Non-adiabaticity of a many-particle Landau-Zener problem: forward and backward sweeps

A.P. Itin and P. Törmä
Department of Applied Physics, Helsinki University of Technology, P.O. Box 5100 02015, Finland

We consider nonlinear dynamics of an interacting many-particle system with a slowly changing parameter: a many-body generalization of the Landau-Zener model. Adiabaticity is destroyed when the parameter crosses a critical value. Applying semiclassical analysis based on concepts of classical adiabatic invariants, we derive a formula which accurately describes particle distributions in the Hilbert space at wide range of parameters and initial conditions of the system. We found striking universal features in the particle distributions which can be probed in an experiment on Feshbach resonance passage or a cavity QED experiment. The dynamics is found to be crucially dependent on the direction of the sweep.

 Destruction of adiabaticity is a central issue in both quantum and classical mechanics. For a single-particle quantum system, very often nonadiabatic dynamics can be described within the exactly solvable Landau-Zener model (LZM) [1], where a probability of transition from an initially occupied instantaneous ground state level to the excited one is exponentially small in the sweeping rate parameter. Experiments with ultracold quantum gases [2] may involve macroscopically large numbers of particles, making semiclassical (SC) treatments justified [3, 4, 5, 6, 7, 8, 9].

Nonadiabatic dynamics in SC models of many-particle systems has been intensively discussed recently [2, 3, 4, 5, 6, 7, 8, 9, 11, 12]. The model (LZM) [1], where a probability of transition from an initially occupied instantaneous ground state level to the excited one is exponentially small in the sweeping rate parameter. Experiments with ultracold quantum gases [2] may involve macroscopically large numbers of particles, making semiclassical (SC) treatments justified [3, 4, 5, 6, 7, 8, 9].

Nonadiabatic dynamics in SC models of many-particle systems has been intensively discussed recently [2, 3, 4, 5, 6, 7, 8, 9, 11, 12]. In many treatments, it was found that exponential LZM-type behaviour for the transition probabilities is replaced with power-laws of the sweeping rates. However, a universal and accurate method for describing nonadiabatic SC dynamics of such many-particle systems is still lacking. Here we present a method based on modelling of a quantum system by an ensemble of classical trajectories and accurate description of its dynamics in a vicinity of a bifurcation, which predicts universal features of the particle distributions amenable for an experimental probe.

We consider a many-particle LZM: time-dependent Dicke model, which has numerous applications in quantum and matter-wave optics [3, 4, 5, 6, 7, 8, 9, 11, 12]. The model can be written as

$$\hat{H} = -\frac{\gamma(t)}{2} \hat{b}^\dagger \hat{b} + \frac{\gamma(t)}{2} \hat{S}^z + \frac{g}{\sqrt{N}} (\hat{b}^\dagger \hat{S}^- + \hat{b} \hat{S}^+),$$

(1)

where $\frac{g}{\sqrt{N}}$ is the coupling strength, $\hat{S}^\pm = \hat{S}_x \pm i \hat{S}_y$ are spin operators, $\hat{b}^\dagger$ and $\hat{b}$ are creation and destruction operators of a bosonic mode, $\gamma(t) = \pm 2\epsilon t$ is detuning, and $\epsilon$ is the sweeping rate of the bosonic mode energy. The spin value $S$ is macroscopically large $S = N/2 \gg 1$: usually the physical origin of the effective spin variable $S$ is a collection of two-level systems (spin-1/2 particles).

Among many possible applications, let us mention the Feshbach resonance passage [13], dynamics of molecular nanomagnets [14], and cavity QED with Bose-Einstein condensates (BEC) [8, 13].

With $N = 1$, one recovers the standard Landau-Zener model. In the context of a Feshbach resonance passage in a Fermi gas, an equivalent realization of the Hamiltonian (1) is $\hat{H} = \epsilon t \sum_{i=1}^N (\hat{n}_{i1} + \hat{n}_{i\dagger}) + \frac{g}{\sqrt{N}} \sum_{i=1}^N \left( \hat{b}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow} + h.c. \right)$, where $\hat{c}_{i\sigma} = \hat{c}_{\uparrow}$ if $\sigma = \uparrow$, and $\hat{c}_{i\sigma} = \hat{c}_{\downarrow}$ if $\sigma = \downarrow$. Coupled atom-molecular BEC are described by a similar model, whose dynamics in the limit of large $N$ becomes equivalent to (1) with the replacement $\gamma \to -\gamma$ [8, 10]. I.e., in the thermodynamic limit of the degenerate model (1) association of Fermi atoms becomes equivalent to dissociation of molecular BEC, and vice versa. We therefore discuss two driving scenarios here: "forward" and "backward" sweeps. In the "forward" sweep, starting in the distant past with some small initial number of bosons $N_b(t)|_{-\infty} \equiv \langle \hat{b}^\dagger \hat{b} \rangle_{-\infty} = N_- \equiv n_-$, we want to calculate the final number of bosons $N_b(t)|_{+\infty} \equiv n_+ N$ and its distribution $P(N_b)$ as a function of the sweeping rate $\epsilon$ and the initial bosonic fraction $n_-$. To be more specific, we start in a number state of (1): $|\psi_{-\infty}\rangle = |N_-,S_\downarrow\rangle = |N_-\rangle |\frac{N}{2} - N_-\rangle$, where $N_-$ can be zero in case we start at the ground state. We consider the sector $S = N/2$ for clarity, but other values of $S$ can be treated analogously (Hilbert space of (1) is decoupled on sectors with definite total spin, or "cooperation number", $S$). Matrix elements of (1) have the form $H_{n,n'} = -\gamma(t) \delta_{n,n'} + n \delta_{n,n'+1} \sqrt{N-n'/\sqrt{N+1}}$.

FIG. 1: The time evolution of the distribution of the rescaled boson number $n$ at a "forward" sweep through the resonance. (a) Quantum calculation with $N=500$. (b) Corresponding ensemble of classical trajectories; sweeping rate is $\epsilon = 0.3$.
$n' \delta_{n,n'-1} \sqrt{N-n}/\sqrt{N}$ (we set $g = 1$ for convenience in this Letter), therefore the model can be referred to the class of generalized Landau-Zener models [16] in the case of linear driving $\gamma(t) \sim t$. In the second dynamical scenario (“backward”), we start in the ground state of (1) at large positive value of $\gamma$ and make an “inverse” sweep to large negative $\gamma$ (see also our supplementary Brief Report [16]). This scenario is relevant to association of Bose atoms in molecular BEC, studied e.g. in [6].

The model and its equivalent realizations have been studied already using various techniques. Diagrammatic methods employed in [8] work well for small $N$ but do not allow to get close to the SC limit for large $N$. Another approach is a SC treatment based on classical adiabatic invariants [7, 8, 9]. At $|t| = \infty$ and $N \to \infty$ the relative number of bosons $N_b/N$ corresponds to a classical action $I$ of an effective Hamiltonian system (see e.g. Eq. (2)), so that for large but finite $N$ the problem can be mapped to the calculation of a change of classical actions of a properly prepared ensemble of trajectories. It is inspiring that calculations with ensembles of trajectories can be mapped to the calculation of a change of classical actions of a properly prepared ensemble of trajectories. Naturally, freedom of choosing a value of the ratio $I_-/\epsilon$ remains. Assuming $I_- \gg \epsilon$ and $1/N, I_- \ll 1$, which corresponds to considerable initial population of the bosonic mode, Ref. [9] applied an approach based on the separatrix crossing theory [19, 20, 21]. From the experimental point of view, however, it is important to analyze also cases of very small initial actions.

Our method for the regime of small initial actions is as follows. To calculate the deviation from adiabaticity, we note that most of the change of the classical action of a phase point happens as it travels near the separatrix and, especially, near the saddle points that arise during the bifurcation as $\gamma$ reaches $-2$. In our new variables, the arising saddle point is located in the origin). Close to the saddle point $n$ is small and one can expand $\sqrt{1-n}$ in series. Let us introduce variables $P = 2\sqrt{n} \cos \phi$, $Y = 2\sqrt{n} \sin \phi$. Near the bifurcation, at $\gamma \approx -2$, we therefore get an effective Hamiltonian $H = -\frac{P^2}{2}(\gamma/2 + 1) - \frac{Y^2}{2}(\gamma/2 - 1) + \frac{P^2}{4}$, where higher order terms in $Y$ and $P$ have been neglected. We neglect also the time-dependence of the coefficient $\gamma/2 - 1$ of the second term. Then, shifting origin of time, we obtain the Hamiltonian $H = \frac{P^2}{2}ct + Y^2 + P^4/16$. After simple rescalings $P = 2^{3/4}P'$, $Y = 2^{3/8}Y'$, $t = t'/3^{3/4}$, $H = 2^{7/3}H'$, the Hamiltonian becomes $H = -\frac{P'^2}{2}ct + \frac{Y'^2}{2} + \frac{P'^4}{4}$ (primes over new variables omitted). We replace also momenta and coordinates: $P \to Y$, $Y \to -P$. Let us now in-
The formula (8), i.e. ∼\( W \) obtained by averaging over the initial distribution (Eq.5). Squares, triangles are numerics for Asymptotics of PII were investigated by Its and Kapaev (3) is [22, 24]. Returning back to the original variables and the Hamiltonian (2), we get the Formula:

\[
\Delta I = \epsilon \left( \frac{I}{\epsilon} - \frac{2}{\pi} \ln \sqrt{\exp \left( \frac{3I}{\epsilon} \right) - 1} \right),
\]

which means that the final number of bosons is \( n_f = 1 - I_\epsilon - \langle \Delta I \rangle_{A_{I_{\epsilon}}} \). It predicts also the final distribution \( P(\Delta I) = P(1 - I_\epsilon - n_f) \). All moments \( M_{k A_{I_{\epsilon}}} = \langle (\Delta I - \langle \Delta I \rangle)^k \rangle_{A_{I_{\epsilon}}} \) are easy to calculate, for instance \( M_{2 A_{I_{\epsilon}}} = \left( \frac{2}{\pi} \right)^2 \int_0^{\pi} d\xi \ln^2(2\sin \pi \xi) = \frac{4}{\pi^2} \).

Introduce a rescaling transformation that makes the essential mathematics of the problem as clear as possible: \( Y = \epsilon^{1/3} \tilde{Y}, \quad P = \epsilon^{2/3} \tilde{P}, \quad t = \epsilon^{-1/3} s, \quad H = \epsilon^{4/3} \tilde{H}. \) The Hamiltonian becomes (omitting tildes over new variables) \( H = -s\frac{\partial^2}{\partial s^2} + \frac{P^2}{2} + \frac{\lambda^2}{2} \). This Hamiltonian does not have a small parameter anywhere, and the loss of adiabaticity is evident. An important property of the bifurcation we are considering is that the effective Hamiltonian leads to the second Painlevé equation (PII)

\[
\frac{d^2 Y}{ds^2} = sY - 2Y^3.
\]

Asymptotics of PII were investigated by Its and Kapaev [22] (see also [24]) using a method of isomonodromic deformations [23]. At \( s \to - \infty \) the asymptotic solution to (3) is [22, 24]

\[
Y(s) = \alpha (-s)^{1/4} \sin \left( \frac{2}{3} (-s)^{3/2} + \frac{3}{4} \alpha^2 \ln (-s) + \phi \right),
\]

and in the limit \( s \to + \infty \) it is

\[
Y(s) = \pm \sqrt{\frac{2}{3}} \pm \rho(2s)^{1/4} \cos \left( \frac{2\sqrt{2}}{3} s^{3/2} - \frac{3}{2} \rho^2 \ln s + \theta \right),
\]

where \((\alpha, \phi)\) and \((\rho, \theta)\) are the “action-angle” variables characterizing the solutions in the limits \( s \to \pm \infty \). As \( s \to \pm \infty \), the adiabatic invariant \( I_\epsilon \) of equation (3) approaches the quantities \( I^-_\epsilon \) or \( I^+_\epsilon \) which are defined (to the lowest order terms) as \( I^-_\epsilon = \alpha^2, \quad I^+_\epsilon = \alpha^2 \). The jump in the adiabatic invariant \( \Delta I_\epsilon = 2I^+_\epsilon - I^-_\epsilon \) can be found from general relations between \( \rho^2 \) and \( \alpha^2 \) as

\[
I^+_\epsilon = \frac{1}{2\pi} \ln \frac{1 + |\rho|^2}{2|\text{Im}(p)|}, \quad p = \sqrt{\epsilon^2 + 1 - \text{Im}(I^-_\epsilon - \phi)} \quad (see \ [22, 24]).
\]

FIG. 3: (a) Change in the action \( \Delta I \) of classical trajectories from the ensemble \( A_{I_{\epsilon}} \) as a function of the initial phase. The change \( \Delta I \) describes the deviation from adiabaticity. We shift all curves horizontally so their maxima are at \( \pi/2 \). We found the change in the action is highly phase-dependent. (b) Average change of the adiabatic invariant \( \langle \Delta I \rangle_{A_{I_{\epsilon}}} \) as a function of the sweep rate \( \epsilon \). Lines are the theoretical curves (Eq.6). Squares, triangles are numerics for the ensemble \( N = 250 \) and \( N = 500 \) (dots); from the formula [5] obtained by averaging over the initial distribution \( W \sim \exp[-2n_b - 2n_b] \) (solid lines). (c) Dispersion of number of bosons for \( N = 250 \); dots: quantum calculations, solid line: the formula [5], i.e. \( N^2(\tilde{n}^2 - \bar{n}^2) = \frac{N^2 \bar{n}^2}{6} \).

\[
\langle \Delta I \rangle_{A_{I_{\epsilon}}} = \epsilon \left( \frac{I}{\epsilon} - \frac{2}{\pi} \ln \sqrt{\exp \left( \frac{3I}{\epsilon} \right) - 1} \right),
\]

where for the ensemble \( A_{I_{\epsilon}} \) \( \pi \xi = (f(I_-) + \phi) \), the function \( f(I_-) \) is not important for our discussion (see [11]); \( \xi \) is a quasi-random variable uniformly distributed on \((0,1)\). The formula predicts the average change in the action to be

\[
\langle \Delta I \rangle_{A_{I_{\epsilon}}} = \epsilon \left( \frac{I}{\epsilon} - \frac{2}{\pi} \ln \sqrt{\exp \left( \frac{3I}{\epsilon} \right) - 1} \right),
\]

which coincides with the result of [9], obtained under the different conditions \( \epsilon \ll I_\epsilon \ll 1 \). Moreover, if \( I_\epsilon \gg \epsilon \), we recover this result of [9], which in the present variables is

\[
\Delta I = -\frac{2\epsilon}{\pi} \ln(2\sin \pi \xi),
\]

where the pseudophase \( \xi \in (0,1) \) is a quasi-random variable. Such a change in the action has zero mean value, nevertheless it introduces spreading in particle distribution since \( \langle \Delta I^2 \rangle \sim \epsilon^2 \). When \( I_\epsilon \ll \epsilon \), we have a qualitatively different result which resembles that of [8] (i.e. \( I_\epsilon = \epsilon \ln I_- / \pi \), with \( I_- = \frac{1}{\epsilon} \)):

\[
\Delta I = -\epsilon \left( \frac{1}{\pi} \ln \left( \frac{\pi I_-}{\epsilon} \right) + 2 \frac{\pi}{\epsilon} \ln(2\sin \pi \xi) \right).
\]

Formula (4) can be used over a wide range of values of \( \epsilon \) and \( I_- \) (we require \( I_- \ll 1 \) and \( \epsilon |\ln I_-| \ll 1 \)). Qualitatively, it is important that the final distributions are determined not only by the average change in the action (5), but also by the phase-dependent part (6), which is therefore important in amplification of quantum fluctuations. This profile has striking universality: we found that several other infinite-range models, e.g. Lipkin model, two-mode BEC with attractive interaction, have analogous behaviour during linear sweep of a control parameter through a critical value. The comparison between the numerical and analytical results for \( L = 0 \)
are given in Figs. 3a,b, where predictions of the Eq. (10) start to deviate from the classical numerics only at large \( \epsilon \) (such that \( -\frac{1}{2} \ln \frac{2\epsilon}{\pi} \sim 1 \)). Then, we take into account distribution of \( L \). We consider a slice of total distribution with equal values of \( x = n + \frac{1}{2} \) and uniform distribution of \( L \in (-2x, 2x) \); averaging over \( \phi \) and \( L \) within the slice, we found that the formula (5) (derived for the “central” point of the slice, i.e. \( L = 0, x = \ldots \)) acquire additional coefficient 2 inside the logarithm: \( I_\ldots \rightarrow 2I_\ldots \). The amplitude of the phase-dependent part is also modified, although it retains its characteristic form shown in Fig. 3a; the final result of averaging over the 3-dimensional distribution (in \( \phi, I_\ldots, L \)) of the initial ensemble of phase points is:

\[
\bar{n} = 1 - \frac{\epsilon}{\pi} \left( \ln \frac{\epsilon N}{\pi} + \gamma \right), \hspace{1cm} \bar{n}^2 - \bar{n}^2 = \frac{\epsilon^2}{6}, \tag{8}
\]

where \( \gamma \) is the Euler constant. Comparison with quantum calculations are given in Figs. 3c,d.

Let us now briefly discuss the inverse sweep (see also [10]), whose properties can also be derived from PII equation. The main feature of the inverse sweep is phase-independence of the change in the action in the limit of small \( I_\ldots \). Deviation from adiabaticity at slow sweeps strictly follows a linear power-law. The coefficient was estimated in [6] to be equal to \( -\frac{\epsilon}{\pi} \approx 0.21 \). The asymptotically exact value of the coefficient was found from mapping to PII in [10]: \( \frac{\epsilon^2}{2\pi} \approx 0.2206 \). The most appealing physical system to implement this process is photonic- or magneto-association of Bose condensates, which was shown to be well described by a two-mode mean-field model. "Forward" sweep would correspond to dissociation of BEC. Experimentally, studying distributions after a sweep could be achieved by making many runs at each particular sweeping rate.

In summary, we have found novel universal features in dynamics of a many-particle LZM using a method that complements the separatrix crossing theory applied to that model in [3]. The results are highly relevant for accurately describing the Feshbach resonance passage in ultracold Fermi and Bose gases and may motivate further experimental activity on that theme. Furthermore, we believe our method will have important applications in the field of dynamics of quantum phase transitions (QPT) [26]. When an underlying quantum system experiences a second order QPT, its mean-field counterpart often experiences a Hamiltonian pitchfork bifurcation. Passage through such a bifurcation leads to PII.

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