Change in the adiabatic invariant in a nonlinear two-mode model of Feshbach resonance passage.

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Mean-field approach has recently been used to model coupled atom-molecular Bose-Einstein condensates (BEC) and coupled Fermi-Bose condensates near Feshbach resonance. Sweeping of magnetic field across the resonance gives a new (nonlinear) version of Landau-Zener problem. We investigate the structure of the corresponding classical phase space and calculate change in the action which corresponds to finite-rate efficiency of the sweep. We consider the case of non-zero initial action, which corresponds to some finite initial molecular fraction.

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I. INTRODUCTION

Adiabatic invariance is very important issue in quantum mechanics [1, 2]. Relation between slow quantum transitions and change in the adiabatic invariant of a linear oscillator has been studied in [3]. Dynamics of Bose-Einstein condensates [4–9] introduces a paradigm of nonlinearity into quantum systems. In many mean-field models related to BEC physics (like nonlinear Landau-Zener models [10, 11], macroscopic quantum self-trapping [12], etc), nonlinear effects that are common to classical nonlinear systems have been revealed. A conceptual phenomenon of classical adiabatic theory is destruction of the adiabatic invariance at separatrix crossings [13] which is encountered in different fields of physics. It is of great importance for BEC physics because change in the classical action of a nonlinear two-state model corresponds to probability of transition between the two states (modes). Here we consider a nonlinear mean-field model of a slow sweep through a Feshbach resonance in a quantum gas of fermionic atoms coupled to BEC of diatomic molecules [14] (for brevity, we call this system a Bose-Fermi condensate). A number of closely related non-stationary problems have come up recently in context of coupled Bose-Fermi condensates ([14–16]) and coupled atom-molecular BEC [17–19]). The mean-field approach to such problems is very interesting and not at all trivial [16]. In [16] the following Hamiltonian describing a fermion-boson condensate is considered:

$$\hat{H} = \sum_{j,\sigma} \varepsilon_j \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma} + \omega \hat{b}^\dagger \hat{b} + g \sum_j \left(\hat{b}^\dagger \hat{c}_{j\downarrow} \hat{c}_{j\uparrow} + \hat{b} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \right), \tag{1}$$

where ε_j are the single-particle energy levels and the operators $\hat{c}_{j\sigma}^\dagger$ $(\hat{c}_{j\sigma})$ create (annihilate) a fermion of one of the two species $\sigma = \uparrow$ or $\downarrow$ in an orbital eigenstate of energy ε_j. In case the single-particle potential is translationally invariant, $|j \uparrow\rangle = |\mathbf{k} \uparrow\rangle$ and $|j \downarrow\rangle = |-\mathbf{k} \downarrow\rangle$ [16]. Operators $\hat{b}^\dagger$ $(\hat{b})$ create (annihilate) quanta of the bosonic field.

The mean-field approximation of (1) amounts to treating the bosonic field classically, i.e. replacing operators $\hat{b}^\dagger$ and $\hat{b}$ with c-numbers in the Heisenberg equations of motion.

This procedure is justified provided the bosonic mode is macroscopically populated. As shown in [16], in this approximation the dynamics of (1) coincides with that of a classical Hamiltonian system (where classical dynamical variables are the time-dependent quantum-mechanical expectation values $\langle \hat{c}_{j\downarrow} \hat{c}_{j\uparrow} \rangle$, $\langle \hat{b} \rangle$, and $\langle \sum_\sigma \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma} \rangle$). The mean-field approximation is also equivalent to replacing operators with classical variables and their commutators with Poisson brackets. It is also shown in [16] that the fermion-oscillator model (1) can be viewed as a generalization of the Dicke (Tavis-Cummings [20]) model of Quantum Optics: the latter model corresponds to zero fermionic bandwidth limit of (1), i.e. to the case when all single-particle levels ε_j are degenerate, $\varepsilon_j = \mu$. To demonstrate this, [16] reformulates (1) as a spin-oscillator model using Anderson's pseudospins (i.e.,

$$2\hat{K}_j^z = \hat{n}_j - 1, \qquad \hat{K}_j^- = \hat{c}_{j\downarrow} \hat{c}_{j\uparrow}, \qquad \hat{K}_j^+ = \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger, \text{ where } \hat{n}_j = \sum_\sigma \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma}), \text{ and obtains the}$$

Hamiltonian

$$\hat{H} = \sum_{j=0}^{n-1} 2\varepsilon_j \hat{K}_j^z + \omega \hat{b}^\dagger \hat{b} + g \sum_{j=0}^{n-1} \left(\hat{b}^\dagger \hat{K}_j^- + \hat{b} \hat{K}_j^+ \right). \tag{2}$$

In the zero bandwidth ("degenerate") limit the Hamiltonian (2) reduces to the Dicke model

$$\hat{H}_{Dicke} = 2\mu \hat{T}_z + \omega \hat{b}^\dagger \hat{b} + g(\hat{b}^\dagger \hat{T}_- + \hat{b} \hat{T}_+), \tag{3}$$

describing an interaction of a single collective spin $\hat{\mathbf{T}} = \sum_j \hat{\mathbf{K}}_j$ with a harmonic oscillator. Mean-field solution of (3) was discussed in [21, 22]. The more general many-body problem (1,2) also turns out to be integrable. Explicit solutions for the mean-field dynamics of the model (1,2) were constructed in [15]. Later, comprehensive solutions for the mean-field dynamics were obtained in [16] using a method of separation of variables [23–25], which allowed to derive a complete set of integrals of motion for (1,2). Quantum solutions of (1) can be obtained by the Bethe ansatz [26, 27]. In [28], quantum model (1) and a more general version which includes s-wave scattering interactions were solved using the boundary quantum inverse scattering method (QISM) as developed by Sklyanin [29];

interesting enough, through the exact solution, the spectrum can be mapped into that of a Schrodinger equation.

In the present paper, we deal only with the mean-field dynamics. The mean-field solutions of [16] describe dynamics of the system that has been prepared in a nonequilibrium state at $t = 0$. To model Feshbach resonance passage converting Fermi atoms to Bose molecules, one may use the model (1) with time-dependent ω. For example, in [14], the model (1) with zero fermionic bandwidth and time-dependent molecular energy was considered using another approach (similar to that of [17]). To be more precise, [14] considers the Hamiltonian $H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \mathcal{E}(t) b_0^{\dagger} b_0 + g \left(\sum_{\mathbf{k}} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow} b_0^{\dagger} + H.c. \right)$, with $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ being the kinetic energy of an atom with mass m, in the degenerate limit where $\epsilon_{\mathbf{k}} = \varepsilon$ for all $\mathbf{k}$. Introducing operators $J_- = \frac{b_0^{\dagger} \sum_{\mathbf{k}} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow}}{(N/2)^{3/2}}$, $J_+ = \frac{\sum_{\mathbf{k}} c_{-\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k},\uparrow}^{\dagger} b_0}{(N/2)^{3/2}}$, $J_z = \frac{\sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} - 2b_0^{\dagger} b_0}{N}$, where $N = 2b_0^{\dagger} b_0 + \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma}$ is the conserved total number of particles, one gets (after certain rescalings) [14] the Heisenberg equations of motion for the association of a quantum-degenerate gas of fermions,

$$
\begin{aligned}
\frac{d}{d\tau} J_x &= -\delta(\tau) J_y \\
\frac{d}{d\tau} J_y &= \delta(\tau) J_x + \frac{3\sqrt{2}}{4} \left(J_z - 1 \right) \left(J_z + \frac{1}{3} \right) - \frac{\sqrt{2}}{N} \left(1 + J_z \right), \\
\frac{d}{d\tau} J_z &= \sqrt{2} J_y,
\end{aligned}
\tag{4}
$$

which depend on the single parameter $\delta(\tau) = (\mathcal{E}(t) - 2\varepsilon)/\sqrt{N} g$. Mean-field limit of (4) is obtained by replacing $J_{x,y,z}$ with their expectation values u, v, w, and omitting the quantum-noise term $\frac{\sqrt{2}}{N} [1 + J_z]$ (which is justified since the mean-field approximation is valid only up to terms of order $1/\sqrt{N}$; the mean-field approach to Feschbach resonance passage is discussed in [30, 31]). The resulting system of equations ($\dot{u} = -\delta(\tau) v$, $\dot{v} = \delta(\tau) u + \frac{\sqrt{2}}{4}(w-1)(3w+1)$, $\dot{w} = \sqrt{2} v$) is analyzed in detail in the present paper (similar models arise in two-mode approximation for coupled atom-molecular BEC [17–19]; also, a three-mode model considered in [32] at certain conditions has very similar phase portraits).

We consider the model of [14], concentrating on the case of non-zero initial molecular

fraction. Within the model, change in the action at the resonance passage gives the remnant atomic fraction as a power-law of a sweeping rate parameter (instead of the exponential law [33] of Landau-Zener linear model). Classical adiabatic theory [13] provides a method to calculate change in the actions in nonlinear systems. It is a well-known fact that action is an adiabatic invariant in a Hamiltonian system that depends on a slowly varying parameter. This result is based on the possibility of averaging over fast motion in the unperturbed [frozen at a certain parameter value] system. The situation is somehow different if the unperturbed system has separatrices on its phase portrait. As the parameter varies, the separatrices slowly evolve on the phase portrait. In particular, the area surrounded by a separatrix may change. Hence, a phase trajectory of the exact system may cross the separatrix of the frozen system. On the separatrix, the period of motion is equal to infinity. This results in breakdown of the averaging method and in this case more accurate study is necessary to describe behavior of the action. It turns out that at the crossing a quasi-random jump in the value of the adiabatic invariant occurs. The asymptotic formula for this jump in a Hamiltonian system depending on a slowly varying parameter was obtained in [34–36]. Later, the theory of adiabatic separatrix crossings was also developed for slow-fast Hamiltonian systems [37], volume preserving systems [38], and was applied to certain physical problems (see, for example, [39–41]). In this paper we use the methods of [36] to obtain a variation of the adiabatic invariant at the separatrix crossing. A separate paper [11] considers four different nonlinear two-mode models related to BEC physics, concentrating on classical non-adiabatic phenomena, and predicts new nonlinear effects there. Section II of the present paper introduces the model and discusses the structure of the classical phase space, while Section III contains calculations of the change of the adiabatic invariant at the resonance passage.

II. MAIN EQUATIONS AND PHASE PORTRAITS

We consider the classical Hamiltonian

$$H = \delta(\tau)w + (1 - w)\sqrt{1 + w}\cos\phi \tag{5}$$

with a slowly varying parameter δ. Such model appears as a mean-field limit of two-mode approximation of coupled atomic and diatomic-molecular Bose-Einstein condensates [17–19] and in the mean-field treatments of coupled degenerate gas of Fermi atoms and BEC of molecules, as discussed in the Introduction. In the latter case, Feshbach resonance passage can be modelled by sweeping the parameter δ, and corresponding change in the classical action is related to the remnant atomic fraction after the sweep.

The system can also be investigated using the equations of motion for a generalized Bloch vector [14]:

$$
\begin{aligned}
\dot{u} &= -\delta(\tau)v, \\
\dot{v} &= \delta(\tau)u + \frac{\sqrt{2}}{4}(w - 1)(3w + 1), \\
\dot{w} &= \sqrt{2}\,v,
\end{aligned}
\tag{6}
$$

where the dot denotes time derivative, $\tau = \varepsilon t$, $0 < \varepsilon \ll 1$ is a small parameter, and $\delta(\tau)$ is a slowly varying parameter corresponding to the [scaled] detuning. Equations of motion (6) restricted to surface (7) are equivalent to equations of motion in Hamiltonian system with the Hamiltonian (5), where canonically conjugated variables are w and ϕ, $\phi = \arctan(v/u)$.

First, we consider equations (6) at frozen values of parameter δ. In this case, these equations possess two first integrals. One of them is $u^2 + v^2 - \frac{1}{2}(w - 1)^2(w + 1) = \text{const}$. Corresponding to the conservation of single-pair atom-molecule coherence, the constant should be taken equal to zero. The equation
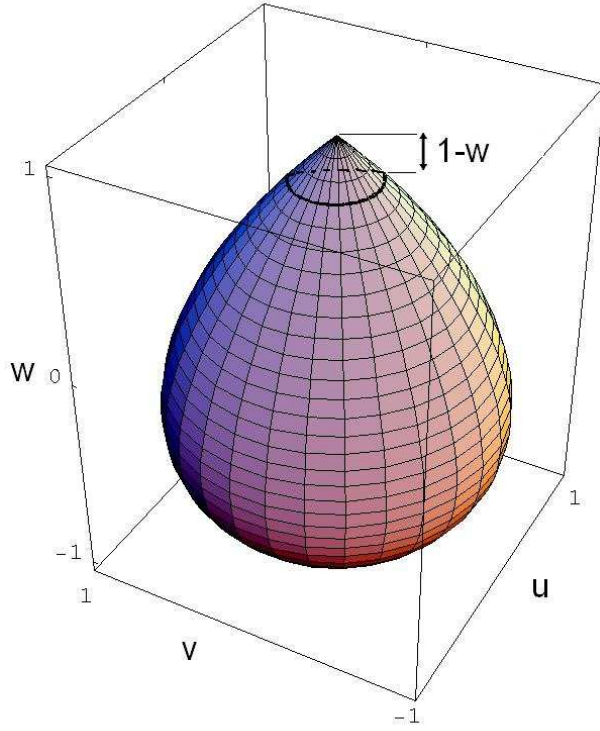
FIG. 1: Geometry of the generalized Bloch sphere (the surface $u^2 + v^2 = \frac{1}{2}(w-1)^2(w+1)$).

$$u^2 + v^2 - \frac{1}{2}(w-1)^2(w+1) = 0. \tag{7}$$

defines a surface of rotation around $w-$axis with a singular [conical] point at (0,0,1) (see Fig.1). Another integral of (6) at a frozen value of δ is given by

$$u + \frac{\delta}{\sqrt{2}}w = \text{const}, \tag{8}$$

and at different values of the constant defines a family of planes parallel to $v-$axis. The angle between these planes and $w-$axis depends on the value of δ. Hence, trajectories of frozen system (6) are given by intersections of surface (7) and planes (8). At $|\delta| < \sqrt{2}$, plane $u = \delta(1-w)/\sqrt{2}$, passing through the singular point (0,0,1) defines a singular
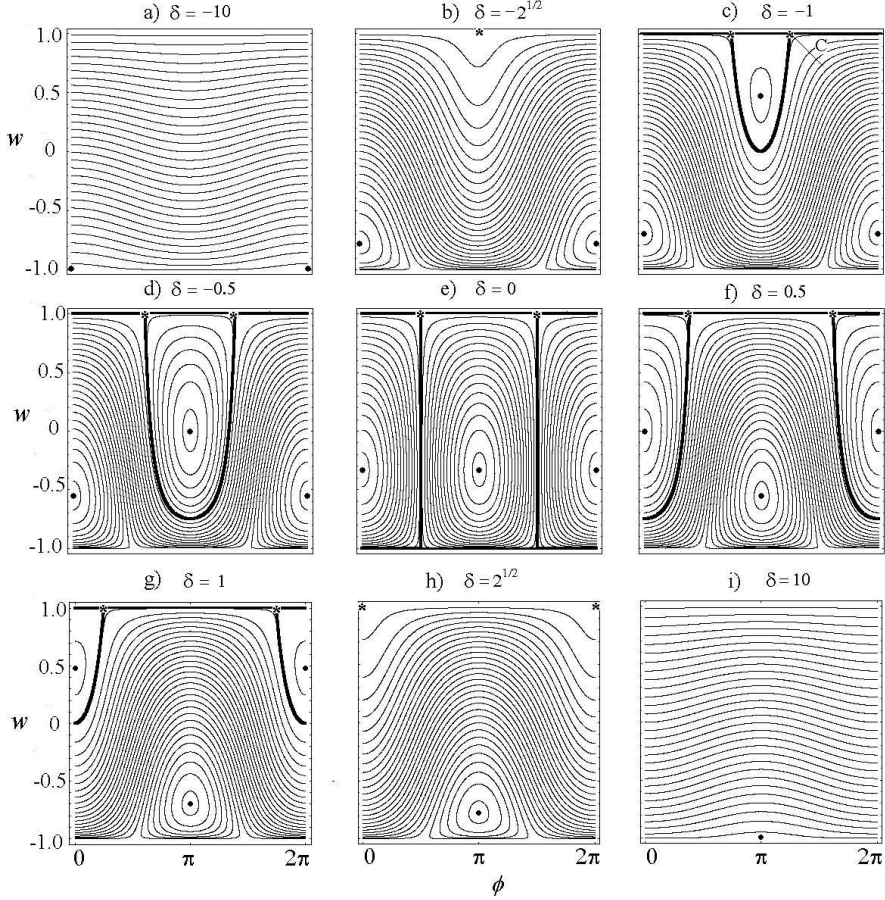
FIG. 2: Phase portraits of the system with Hamiltonian (5) frozen at different values of parameter δ.

trajectory on surface (7).

Consider phase portraits of the system with Hamiltonian (5) frozen at different values of parameter δ [see Figure 2]. In these portraits, points (0,0,1) and (0,0,-1) of the (u, v, w) space are represented as segments $w = 1$ and $w = -1$ correspondingly. Point (0,0,1) is always a stable point of (6), but formally speaking this is not true for the points of the segment $w = 1$ on phase portraits of the system with Hamiltonian (5). If δ is negative and $|\delta| > \sqrt{2}$, there is only one stable elliptic point on the phase portrait, at $\phi = 0$ and

w not far from -1 [see Figure 2a]. It may seem that there are also two singular points at $w = -1, \phi = \pi/2,\ 3\pi/2$, but they are just an artefact of the representation in variables w, ϕ; the phase trajectory passing through these points corresponds to the trajectory of (6) passing through (0,0,-1), and the period of motion on this trajectory is finite.

At $\delta = -\sqrt{2}$ a bifurcation takes place, and at $0 > \delta > -\sqrt{2}$ the phase portrait looks as shown in Figs.2c,d. There are two saddle points at $w = 1, \cos\phi = \delta/\sqrt{2}$ and a newborn elliptic point at $\phi = \pi$. The trajectory connecting these two saddles corresponds to the singular trajectory on the surface (7). On the phase portrait of the system with Hamiltonian (5) it separates rotations and oscillating motions and we call it the separatrix of the frozen system. Below, we will consider "shifted" Hamiltonian $E = H - \delta$; E equals zero on the separatrix.

At $\delta = 0$ the singular trajectory on the surface (7) is passing through (0,0,-1), and correspondingly on the phase portrait the segment $w = -1$ belongs to the separatrix [Figure 2 e]. At $0 < \delta < \sqrt{2}$ the phase portrait looks as shown in Figs. 2 f,g. Finally, at large positive values of δ, again there is only one elliptic stationary point at $\phi = \pi$, and w close to -1.

It may be easier to understand the transition between Figure 2 h and Figure 2 i using also the (u, v, w) representation (see Figure 1). The elliptic point in Figure 2 h corresponds to the elliptic point on the surface (7). This latter elliptic point is close to the pole $(0, 0, -1)$ of the surface (7). As parameter δ grows, this elliptic point approaches to the pole. Consider a closed trajectory of small enough diameter on the surface (7), surrounding this elliptic point. This trajectory is given by an intersection of surface (7) and one of the planes (8) defined by a certain value of the constant. While δ is not large enough, this trajectory does not embrace the pole. The corresponding phase trajectory in Figure 2 h surrounds the elliptic point. At δ large enough, the trajectory on surface (7) corresponding to the same value of the constant in (8) embraces the pole. Along the corresponding phase trajectory in Figure 2 i, value of ϕ varies from 0 to 2π.

Consider now a phase trajectory on a phase portrait frozen at a certain value of δ. If the trajectory is closed, the area S inside of it is connected with the action I of the system by a simple relation $S = 2\pi I$. If the trajectory is not closed, we define the action as follows. If the area S bounded by the trajectory and lines $w = 1, \phi = 0, \phi = 2\pi$ is smaller than 2π, we still have $S = 2\pi I$. If S is larger than 2π, we put $2\pi I = 4\pi - S$. Defined in this way, I is a continuous function of the coordinates.

In system with Hamiltonian (5) with $\tau = \varepsilon t$, the action I is an adiabatic invariant of motion (see, for example, [13]). Far from the separatrix, it undergoes oscillations of order ε.

In the following, we will use the so called improved adiabatic invariant $J = I + \varepsilon \tilde{u}(w, \phi, \tau)$ rather than I. The function u is defined as follows [see, for example, [36]]:

$$\tilde{u} = \tilde{u}(w, \phi, \tau) = \frac{1}{2\pi} \int_0^T \left(\frac{T}{2} - t \right) \frac{\partial E}{\partial \tau} dt. \tag{9}$$

The integral in (9) is computed along the unperturbed trajectory passing through the point (w, ϕ) at the time moment $t = 0$; T is the period of motion on this trajectory. If the trajectory is not closed, T is the time necessary for a phase point on this trajectory to cover the distance of 2π along the ϕ-axis. [Definition (9) is valid provided that on this trajectory the action I and the area on the phase portrait are related simply as $S = 2\pi I$; in the following calculations of the jump in the adiabatic invariant, we need to consider only such trajectories.] Far from the separatrices, variation of J along a phase trajectory is of order ε^2.

As the slow time τ grows, the area bounded by the separatrix $S^*(\tau)$ slowly changes. On the other hand, a value of the adiabatic invariant associated with a certain phase trajectory stays well-preserved. Accordingly, phase trajectories of (5) can cross the separatrix. Let initially δ be large in magnitude and negative, so that the phase portrait is similar to one shown in Figure 2a. Consider a trajectory rotating close to the singular point on surface (7). Along the corresponding phase trajectory on the plane (ϕ, w), value of w

is close to 1. We assume $1 - w$ on this trajectory to be small, yet finite. Hence, the initial value J_- of improved action J is also small. As the time goes, value of parameter δ grows, and at $\delta = -\sqrt{2}$ the separatrix loop appears. The area $S^*(\tau)$ surrounded by the separatrix grows with time, and the action associated with the phase trajectory stays approximately constant. In the so called improved adiabatic approximation this action is conserved at $J = J_-$, and at the slow time moment $\tau = \tau_*$ such that $S^*(\tau_*) = 2\pi J_-$ the phase trajectory crosses the separatrix. Phenomena that take place at such crossing are considered in the following section.

III.   VARIATION OF THE ADIABATIC INVARIANT AT THE SEPARATRIX CROSSING

First, consider the motion in the frozen system along a phase trajectory close to the separatrix. Let on this trajectory $E = h$, $|h| \ll 1$. [We consider such values of δ that h is positive outside the separatrix and is negative inside.] The main part of the time a phase point on this trajectory spends in a neighborhood of the saddle points at $w = 1$. Linearizing the system near the saddle points, we find that in the main approximation the period of motion along this trajectory is

$$T = -\frac{2}{\sqrt{2 - \delta^2}}\ln|h| + b. \tag{10}$$

Here b is a smooth function of δ; its form is not important for the rest of the argument. In agreement with the formula $T = 2\pi\partial I/\partial h$ we find for the adiabatic invariant I in the main approximation

$$2\pi I = S^* - \frac{2}{\sqrt{2 - \delta^2}}h\ln|h| + (b + \frac{2}{\sqrt{2 - \delta^2}})h. \tag{11}$$

Now compute the function $\tilde{u}$ at a point of the vertex bisecting the angle between incoming and outgoing separatrices of the saddle point (see Figure 2c). From (9), (10)

one obtains in the main approximation:

$$2\pi\tilde{u} = \frac{\Theta}{2\sqrt{2-\delta^2}}\ln|h| - b\frac{\Theta}{4} + d, \qquad \Theta = \frac{\partial S^*}{\partial \tau}. \tag{12}$$

Here d is a smooth function of δ; its form is not important for the rest of the argument. Consider now the separatrix crossing in the exact system with Hamiltonian E. On the relevant interval of slow time we have $\Theta(\tau) > 0$ [the area inside the separatrix loop grows]. Initial values of the Hamiltonian and the improved adiabatic invariant at $\tau = \tau_-$ are h_-, J_-. The phase point rotates close to the separatrix. As the area bounded by the separatrix grows, the point comes closer to the separatrix with each turn. Denote by $h_n, I_n, \tilde{u}_n$ values of the corresponding functions at time moments τ_n when the trajectory crosses the vertex bisecting the angle between incoming and outgoing separatrices of the saddle point C outside the separatrix loop (see Figure 2c). We enumerate τ_n as follows: τ_0 is the time of the last crossing of the vertex before crossing the separatrix, other τ_n have negative numbers $\tau_0 > \tau_{-1} > ... > \tau_{-N} \geq \tau_-$. Here $N \gg 1$ is a large integer. Its exact value does not influence the result in the main approximation. After crossing the separatrix, the phase point continues its motion inside the separatrix loop. As the loop grows, the phase point goes deeper and deeper inside, rotating around the elliptic point. At time moments τ_n, $1 \leq n \leq N$, the trajectory crosses the vertex bisecting the angle between incoming and outgoing separatrices of the saddle point C inside the separatrix loop. The corresponding values of $h, I, \tilde{u}$ are $h_n, I_n, \tilde{u}_n$.

It follows from (10) - (12), that in the main approximation the following expressions are valid:

$$\begin{aligned}
h_{n+1} &= h_n - \varepsilon\Theta, \\
\tau_{n+1} &= \tau_n - \frac{\varepsilon}{2\sqrt{2-\delta_*^2}}\left[\ln|h_n| + 3\ln|h_n - \varepsilon\Theta|\right] + \varepsilon b,
\end{aligned} \tag{13}$$

$$2\pi I_n = S^*(\tau_0) - \Theta(\tau_0 - \tau_n) - \frac{2}{\sqrt{2 - \delta_*^2}}h_n\ln|h_n| + (b + \frac{2}{\sqrt{2 - \delta_*^2}})h,$$

$$2\pi\tilde{u}_n = \frac{\Theta}{2\sqrt{2 - \delta_*^2}}\ln|h_n| - b\frac{\Theta}{4} + d.$$

Here and below the values of Θ, b, and d are calculated at $\tau = \tau_*$, the time of separatrix crossing in the adiabatic approximation, δ_* is also the value of δ at $\tau = \tau_*$. Summing the above expressions (13) from $n = -N$ to $n = 0$, we find the change of the improved adiabatic invariant before the separatrix crossing in the main approximation:

$$2\pi(J_0 - J_{-N}) = \frac{\varepsilon\Theta}{\sqrt{2 - \delta_*^2}}\left[\ln\xi - 2\xi\ln\xi + 2\xi - 2\ln(\sqrt{2\pi}/\Gamma(\xi))\right], \qquad (14)$$

where $\xi = |h_0/(\varepsilon\Theta)|$, $\Gamma(\cdot)$ is the gamma function. At the separatrix crossing we obtain:

$$2\pi(J_1 - J_0) = \frac{\varepsilon\Theta}{\sqrt{2 - \delta_*^2}}\left[-\ln\xi - \ln(1 - \xi) + 2(1 - \xi)\ln(1 - \xi) + 2\xi\ln\xi\right]. \qquad (15)$$

For the change of J after the separatrix crossing we find

$$2\pi(J_N - J_1) = \frac{\varepsilon\Theta}{\sqrt{2 - \delta_*^2}}\left[\ln(1 - \xi) - 2(1 - \xi)\ln(1 - \xi) - 2\xi - 2\ln(\sqrt{2\pi}/\Gamma(1 - \xi))\right]. \quad (16)$$

Far from the separatrix, the variation of J is of order ε^2 on time periods of order $1/\varepsilon$. Hence, to obtain in the main approximation the jump of J at the separatrix crossing, one has to sum up expression (14) - (16). Thus, we find:

$$2\pi\Delta J = -2\frac{\varepsilon\Theta}{\sqrt{2 - \delta_*^2}}\ln(2\sin\pi\xi). \qquad (17)$$

Note, that this result is similar to one obtained for a symmetrical double well (see [35, 36]), though the geometry here is different. According to [35, 36], the error of formula (17) is $O(\varepsilon^{3/2}|\ln\varepsilon|)$.

Formula (17) can be simplified. The separatrix is defined by equation $E = 0$. Thus, the area inside the separatrix loop can be calculated as

$$S^*(\delta) = 2 \int_{\delta^2 - 1}^{1} \left[\pi - \arccos \left(\frac{\delta}{\sqrt{1 + w}} \right) \right] dw \tag{18}$$

We are interested in derivative of $S^*(\delta)$ over δ. Differentiating the above integral over parameter δ one obtains:

$$\frac{\partial S^*}{\partial \delta} = -2 \int_{\delta^2}^{2} \frac{-dx}{\sqrt{x - \delta^2}} = 4\sqrt{2 - \delta^2} \tag{19}$$

We have

$$\Theta = \frac{\partial S^*}{\partial \delta} \cdot \delta', \tag{20}$$

where $\delta' \equiv \partial \delta / \partial \tau$. Therefore, formula (17) takes the following form:

$$\Delta J = -\frac{4\varepsilon \delta'_*}{\pi} \ln(2 \sin \pi \xi). \tag{21}$$

Here δ'_* is the value of δ' calculated at time $\tau = \tau_*$.

The value ξ strongly depends on initial conditions: a small of order ε variation of initial conditions results generally in variation of ξ of order 1. Hence, this value can be considered as a random variable; its distribution should be treated as uniform on the segment $(0, 1)$ [see [36], [37], see also [40] for numerically found distribution of ξ in a similar problem]. Formula (21) is valid provided that ξ is not too close to the ends of the interval $(0, 1)$: $k\sqrt{\varepsilon} < \xi < 1 - k\sqrt{\varepsilon}$, where k is a positive constant, see [36]. The value ΔJ in (21) should also be treated as random; we find its dispersion below.

After the separatrix crossing, the phase point rotates around the elliptic point inside the separatrix loop and slowly drifts with this point to the bottom of the phase portrait. If $\delta(\tau)$ is a monotonous function, the phase trajectory will never again cross the separatrix. Assume that $\delta(\tau)$ is a smooth function and $\delta = \delta_- = \text{const}$ at $\tau < \tau_-$, $\delta = \delta_+ = \text{const}$ at $\tau > \tau_+$. [It is assumed that $\delta_- < 0$, $\delta_+ > 0$.] In other words, parameter δ is slowly monotonically varying between two border values. Then $\partial E / \partial \tau = 0$ at $\tau = \tau_{\pm}$, and

action I coincides with J. Hence, formula (21) gives the variation in action I. Let the magnitudes of δ_- and δ_+ be large enough. If the initial value of $w = w_-$ is close enough to 1, the corresponding unperturbed phase trajectory is an almost straight line (cf. Fig. 2 a). Hence, $I_- \approx (1 - w_-)$. Similarly, $I_+ \approx (-1 - w_+)$. Thus, variation in action I corresponds to the remnant atomic fraction. In the adiabatic limit, value of atom-molecular imbalance is reversed at the passage, while the change in the action produce nonadiabatic correction to this result. A typical jump in the action is shown in Fig.3.

Dispersion of jumps in the action can be predicted using formula (21):

$$\sigma^2 = 16\varepsilon^2(\delta'_*)^2\pi^{-2}\int_0^1 \ln^2(2\sin\pi\xi)\,d\xi = \frac{4\varepsilon^2(\delta'_*)^2}{3} \tag{22}$$

To check numerically the scaling of the jumps with ε and the dispersion, we calculated bunches of trajectories with close initial conditions (see Fig.4). For the numerical calculations, we used linear sweeping with $\delta' = 1$, therefore the predicted value of dispersion is $\sigma^2 = (4/3)\varepsilon^2$. Numerically found coefficient is equal to 1.30, which is in reasonable (2% accuracy) agreement with theoretical prediction $4/3 = 1.3333$.

Consider now briefly the case when the external parameter δ varies slow periodically between a positive and a negative values of large magnitudes. In this situation a phase trajectory crosses the separatrix once on each period of variation of δ. Each crossing can be characterized by two values, namely J and ξ. Consider two subsequent crossings of the separatrix. Assume that $J = J_1$ well before the first crossing, and the corresponding value of ξ is ξ_1. Let J_2, ξ_2 characterize the second crossing. In the main approximation, we have the following map:

$$J_2 = J_1 + \varepsilon F(\xi_1) \tag{23}$$

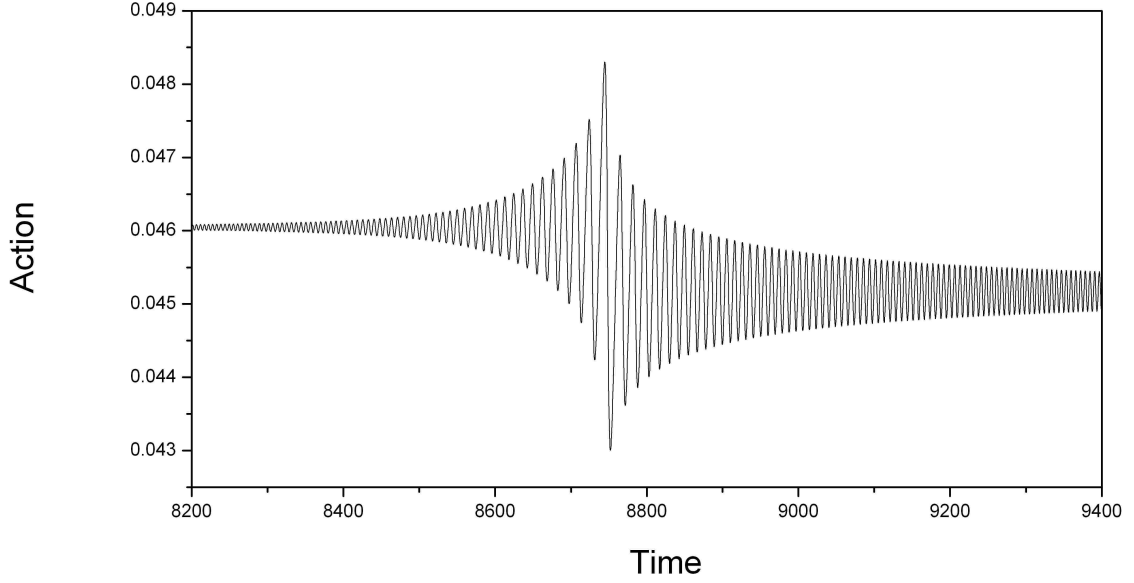$$\xi_2 = \xi_1 + \varepsilon^{-1}G(J_2) \mod 1, \tag{24}$$

FIG. 3: Typical jump of the adiabatic invariant (action) at separatrix crossing.

where

$$F(\xi) = -\frac{\Theta}{\pi\sqrt{2 - \delta_*^2}}\ln(2\sin\pi\xi),$$

$$G(J) = \frac{1}{2\pi}\int_{\tau_1}^{\tau_2}\omega(J,\tau)\,d\tau,$$

τ_1, τ_2 are values of the slow time τ corresponding to the first and the second separatrix crossings, calculated in the adiabatic approximation; ω is a frequency of the fast motion. Suppose that the value ξ_1 gets a small variation $\Delta\xi_1$. According to (23), this leads to variation of the jump in the improved adiabatic invariant by a value $\varepsilon F'(\xi_1)\Delta\xi_1$, where F' denotes derivative of function $F(\xi)$. Thus, as follows from (24), the value ξ_2 obtains a variation $\Delta\xi_2 = \Delta\xi_1 + G'(J_2)F'(\xi_1)\Delta\xi_1$, and

$$\frac{\Delta\xi_2}{\Delta\xi_1} - 1 \sim G'F'. \tag{25}$$

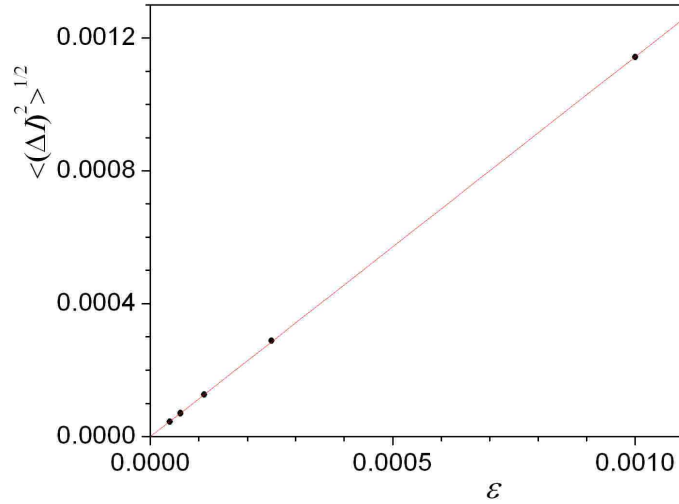FIG. 4: Scaling of jumps in improved adiabatic invariant with ε. For each point on the plot, we take a set of 100 trajectories with initial (at $\delta = -10$) values of w being closely distributed around $w = 0.99 = 1 - 10^{-2}$. Final values of improved action were taken far from the separatrix (at $\delta = 0$). The line on the plot is a linear fit to data, and a perfect linear scaling can be seen. The slope of the line gives $\sigma \approx 1.14\varepsilon$, and the coefficient is in good agreement with the theoretical value $\sqrt{4/3} \approx 1.15$.

This latter value can be used to describe the phase mixing in the system. If it is large, values ξ_1 and ξ_2 are statistically independent. This is the case when ξ_1 is close enough to 0 or to 1. Assume first that in the process of iterations of the map (23), (24) all the values ξ_i are statistically independent. Then the dynamics in the system results in diffusion of the adiabatic invariant and mixing in the phase space. Indeed, the process can be roughly modelled as a random walk in adiabatic invariant: the time interval between two subsequent steps is of order ε^{-1}, and the length of each step is of order ε. Hence, total variation in J after N steps is $\sqrt{N}\varepsilon$. After $N \sim \varepsilon^{-2}$ steps, which takes time of order ε^{-3}, the value of J (and hence the remnant part of the atomic fraction) will change by a value
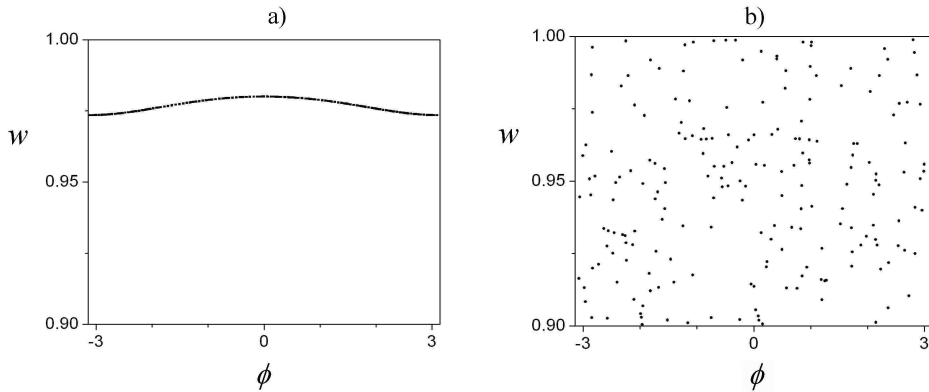
FIG. 5: Stroboscopic shots of two trajectories without/with separatrix crossings (a)/b) correspondingly), and with the same initial conditions. Parameters: $\varepsilon = 0.002$, $\delta_0 = -10$. In (a), value of δ was modulated as $\delta = \delta_0(0.75 + 0.25\cos\varepsilon t)$, so no separatrix crossing occur. In (b), $\delta = \delta_0\cos\varepsilon t$, so multiple separatrix crossings result in diffusion of adiabatic invariant as described in the text.

of order one.

An example of such diffusion is shown in Fig. 5b. The figure demonstrates the result of integration along one phase trajectory over a long period of time with δ being modulated as $\delta = \delta_0\cos(\tau)$, $\delta_0 = -10$. For the presentation, we plot the corresponding phase points on this trajectory at instances of time when $\delta = \delta_0$. For the comparison, we plot the results for a trajectory with the same initial conditions, but with δ being modulating as $\delta = \delta_0(0.75 + 0.25\cos(\tau))$, $\delta_0 = -10$, i.e. without the separatrix crossings (Fig. 5a). The same stroboscopic shots produce smooth curve: the adiabatic invariant is eternally conserved in this system at sufficiently small ε [13].

It is interesting to note that (for system with separatrix crossings) the variations in ξ may be correlated along certain trajectories. As it was shown in [42] in a more general case, this results in existence of stable periodic trajectories and stability islands in the domain of the separatrix crossings. Total measure of these islands does not tend to zero

as $\varepsilon \to 0$, yet it is small. Along a phase trajectory with initial conditions inside such an island, the value of the adiabatic invariant undergoes only periodic oscillations with amplitude of order ε [42].

IV. ACKNOWLEDGEMENTS

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