_u + k_v \phi_v, \quad K = l_v I_u - l_u I_v,$$

$$\psi = l_u \phi_u + l_v \phi_v, \quad J = -k_v I_u + k_u I_v. \tag{22}$$

Variables P_R, R remain unchanged under this transformation. The transformation (22) produces slow (γ) and fast (ψ) phases from initial phases ϕ_u, ϕ_v in the vicinity of (k_u, k_v)-resonance. Such transformations are often used in systems with slow and fast variables [18]. The new Hamiltonian has the form

$$\mathcal{H} = \mathcal{H}_0(K, J, P_R, R) + \epsilon \mathcal{H}_1(K, J, \gamma, \psi, P_R, R) + O(\epsilon^2). \tag{23}$$

(We keep old notations for the Hamiltonian in the new variables.) The new phase $\gamma = k_u \phi_u + k_v \phi_v$ is called a resonant phase. In a resonant zone the resonant phase γ changes slowly and ψ changes rapidly; $\dot{\gamma} \sim \sqrt{\epsilon}, \dot{\psi} \sim 1$. So that we can perform the averaging of the Hamiltonian over ψ [16,18]. To this end, we should perform in the resonant zone a canonical transformation of variables

$$(K, J, \gamma, \psi, P_R, R) \rightarrow (\overline{K}, \overline{J}, \overline{\gamma}, \overline{\psi}, \overline{P}_R, \overline{R}), \tag{24}$$

which is close to identity in (K, J, γ, ψ) by $O(\epsilon)$ and close to identity in (P_R, R) by $O(\epsilon^2)$ [16]. In the new variables the Hamiltonian has the form (bars over new variables are omitted)

$$\mathcal{H} = \mathcal{H}_0(K, J, P_R, R) + \epsilon \overline{\mathcal{H}_1}(K, J, \gamma, P_R, R) + O(\epsilon^2). \tag{25}$$

Here, $\overline{\mathcal{H}_1}$ is the average of $\mathcal{H}_1|_{\epsilon=0}$ over ψ (or, equivalently, the sum of the resonant harmonics in the Fourier series expansion for $\mathcal{H}_1|_{\epsilon=0}$ [16]). The differential equation for J has now the form

$$\dot{J} = O(\epsilon^2). \tag{26}$$

Therefore, J is well conserved in the resonant zone [its variation during a time $O(1/\epsilon)$ in a resonant zone is $O(\epsilon)$]. The resonant surface is defined now by the equation $\partial \mathcal{H}_0 / \partial K = 0$. Let us assume that condition $\partial^2 \mathcal{H}_0 / \partial K^2 \neq 0$ is fulfilled on this surface. Then, locally the equation of the resonant surface can be represented in the form $K = a(P_R, R, J)$. An expansion of $\mathcal{H}$ near the resonant surface yields [16]

$$\mathcal{H} = \Lambda(P_R, R, J) + \frac{1}{2} g(P_R, R, J)[K - a(P_R, R, J)]^2 + \epsilon f(\gamma, P_R, R, J) + O_\gamma(|K - a|^3 + \epsilon |K - a|) + O(\epsilon^2). \tag{27}$$

Here, Λ, f, g are restrictions of $\mathcal{H}_0, \overline{\mathcal{H}_1}, \partial^2 \mathcal{H}_0 / \partial K^2$ to the resonant surface. Index γ in $O_\gamma(\cdot)$ indicates functions that do not depend on ψ. Performing a simple transformation described in Ref. [16], we obtain that dynamics in the resonant region is determined by the Hamiltonian

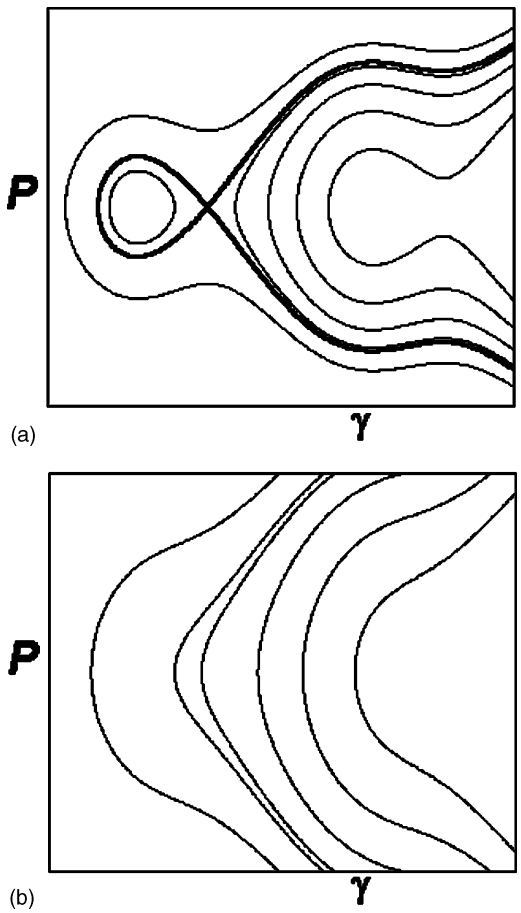

FIG. 2. Typical phase portraits of the Hamiltonian F_0 from Eq. (28). From left to right: (a) The phase portraits have an oscillatory domain [the inequality $\min_\gamma(\partial f/\partial\gamma) < -b < \max_\gamma(\partial f/\partial\gamma)$ is satisfied]. (b) There is no such a domain on the phase portrait.

$$F = \epsilon^{-1} \Lambda(P_R, R, J) + F_{01}(P, \gamma, P_R, R, J) + O(\epsilon),$$

$$F_{01} = F_0 + O_\gamma(\sqrt{\epsilon}),$$

$$F_0 = \frac{1}{2} g(P_R, R, J) P^2 + f(\gamma, P_R, R, J) + b(P_R, R, J)\gamma, \tag{28}$$

where $b = \{a, \Lambda\}$ ($\{\cdot\}$ means Poisson brackets), canonically conjugated variables are (P, γ), $(\epsilon^{-3/2} P_R, R)$, and $(J, \epsilon^{-1/2}\psi)$ (a new time $\theta = \sqrt{\epsilon} t'$ was introduced). Approximate equations of motions have the following form [16]:

$$P_R' = -\sqrt{\epsilon} \frac{\partial \Lambda}{\partial R}, \quad R' = \frac{\partial \Lambda}{\partial P_R},$$

$$P' = -\frac{\partial F_0}{\partial \gamma}, \quad \gamma' = \frac{\partial F_0}{\partial P},$$

$$J = \text{const}, \tag{29}$$

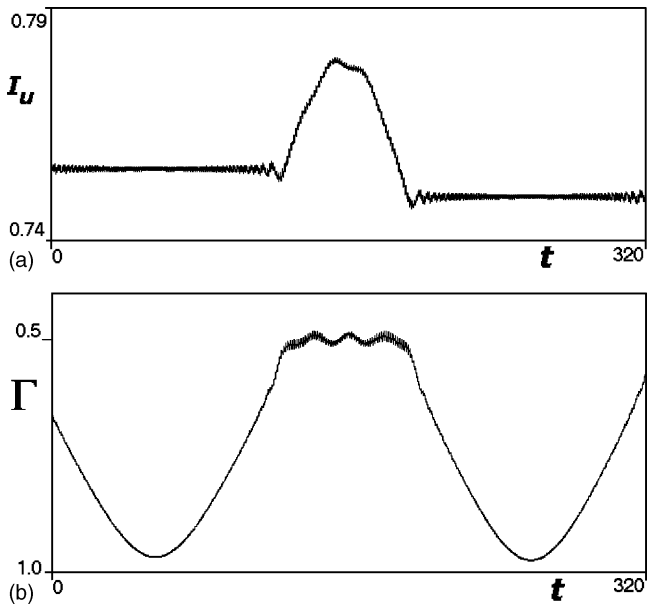

FIG. 3. Capture of a phase point into a (2,1) resonance and escape from the resonance. The captured point moves along a resonant curve in the phase space until it escapes from the resonance. Parameters of the system: $m=1$, $M=24000$, $P'_\Theta=0.4$, $E=-2.62$. From top to bottom: (a) Dynamics of the adiabatic invariant I_u. (b) Dynamics of the frequencies ratio $\Gamma=\omega_u/\omega_v$.

where primes denote differentiating over new time θ. Hence, evolution of slow variables P_R, R is governed by a Hamiltonian system; the Hamiltonian $\sqrt{\epsilon}\Lambda(P_R,R,J)$ of this system depends on the parameter J. This system determines the flow on the resonant surface, which is called "a resonant flow" [16]. Behavior of P,γ is governed by the Hamiltonian $F_0(P,\gamma,P_R,R,J)$. This Hamiltonian depends on the parameter $J=$const and on the slowly varying parameters P_R,R. Consider subsystem for P,γ in Eq. (29) with frozen P_R,R. We get a Hamiltonian system with one degree of freedom which is called a pendulumlike system because the Hamiltonian F_0 resembles a Hamiltonian of a pendulum under the action of a constant torque [16](for a pendulum $F_0=\frac{1}{2}gP^2-\cos\gamma+b\gamma$). There are two basic types of the phase portraits of the Hamiltonian F_0: with oscillation regions and without such regions. If in Eq. (28) $\min_\gamma(\partial f/\partial\gamma)<-b<\max_\gamma(\partial f/\partial\gamma)$, then there are stable and unstable stationary points on the phase portrait. The separatrices of the unstable stationary points enclose the oscillation regions. If this inequality is not satisfied, there are no oscillation regions. Typical phase portraits are presented in Fig. 2.

Motion in oscillation regions correspond to captured into a resonance motion of phase points. Motion outside such regions (motion in the rotation region) correspond to the phase points that cross the resonant zone without being captured. Now let us take into account slow change of the parameters P_R,R along the resonant flow in system (29). Let the area of an oscillation region grow along the resonant flow. Then additional space appears inside the oscillation region. Due to conservation of phase volume in Hamiltonian systems, this space will not be occupied by the phase points that were captured into resonance earlier. Therefore, some

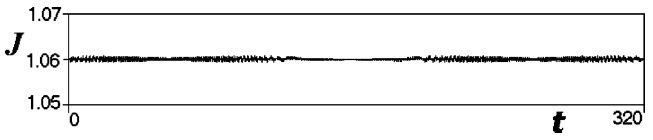

FIG. 4. Dynamics of the adiabatic invariant J. Parameters and initial conditions are the same as in Fig. 3.

phase points of Eq. (29) cross a separatrix of the phase portrait of F_0, and change the regime of motion from a rotation to an oscillation. This means capture into resonance. If area of an oscillation region decreases along the resonant flow, then phase points leave this oscillation region and leave the resonant zone. This is escape from the resonance. We found these phenomena in numerical investigations of the system (7). The results are demonstrated in Fig. 3, where capture into a (2,1) resonance and escape from the resonance are shown. The same phenomenon was investigated recently in Refs. [23,25,26]. For a three-body Coulomb system similar to a hydrogen molecular ion, the phenomenon of capture into a resonance is numerically demonstrated and analytically explained. While moving in oscillating region the captured phase point has two adiabatic invariants [16] : J and "action" variable ρ for the pendulumlike system in the oscillat-

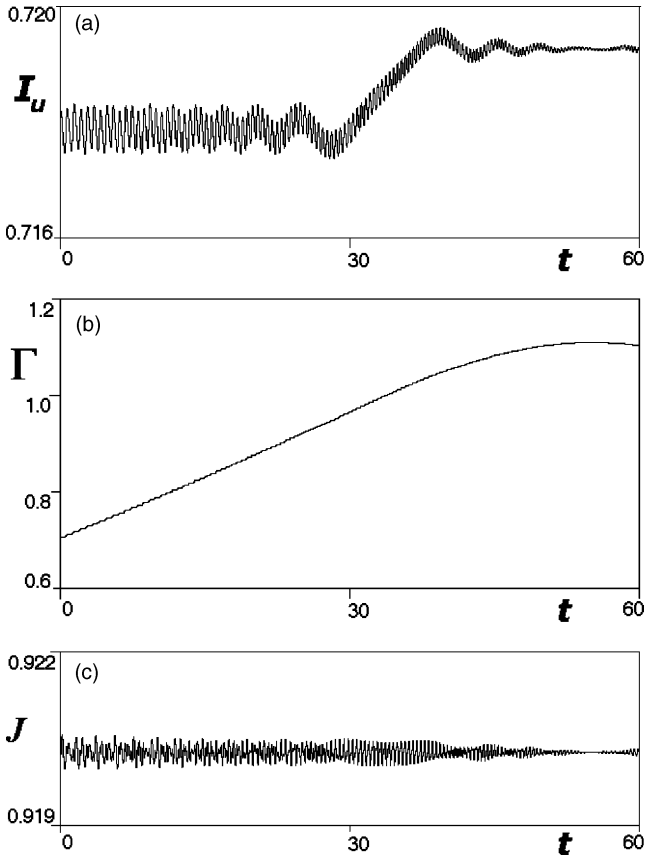

FIG. 5. A single jump of the adiabatic invariant I_u on a (1,1) resonance. Parameters of the system: $m=1$, $M=24000$, $P'_\Theta=0.001$, $E=-2.786$. From top to bottom: (a) Dynamics of the adiabatic invariant I_u. (b) Dynamics of the frequencies ratio $\Gamma=\omega_u/\omega_v$. (c) Dynamics of the adiabatic invariant J.

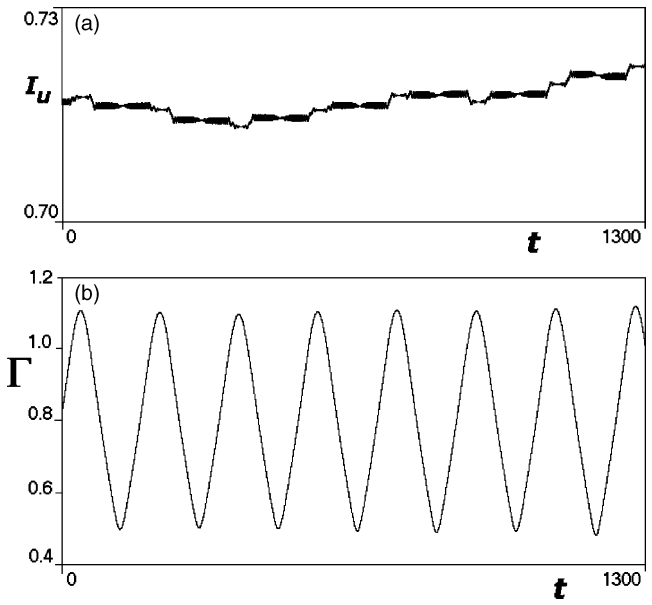

FIG. 6. Jumps of the adiabatic invariant I_u. Parameters of the system: $m=1$, $M=24000$, $P'_\Theta=0.001$, $E=-2.786$. From top to bottom: (a) Dynamics of the adiabatic invariant I_u. (b) Dynamics of the frequencies ratio $\Gamma=\omega_u/\omega_v$.

ing region [i.e., the area on (P,γ) plane encircled by a line of constant F_0 passing through the phase point, divided by 2π].

The goodness of conservation of the adiabatic invariant J is demonstrated in Fig. 4. The goodness of conservation of the ''internal'' adiabatic invariant ρ in a similar problem was demonstrated numerically in Ref. [23].

Phase points that cross the resonance without being captured undergo a jump of adiabatic invariant K of order $\sqrt{\epsilon}$ [16] and, therefore, jumps of $I_{u,v}$ (since $I_u=k_uK+l_uJ$, $I_v=k_vK+l_vJ$, and the magnitude of J is well conserved during passage through the resonance). This phenomenon is called a *scattering on a resonance*. We present corresponding results of numerical investigations of the system (7) in Fig. 5, where a single jump of the adiabatic invariant I_u on a (1,1) resonance is shown, and Fig. 6, where several jumps are shown. Although there are passages through other resonances in Fig. 6, including (3,5) resonance, they are not visible in the figure (there are no distinguishable jumps of the adiabatic invariants on the other resonances). The reason for this is fast decay of the resonant harmonics of $\overline{\mathcal{H}_1}$ in Eq. (25) with increasing the order of a resonance (see Ref. [16]). In the adiabatic approximation a value of the unperturbed frequencies ratio $\Gamma=\omega_u/\omega_v$ evolves periodically in time. In Fig. 6(b) small deviations from periodicity can be seen.

Both capture into a resonance and scattering on a resonance are probabilistic phenomena, and they are usual in systems with resonance crossings (see Refs. [16,18,25,26]). For a phase point approaching the resonance the probability to be captured is a value of order of $\sqrt{\epsilon}$. So, a phase point in (I_u,I_v,P_R,R) space moves in a following way: while it is far from low-order resonant surfaces $k_u\omega_u(I_u,P_R,R)+k_v\omega_v(I_v,P_R,R)=0$ and separatrices, it moves in a vicinity of an adiabatic curve $I_{u,v}=\text{const}$. When it nears a resonant surface (enters a resonant zone), it leaves the adiabatic curve and can be either captured into the resonance or pass through the resonance region without capture. In the case of capture the phase point continues to move in the vicinity of a resonant surface until it becomes ejected from the resonance. For the captured phase point, variables R,P_R evolve along a resonant flow trajectory $\{\overline{R}(\epsilon t),\overline{P}_R(\epsilon t)\}$ so the area $\mathcal{S}$ of the oscillating region slowly evolves as $\mathcal{S}(\overline{R}(\epsilon t),\overline{P}_R(\epsilon t))$. In the first-order approximation $\rho=\text{const}$ along the trajectory of the phase point in the oscillation region. At the time of capture into the oscillating region $2\pi\rho=\mathcal{S}(R,P_R)$. The phase point will be ejected from the oscillating region when $\mathcal{S}(R(\epsilon t),P_R(\epsilon t))$ is equal to $2\pi\rho$ again, so the times of capture and escape from the resonance are two nearby roots of the equation $\mathcal{S}(\overline{R}(\epsilon t),\overline{P}_R(\epsilon t))=2\pi\rho$ [16]. Along the captured phase trajectories, adiabatic invariants I_α may change by values of order 1.

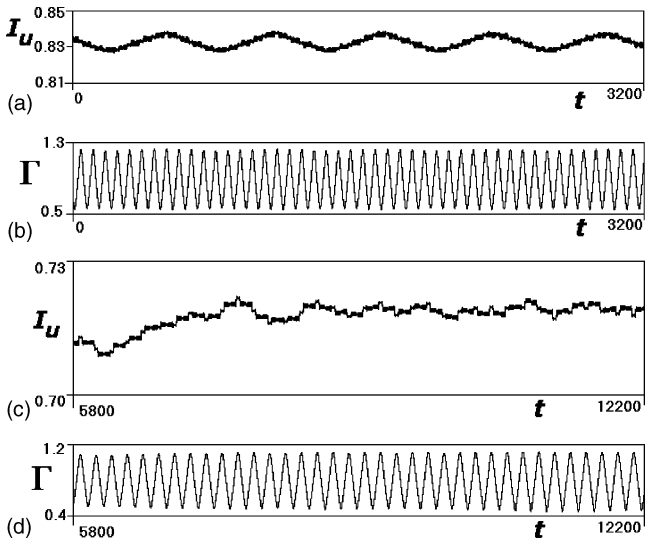

FIG. 7. Regular and diffusionlike behavior of approximate adiabatic invariants. From top to bottom: (a) Regular dynamics of the adiabatic invariant I_u. Parameters of the system, $m=1$, $M=2000$, $P'_\Theta=0.05$, $E=-2.84$. Initial values of adiabatic invariants; $I_u=8.34\times10^{-1}$, $I_v=6.36\times10^{-2}$. (b) Dynamics of the frequencies ratio $\Gamma=\omega_u/\omega_v$ [parameters and initial conditions are the same as in (a)]. (c) Diffusionlike dynamics of the adiabatic invariant I_u. Parameters of the system; $m=1$, $M=24000$, $P'_\Theta=0.001$, $E=-2.786$. Initial values of adiabatic invariants; $I_u=7.17\times10^{-1}$, $I_v=1.44\times10^{-1}$. (d) Dynamics of the frequencies ratio $\Gamma=\omega_u/\omega_v$ [parameters and initial conditions are the same as in (c)].

For the captured phase point, variables R,P_R evolve along a resonant flow trajectory $\{\overline{R}(\epsilon t),\overline{P}_R(\epsilon t)\}$ so the area $\mathcal{S}$ of the oscillating region slowly evolves as $\mathcal{S}(\overline{R}(\epsilon t),\overline{P}_R(\epsilon t))$. In the first-order approximation $\rho=\text{const}$ along the trajectory of the phase point in the oscillation region. At the time of capture into the oscillating region $2\pi\rho=\mathcal{S}(R,P_R)$. The phase point will be ejected from the oscillating region when $\mathcal{S}(R(\epsilon t),P_R(\epsilon t))$ is equal to $2\pi\rho$ again, so the times of capture and escape from the resonance are two nearby roots of the equation $\mathcal{S}(\overline{R}(\epsilon t),\overline{P}_R(\epsilon t))=2\pi\rho$ [16]. Along the captured phase trajectories, adiabatic invariants I_α may change by values of order 1.

In the case of passing through the resonant region without capture the adiabatic invariants I_u,I_v of the phase point undergo jumps $\sim\sqrt{\epsilon}$, and after passage through the resonant zone the particle continues to move along other adiabatic curve.

Performing numerical investigations of the system (7), we have observed phenomena of scattering on resonances for systems with particle mass ratio m/M ranging from 10^{-3} to 10^{-7}, both in systems with $L=0$ and $L\neq0$. So far we have observed the phenomena of capture into a resonance only in systems with $L\neq0$.

In the present paper, we investigate passages of phase

points of our system through resonances, but not separatrices. Separatrix crossings may also lead to breakdown of adiabatic invariance [27]. It is known that in systems with two degrees of freedom behavior of the breakdown of adiabaticity near separatrices is different from that near resonances (see Refs. [19,20,27,28]). For multidimensional systems, there is presently no rigorous theory of dynamics of adiabatic invariants at separatrix crossings. We are going to investigate separatrix crossings in the TBC problem in a separate paper.

We would like to mention that systems with passages through resonances were investigated also in a different way in Refs. [29,30] (see also references therein).

IV. LONG-TIME DYNAMICS

In accordance with Ref. [16], the actions $I_{u,v}$ are almost adiabatic invariants over the time interval $(0,O(1/\epsilon))$ (which is of order of a typical period of nuclei oscillations). On longer time intervals adiabatic invariance is destroyed for the majority of initial conditions due to captures into resonances and scattering on resonances. Consider this topic using the estimates given in Ref. [16], which explain destruction of adiabatic invariance in a large part of the phase space of systems with passage through a single resonance. Consider a stable periodic adiabatic trajectory $\mathcal{P}$ of our system that crosses a low-order resonant surface. Let us neglect influence of all other resonant surfaces. A phase point that moves near $\mathcal{P}$ crosses the resonant surface repeatedly. Let us also suppose that the probability of capture into the resonance is equal to 0 at the points of intersection of $\mathcal{P}$ with the resonant surface.

An asymptotic formula for the jump of the adiabatic invariant K has the following form [16]:

$$\Delta K = 2\sqrt{\epsilon} s \int_{\pm\infty}^{\gamma^*} \frac{(\partial f/\partial \gamma) d\gamma}{\sqrt{2g[h_* - f(\gamma, P_{R_*}, R_*, J) - b\gamma]}} + O(\epsilon), \tag{30}$$

where P_{R_*}, R_* are the values of slow variables at the point of intersection of the adiabatic trajectory $\mathcal{P}$ with the resonant surface; γ_* denote the value of γ at the point of intersection of the exact trajectory with the resonant surface; h_* is the value of the Hamiltonian F_0 at the resonant surface [i.e., $h_* = f(\gamma_*, P_{R_*}, R_*, J) + b\gamma_*$]; the sign in $\pm\infty$ is given by $s = -\mathrm{sgn}(bg)$. Consider two successive crossings with the resonant surface. Let these crossings occur at values of the resonance phase $\gamma_* = \gamma_1$ and $\gamma_* = \gamma_2$ correspondingly.

Now a small variation $\delta\gamma_1$ of γ_1 produces the variation of the jump value of K: $\delta\Delta K \sim \sqrt{\epsilon}\delta\gamma_1$. As a result, the time period between two crossings changes by $\delta t \sim \delta\Delta K/\epsilon$, producing a variation $\delta\gamma_2 \sim \delta\Delta K/\epsilon$. Hence, we get $\delta\gamma_2 \gg \delta\gamma_1$ and values of γ_1 and γ_2 can be considered as independent. The jump value of K is the function of γ_* and is also the probabilistic value (see Ref. [16] for details). Jumps of K at resonance crossings can be considered as random walks with steps of order $\sqrt{\epsilon}$. Accumulation of such jumps produces a diffusion [see Fig. 7(c)].

For some initial points the above-mentioned estimates are not valid (the measure of such initial points is small for systems with a single resonance [16]).

We have found an interesting example of regular dynamics of actions I_α in our system (see Fig. 7). Consequent jumps of I_α are correlated in such a way that I_α evolve along periodic in time curves. This regime is effectively stable: it lasts for thousands of nuclei oscillations at least. However, then a value of ϵ is lessen, dynamics of the phase point (with the same initial conditions) becomes irregular, like in Fig. 7(c).

We are going to investigate long-time dynamics of the adiabatic invariants in the system more thoroughly in future studies. Note that an accurate description of statistical properties of jumps of adiabatic invariants in multiresonance systems is still the unsolved question.

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