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Fast forward to the classical adiabatic invariant

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Abstract

We show how the classical action, an adiabatic invariant, can be preserved under non-adiabatic conditions. Specifically, for a time-dependent Hamiltonian $H = p^2/2m + U(q, t)$ in one degree of freedom, and for an arbitrary choice of action I_0 , we construct a “fast-forward” potential energy function $V_{\text{FF}}(q, t)$ that, when added to H , guides all trajectories with initial action I_0 to end with the same value of action. We use this result to construct a local dynamical invariant $J(q, p, t)$ whose value remains constant along these trajectories. We illustrate our results with numerical simulations. Finally, we sketch how our classical results may be used to design approximate quantum shortcuts to adiabaticity.

For a classical system in one degree of freedom, the action variable $I = \oint p \cdot dq$ is an adiabatic invariant [1]. As an example, when the length of a pendulum is slowly varied, both its energy E and frequency of oscillation ω change with time, but their ratio E/ω , which is proportional to the action, remains constant. The adiabatic invariant can be visualized in phase space by imagining a collection of trajectories evolving under a slowly time-dependent Hamiltonian, H . If all initial conditions are sampled from a single energy shell (that is, a level curve) of $H(q, p, 0)$, then a snapshot of these trajectories at a later time t will find them located on a single energy shell of $H(q, p, t)$, with the same action as the initial shell, as shown in Fig. 1.

In this paper we pose and answer the question: how can the adiabatic invariant be preserved under non-adiabatic driving conditions? We consider a Hamiltonian $H(q, p, t) = p^2/2m + U(q, t)$ that varies at an arbitrary rate. Under the evolution generated by this Hamiltonian, the action $I(q, p, t)$ does not remain constant: if at time $t = 0$ we launch a collection of trajectories, each with the same initial action I_0 , then at later times their actions will generally differ from one another, and from the initial action. Thus under non-adiabatic driving, trajectories wander away from the energy shell associated with the action I_0 . But suppose we want these trajectories to “return home” at a specified later time τ , i.e. we demand that the action of each trajectory be equal to I_0 at $t = \tau$, given that its action had this value at $t = 0$. In this paper we solve for the additional forces that are required to steer the trajectories back to the action I_0 at $t = \tau$. More precisely, we show how to construct an auxiliary “fast-forward” potential $V_{\text{FF}}(q, t)$ with the following property. Under

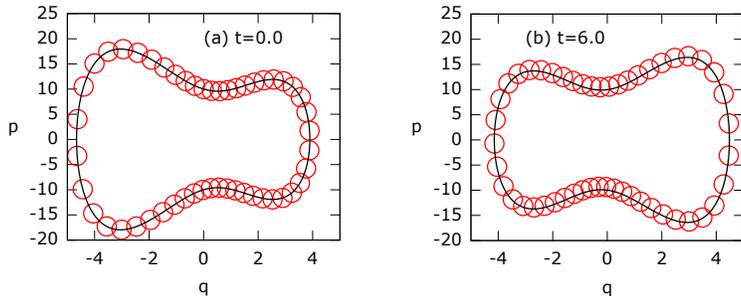


FIG. 1. Illustration of the classical adiabatic invariant. Fifty trajectories evolving under a slowly varying Hamiltonian are shown at an initial time and a later time. The closed curves are instantaneous *energy shells* – level curves of H – with identical values of the action $I = \oint p \cdot dq$. Trajectories were generated using $H(q, p, t)$ given by Eq. 22, setting $\tau = 10.0$ to achieve slow driving.

the dynamics generated by the Hamiltonian $H_{\text{FF}} = H + V_{\text{FF}}$, *all trajectories that begin with action I_0 at $t = 0$ will end the same action, I_0 , at $t = \tau$* . Throughout this paper, the action $I(q, p, t)$ is defined with respect to the original Hamiltonian $H(q, p, t)$.

We were led to this topic through our interest in quantum *shortcuts to adiabaticity* [2], and (as we briefly discuss later) we expect our results will prove useful in the design of such shortcuts for guiding a quantum system to a desired energy eigenstate. The primary focus of this paper, however, is a self-contained problem of general theoretical interest in elementary classical dynamics, for which we obtain a simple and appealing solution (Eq. 10).

Consider a classical system in one degree of freedom, described by a kinetic-plus-potential Hamiltonian

$$H(z, t) = \frac{p^2}{2m} + U(q, t) \quad , \quad z = (q, p) \quad (1)$$

H varies with time during the interval $0 \leq t \leq \tau$, but is constant outside this interval. We assume that H is twice continuously differentiable with respect to time, hence both $\partial H / \partial t$ and $\partial^2 H / \partial t^2$ vanish at $t = 0$ and $t = \tau$. In Appendix A, we discuss how this assumption can be relaxed.

The term *energy shell* will denote a level curve of $H(z, t)$, that is the set of all points where H takes on a particular value, E , at time t . We will assume that each energy shell forms a simple, closed loop in phase space. The function

$$\Omega(E, t) = \int dz \theta [E - H(z, t)] = \oint_E p \cdot dq \quad (2)$$

is the volume of phase space enclosed by the energy shell E of $H(z, t)$, and the *action*,

$$I(z, t) = \Omega(H(z, t), t), \quad (3)$$

is the volume enclosed by the energy shell that contains the point z . Eq. 3 implies

$$\{I, H\} \equiv \frac{\partial I}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial I}{\partial p} \frac{\partial H}{\partial q} = 0 \quad (4)$$

which will prove useful.

Let us choose an arbitrary action value $I_0 > 0$, and define the *adiabatic energy* $\bar{E}(t)$ by

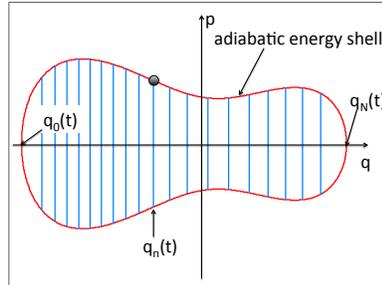


FIG. 2. The region of phase space enclosed by the adiabatic energy shell $\mathcal{E}(t)$ is divided by line segments at $\{q_n(t)\}$ into vertical strips of equal phase space volume. The motion of these lines is described by velocity and acceleration fields $v(q, t)$ and $a(q, t)$.

the condition

$$\Omega(\bar{E}(t), t) = I_0 \quad (5)$$

The *adiabatic energy shell* $\mathcal{E}(t) = \{z | H(z, t) = \bar{E}(t)\}$ is the level curve of $H(z, t)$ with the value $\bar{E}(t)$, enclosing a phase space volume I_0 . Hence $I(z, t) = I_0$ for all $z \in \mathcal{E}(t)$.

At $t = 0$, the adiabatic energy shell $\mathcal{E}(0)$ defines a set of initial conditions that form a closed loop in phase space. As trajectories evolve under $H(z, t)$ from these initial conditions, this loop evolves in time,

$$\mathcal{L}(t) = \{z = z_t(z_0) | z_0 \in \mathcal{E}(0)\} \quad (6)$$

where $z_t(z_0)$ indicates the trajectory that evolves under $H(z, t)$ from initial conditions z_0 . If H varies slowly with time, then these trajectories remain close to the adiabatic energy shell, but under more general conditions the loop $\mathcal{L}(t)$ strays away from $\mathcal{E}(t)$ for $t > 0$.

Now consider an auxiliary potential $V_{\text{FF}}(q, t)$, let $z_t^{\text{FF}}(z_0)$ indicate evolution under $H_{\text{FF}} = H + V_{\text{FF}}$, and consider the loop

$$\mathcal{L}_{\text{FF}}(t) = \{z = z_t^{\text{FF}}(z_0) | z_0 \in \mathcal{E}(0)\} \quad (7)$$

that evolves under H_{FF} from the initial conditions defined by $\mathcal{E}(0)$. Our aim is to construct $V_{\text{FF}}(q, t)$ such that $\mathcal{L}_{\text{FF}}(\tau) = \mathcal{E}(\tau)$: we want the auxiliary potential to guide trajectories faithfully back to the adiabatic energy shell at the final time $t = \tau$. The notation FF, for “fast-forward” [3–10], indicates that V_{FF} drives the system rapidly to a destination that it would otherwise have reached during a slow process. We now describe how to construct a potential $V_{\text{FF}}(q, t)$ with this property.

Imagine a set of line segments at locations $q_1(t), \dots, q_{N-1}(t)$, that divide the region of phase space enclosed by the adiabatic energy shell $\mathcal{E}(t)$ into $N \gg 1$ narrow strips of equal phase space volume; see Fig. 2. Let $q_0(t)$ and $q_N(t)$ denote the left and right turning points of the adiabatic energy shell. In the limit $N \rightarrow \infty$, the parametric time-dependence of these line segments defines a velocity field $v(q, t)$ and an acceleration field $a(q, t)$:

$$\frac{dq_n}{dt} = v(q_n, t) \quad , \quad \frac{d^2q_n}{dt^2} = a(q_n, t) = \frac{\partial v}{\partial q}v + \frac{\partial v}{\partial t} \quad (8)$$

Since $\partial H/\partial t = \partial^2 H/\partial t^2 = 0$ at $t = 0$ and $t = \tau$ (see comments following Eq. 1) we have

$$v(q, 0) = v(q, \tau) = 0 \quad , \quad a(q, 0) = a(q, \tau) = 0 \quad (9)$$

We now claim that the desired fast-forward potential satisfies

$$-\frac{\partial V_{\text{FF}}}{\partial q} = ma \quad (10a)$$

therefore it is given by ¹

$$V_{\text{FF}}(q, t) = - \int_{q_0(t)}^q dq' ma(q', t) \quad (10b)$$

By Eq. 9, $V_{\text{FF}}(q, t)$ vanishes at the start and end of the process. Since $v(q, t)$ and $a(q, t)$ depend on the value I_0 , different choices of I_0 generally produce different fast-forward potentials $V_{\text{FF}}(q, t)$. We now show that an auxiliary potential given by Eq. 10 will indeed produce the desired result, for an arbitrary but fixed I_0 .

We begin by solving for the velocity field $v(q, t)$. The volume of the region of phase space that is enclosed by the energy shell, and is located to the left of a point $q \in [q_0, q_N]$, is given by

$$S(q, t) = 2 \int_{q_0(t)}^q dq' \bar{p}(q', t) \quad (11)$$

where $\bar{p}(q, t) = [2m(\bar{E} - U)]^{1/2}$ specifies the upper branch of the adiabatic energy shell. By construction, $v(q_n(t), t)$ is the velocity of a line segment $q_n(t)$ that evolves at fixed S : $(d/dt)S(q_n(t), t) = 0$. Hence

$$v(q, t) = \left. \frac{dq}{dt} \right|_S = - \frac{\partial_t S}{\partial_q S} \quad (12)$$

¹ The choice of setting the lower bound of integration at $q_0(t)$ is arbitrary. A different choice would modify $V_{\text{FF}}(q, t)$ by an additive function $\phi(t)$ having no effect on the dynamics.

Now consider a point in phase space, $(q_n(t), p_n(t))$, attached to the top of the n 'th line segment: $p_n = \bar{p}(q_n, t)$ (see Fig. 2). As the shape of the energy shell and the locations of the line segments vary parametrically with time, this point (q_n, p_n) moves in phase space, “surfing” the upper branch of the energy shell. This motion is described by the equations

$$\dot{q}_n = v(q_n, t) \quad , \quad \dot{p}_n = -p_n v'(q_n, t) \quad (13)$$

where the equation for \dot{p}_n is obtained by demanding that the phase space volume of the strip between neighboring vertical lines, $\delta S_n \equiv 2p_n(q_{n+1} - q_n)$, remain constant. In Eq. 13 and throughout the paper, dots and primes denotes derivatives with respect to t and q , respectively. Eq. 13 also describes the motion of a point attached to the bottom of one of the vertical lines. We easily verify that Eq. 13 is generated by a Hamiltonian

$$K(q, p, t) = pv(q, t) \quad (14)$$

Therefore if we start with initial conditions distributed over the energy shell $\mathcal{E}(0)$, and we evolve trajectories from these initial conditions under the Hamiltonian $K(q, p, t)$, then these trajectories cling to the evolving adiabatic energy shell, with each trajectory attached to the upper or lower end of one of the vertical line segments. Hence the flow generated by K *preserves the adiabatic energy shell*, in the following sense: for each time step δt , this flow maps points on $\mathcal{E}(t)$ to points on $\mathcal{E}(t + \delta t)$. This implies that the action $I(z, t)$ is conserved under this flow, for those trajectories with action I_0 . Therefore we have:

$$0 = \frac{\partial I}{\partial t} + \frac{\partial I}{\partial q} \dot{q} + \frac{\partial I}{\partial p} \dot{p} = \frac{\partial I}{\partial t} + \{I, K\} \quad \forall z \in \mathcal{E}(t) \quad (15)$$

Next, we construct a Hamiltonian $G(z, t) \equiv H + K$, which generates equations of motion

$$\dot{q} = \frac{p}{m} + v(q, t) \quad , \quad \dot{p} = -U'(q, t) - pv'(q, t) \quad (16)$$

Along a trajectory $z(t)$ obeying these dynamics, we have

$$\dot{I} = \frac{d}{dt} I(z(t), t) = \frac{\partial I}{\partial t} + \{I, H\} + \{I, K\} \quad (17)$$

Eqs. 4, 15 and 17 imply that $\dot{I} = 0$ for all $z \in \mathcal{E}(t)$. Thus the flow generated by $G = H + K$ preserves the adiabatic energy shell. This is easily understood: with each time step δt , the term $K(z, t)$ generates a flow that maps $\mathcal{E}(t)$ onto $\mathcal{E}(t + \delta t)$ while the term $H(z, t)$ generates flow parallel to the adiabatic energy shell. As a consistency check, we can verify directly from Hamilton's equations that the flow generated by G preserves the adiabatic energy shell (see Appendix B).

To this point, we have constructed a Hamiltonian $G = H + K$ that generates trajectories which cling to the adiabatic energy shell $\mathcal{E}(t)$. Along these trajectories, $I(z, t)$ remains constant. We now introduce a change of variables that effectively transforms $K(z, t)$ into the potential energy function $V_{\text{FF}}(q, t)$ that we seek.

Consider the evolution of the observables

$$Q(q, p, t) = q \quad , \quad P(q, p, t) = p + mv(q, t) \quad (18)$$

along a trajectory that evolves under Eq. 16. By direct substitution we get

$$\frac{dQ}{dt} = \frac{P}{m} \quad , \quad \frac{dP}{dt} = -U'(Q, t) + ma(Q, t) \quad (19)$$

using Eq. 8. Eq. 19 is generated by the Hamiltonian

$$H_{\text{FF}}(Z, t) = H(Z, t) + V_{\text{FF}}(Q, t) \quad (20)$$

where $Z = (Q, P)$ and V_{FF} satisfies Eq. 10. Thus Eq. 18 defines a time-dependent transformation $\mathcal{M}_t : z \rightarrow Z$, which maps any trajectory $z(t)$ evolving under $G(z, t)$ to a counterpart trajectory $Z(t)$ evolving under $H_{\text{FF}}(Z, t)$. Now consider specifically a trajectory $z(t)$ that evolves, under G , from initial conditions on the adiabatic energy shell $\mathcal{E}(0)$. As we have already seen, this trajectory remains on the adiabatic energy shell $\mathcal{E}(t)$ for all times $t \in [0, \tau]$. Under the mapping \mathcal{M}_t , its image $Z(t)$ (which evolves under H_{FF}) is displaced along the momentum axis by an amount $mv(q, t)$ (Eq. 18). By Eq. 9, $Z(t)$ begins and ends on the adiabatic energy shell: $Z(0) \in \mathcal{E}(0)$, $Z(\tau) \in \mathcal{E}(\tau)$. This is precisely the behavior we desired to generate, which concludes our proof.

In Eq. 7 we used $\mathcal{L}_{\text{FF}}(t)$ to denote a loop in phase space evolving under H_{FF} . The results

of the previous paragraph can be written compactly as follows:

$$\mathcal{M}_t : \mathcal{E}(t) \rightarrow \mathcal{L}_{\text{FF}}(t) \quad (21)$$

At any time t , $\mathcal{L}_{\text{FF}}(t)$ is the image of $\mathcal{E}(t)$ under the transformation defined by Eq. 18 (see Fig. 4 below). This result implies that the function $J(q, p, t) \equiv I(q, p - mv(q, t), t)$ is a *local dynamical invariant*. That is, if a trajectory $z(t)$ is launched from the energy shell $\mathcal{E}(0)$ and then evolves under H_{FF} , then the value of J is conserved along this trajectory: $J(z(t), t) = I_0$. For consistency, we can verify directly from Hamilton's equations that $dJ/dt = 0$ for any point $z \in \mathcal{L}_{\text{FF}}$ (see Appendix C).

To illustrate our results, we chose the dimensionless Hamiltonian

$$H(z, t) = \frac{p^2}{2} + q^4 - 16q^2 + \alpha(t)q \quad (22a)$$

with

$$\alpha(t) = 4 \cos(\pi t/\tau)[5 - \cos(2\pi t/\tau)] \quad (22b)$$

This Hamiltonian describes a particle in a double-well potential, with a linear contribution whose slope $\alpha(t)$ evolves from +16 at $t = 0$, to -16 at $t = \tau$, with $\dot{\alpha} = \ddot{\alpha} = 0$ at initial and final times. As illustrated in Fig. 1, when $\tau = 10.0$ the driving is sufficiently slow for the adiabatic invariant to be conserved with high accuracy. For the simulations described in the following paragraph, we set $\tau = 1.0$ to obtain non-adiabatic driving.

We considered an initial adiabatic energy shell $\mathcal{E}(0)$ with energy $\bar{E}(0) = 50.0$, which corresponds to $I_0 = 214.035$. We numerically determined the fields $v(q, t)$ and $a(q, t)$ and constructed $V_{\text{FF}}(q, t)$ according to Eq. 10. We then generated 50 initial conditions on the energy shell $\mathcal{E}(0)$, shown in Fig. 3(a), and we performed two sets of simulations. In the first set, trajectories were evolved from these initial conditions under $H(z, t)$. In the second set, trajectories were evolved from the same initial conditions under the Hamiltonian $H_{\text{FF}} = H + V_{\text{FF}}$. In the absence of the fast-forward potential V_{FF} , the trajectories belonging to the first set have final actions $I(z, \tau)$ that span a range of values, as seen in Fig. 3(b). By contrast, the addition of V_{FF} guides the second set of trajectories back to the adiabatic energy shell $\mathcal{E}(\tau)$, where each trajectory ends with $I(z, \tau) = I_0$; see Fig. 3(c). Note, however, that while the initial conditions in Fig. 3(a) are spaced uniformly with respect to the microcanonical

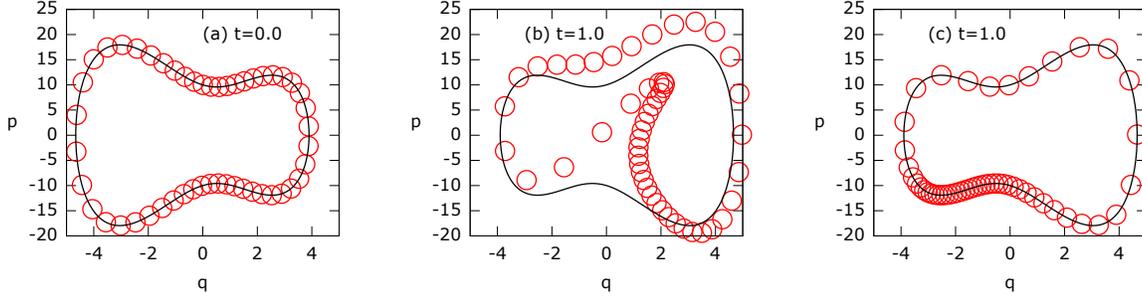


FIG. 3. Initial (a) and final (b,c) conditions for trajectories launched from a single energy shell $\mathcal{E}(0)$. The trajectories in panel (b) evolved under $H(z, t)$ (Eq. 22), while those in panel (c) evolved under $H_{\text{FF}} = H + V_{\text{FF}}$, with $\tau = 1.0$. The solid black curves show the adiabatic energy shell $\mathcal{E}(t)$ at initial and final times.

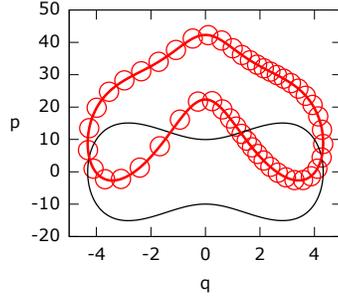


FIG. 4. A snapshot, at $t = \tau/2$, of 50 trajectories evolving under $H_{\text{FF}}(z, t)$ using a rapid protocol, with $\tau = 0.2$ (see text). The closed black loop is the adiabatic energy shell $\mathcal{E}(t)$, and the red loop above it is constructed by displacing each point on the lower loop by an amount $mv(q, t)$ along the p -axis. As predicted by Eq. 21, the trajectories coincide with the red loop.

measure, this is not the case for the final conditions in Fig. 3(c). As discussed in the Appendix D, this non-uniformity is due to the fact that $V_{\text{FF}}(q, t)$ depends on the choice of I_0 .

We also performed simulations with a shorter duration, $\tau = 0.2$. After constructing $V_{\text{FF}}(q, t)$ for this faster protocol, we simulated 50 trajectories evolving under $H_{\text{FF}} = H + V_{\text{FF}}$, using the initial conditions in Fig. 3(a). Fig. 4 depicts a snapshot of these trajectories at $t = \tau/2$. The two closed curves show the adiabatic energy shell $\mathcal{E}(t)$ and its image under the mapping $p \rightarrow p + v(q, t)$ (see Eq. 18). This figure confirms Eq. 21: the trajectories evolving under $H_{\text{FF}} = H + V_{\text{FF}}$ are located on a loop $\mathcal{L}_{\text{FF}}(t)$ that is obtained by “shearing” the instantaneous energy shell $\mathcal{E}(t)$ along the momentum axis, by an amount $mv(q, t)$.

For so-called *scale-invariant driving* [11], the time-dependence of $U(q, t)$ is described by

scaling and translation parameters $\gamma(t)$ and $f(t)$:

$$U(q, t) = \frac{1}{\gamma^2} U_0 \left(\frac{q - f}{\gamma} \right) \quad (23)$$

We then obtain $v(q, t) = (\dot{\gamma}/\gamma)(q - f) + \dot{f}$ and

$$V_{\text{FF}}(q, t) = -\frac{m}{2} \frac{\ddot{\gamma}}{\gamma} (q - f)^2 - m\ddot{f}q \quad (24)$$

which does not depend on I_0 . [11] In this rather special case, every trajectory evolving under H_{FF} returns to its adiabatic energy shell at $t = \tau$, $J(z, t)$ is a *global* dynamical invariant – it is the Lewis-Riesenfeld invariant [12, 13] – and microcanonical initial distributions are mapped to microcanonical final distributions.

The problem that we have studied has a quantum analogue, introduced by Masuda and Nakamura [3, 4]: given a Hamiltonian

$$\hat{H}(t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + U(q, t) \quad (25)$$

construct $V_{\text{FF}}^{(n)}(q, t)$ such that evolution under $\hat{H} + V_{\text{FF}}^{(n)}$ causes a selected eigenstate $\varphi_n(q, 0) \equiv \langle q | n(0) \rangle$ of $\hat{H}(0)$ to evolve to the corresponding eigenstate $\varphi_n(q, \tau)$ of $\hat{H}(\tau)$. This problem has been solved for both Schrödinger [3–9] and Dirac [10] dynamics, but the solution generically becomes singular at the nodes of $\varphi_n(q, t)$ (see e.g. Eq. 5 of Ref. [5]), hence a well-behaved $V_{\text{FF}}^{(n)}(q, t)$ cannot generally be constructed for $n > 0$.² Our result offers an alternative approach: for the corresponding classical Hamiltonian $H(z, t) = p^2/2m + U(q, t)$, choose $I_0 = 2\pi\hbar[n + (1/2)]$ and construct the fast-forward potential $V_{\text{FF}}^{(n)}(q, t)$ using the method developed in this paper. This potential is free from singularities, and for large n the Correspondence Principle suggests that evolution under $\hat{H} + V_{\text{FF}}^{(n)}$ will cause the initial eigenstate $\varphi_n(q, 0)$ to evolve approximately to the final eigenstate $\varphi_n(q, \tau)$. Preliminary numerical results support this expectation [14].

It is also interesting to compare our analysis with the *counter-diabatic* approach, where the quantum eigenstate $|n(t)\rangle$ [15, 16] or the classical action $I(z, t)$ [17–19] is preserved along the entire trajectory. In the classical case this is achieved at the cost of adding a

² The special case of scale-invariant driving is an exception to this statement.

momentum-dependent term $H_{\text{CD}}(z, t)$ rather than a potential $V_{\text{FF}}(q, t)$, to the Hamiltonian. For scale-invariant driving [11], H_{CD} coincides with our term K (Eq. 14), but more generally H_{CD} is a nonlinear function of both q and p , which may be complicated [19] and difficult to implement experimentally.

It is natural to ask whether our results can be applied to systems with $d > 1$ degrees of freedom. In certain situations of experimental relevance, such as ultracold gases in optical lattices, a separation of variables reduces a three-dimensional problem to an effectively one-dimensional one [7, 20], providing a potential platform to test our predictions. More generally, the distinction between integrable, chaotic, and mixed phase space systems becomes crucial for d -dimensional systems [21]. For integrable systems, the transformation to action-angle variables [1] may provide a useful first step to extending our results, but for chaotic or mixed systems the task is likely to be more challenging.

Adiabatic invariants enjoy a distinguished history in quantum and classical mechanics [22], but the problem of how to achieve adiabatic invariance under non-adiabatic conditions has gained attention only recently. Here we have shown how to construct a potential $V_{\text{FF}}(q, t)$ that guides trajectories launched from a given energy shell of an initial Hamiltonian to the corresponding energy shell of the final Hamiltonian, so that the initial and final values of action are identical for every trajectory.

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A. APPENDICES

A. A. Continuity conditions on $H(z, t)$

In the main text, we specified that $H(z, t)$ is constant in time for $t < 0$, then varies between $t = 0$ and $t = \tau$, then remains constant in time for $t > \tau$. As a result, H cannot be an entirely smooth function of time: for some $n \geq 0$, the derivative $\partial^n H / \partial t^n$ must be

discontinuous. We explicitly assumed that this discontinuity occurs at $n \geq 3$, giving us

$$\frac{\partial H}{\partial t}(z, 0) = \frac{\partial H}{\partial t}(z, \tau) = 0 \quad (26a)$$

$$\frac{\partial^2 H}{\partial t^2}(z, 0) = \frac{\partial^2 H}{\partial t^2}(z, \tau) = 0 \quad (26b)$$

leading to Eq. 9 of the main text.

The assumption that H is twice continuously differentiable was made both for clarity of presentation, and because it arises in proofs of the adiabatic invariance of the action [23]. In our context, however, the assumption is not necessary, therefore in the following we will discuss how Eq. 26 can be relaxed. We will continue to require that H itself is a continuous function of time. Without loss of generality, we will assume that discontinuities in $\partial H/\partial t$ and $\partial^2 H/\partial t^2$ occur only at $t = 0$ and $t = \tau$, and not within the time interval $0 < t < \tau$.

We first consider the simpler case, in which the above-mentioned discontinuity occurs at $n = 2$, i.e. Eq. 26a holds but 26b is violated. Then $v(q, 0) = v(q, \tau) = 0$, but $a(q, t)$ changes abruptly at $t = 0$ and/or $t = \tau$. In this situation the fast-forward potential will also be discontinuous at these times (see Eq. 10) but otherwise the analysis in the main text remains valid. Thus the violation of Eq. 26b simply implies that $V_{\text{FF}}(q, t)$ is turned on and/or off suddenly rather than continuously.

Now consider the case in which the discontinuity occurs at $n = 1$, hence Eq. 26a is violated. Specifically, suppose the time-dependence of the Hamiltonian is turned on abruptly: $\partial H/\partial t \neq 0$ at $t = 0^+$, hence

$$v_0(q) \equiv v(q, 0^+) \neq 0 \quad (27)$$

The velocity field changes suddenly from $v(q, 0^-) = 0$ to $v(q, 0^+) = v_0(q)$. The term $\partial v/\partial t$ in Eq. 9 then leads to a singular term $v_0(q)\delta(t)$ in the acceleration field $a(q, t)$. By Eq. 10, this term leads to a contribution to V_{FF} that is proportional to $\delta(t)$, which produces an impulsive force field at $t = 0$:

$$-\frac{\partial V_{\text{FF}}}{\partial q}(q, t) = mv_0(q)\delta(t) + [\text{other terms}] \quad (28)$$

The effect of this impulse is simple to state: a trajectory located at (q, p) at time $t = 0^-$ is instantaneously “boosted” to $(q, p + mv_0(q))$ at time $t = 0^+$ as it evolves under H_{FF} .

Similar comments apply if $\partial H/\partial t \neq 0$ at $t = \tau^-$. Then

$$v_\tau(q) \equiv v(q, \tau^-) \neq 0 \quad (29)$$

and we get a singular term in V_{FF} that produces an impulsive force

$$-mv_\tau(q)\delta(t - \tau) \quad (30)$$

Now consider a collection of trajectories that, for $t < 0$, are found on the adiabatic energy shell $\mathcal{E}(0)$. As in the main text, let the loop $\mathcal{L}_{\text{FF}}(t)$ describe the evolution of these trajectories, under $H_{\text{FF}}(z, t)$. At $t = 0$, the impulsive force in Eq. 28 boosts these trajectories from $\mathcal{L}_{\text{FF}}(0^-) = \mathcal{E}(0)$ to a loop $\mathcal{L}_{\text{FF}}(0^+)$ that is displaced along the momentum axis by an amount $mv_0(q)$. Subsequently, this loop evolves exactly as described in the main text: for $0 < t < \tau$, $\mathcal{L}_{\text{FF}}(t)$ is displaced from the adiabatic energy shell $\mathcal{E}(t)$ by an amount $mv(q, t)$ (Eq. 21). In particular, at $t = \tau^-$ this loop is displaced from $\mathcal{E}(\tau)$ by $mv_\tau(q)$. The final impulse at $t = \tau$ (Eq. 30) instantaneously brings the collection of trajectories from $\mathcal{L}_{\text{FF}}(\tau^-)$ to $\mathcal{L}_{\text{FF}}(\tau^+) = \mathcal{E}(\tau)$.

Thus, non-vanishing derivatives $\partial H/\partial t$ at initial and final times can be accommodated by impulse-like terms in $V_{\text{FF}}(q, t)$. See Section III.A. of Ref. [11] for an example that illustrates this point in the context of scale-invariant driving.

B. Flow under G preserves the adiabatic energy shell

The Hamiltonian $G(z, t) = H + K$ generates the flow (Eq. 16)

$$\dot{q} = \frac{p}{m} + v(q, t) \quad , \quad \dot{p} = -\frac{\partial U}{\partial q}(q, t) - p\frac{\partial v}{\partial q}(q, t) \quad (31)$$

Let $\dot{H}(q, p, t)$ denote the instantaneous rate of change of H , along a trajectory that passes through the point (q, p) at time t as it evolves under these dynamics:

$$\begin{aligned} \dot{H}(q, p, t) &\equiv \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial t} \\ &= \frac{\partial U}{\partial q}v - \frac{p^2}{m}\frac{\partial v}{\partial q} + \frac{\partial U}{\partial t} \end{aligned} \quad (32)$$

To establish that the flow given by Eq. 31 preserves the adiabatic energy shell, we must show that

$$\dot{H}(q, p, t) = \frac{d}{dt}\bar{E}(t) \quad \text{when } (q, p) \in \mathcal{E}(t) \quad (33)$$

We evaluate \dot{H} at a point $(q, p) \in \mathcal{E}(t)$, by setting $p = \pm\bar{p}(q, t) = \pm [2m(\bar{E} - U)]^{1/2}$:

$$\begin{aligned} \dot{H}(q, \pm\bar{p}, t) &= \frac{\partial U}{\partial q}v - 2(\bar{E} - U)\frac{\partial v}{\partial q} + \frac{\partial U}{\partial t} \\ &= -\frac{1}{v}\frac{\partial}{\partial q} [(\bar{E} - U)v^2] + \frac{\partial U}{\partial t} \\ &= \frac{\partial_q S}{\partial_t S} \frac{\partial}{\partial q} \left[\frac{\bar{p}^2}{2m} \left(\frac{\partial_t S}{\partial_q S} \right)^2 \right] + \frac{\partial U}{\partial t} \\ &= \frac{\bar{p}}{2m} \partial_q \partial_t S + \frac{\partial U}{\partial t} = \frac{\bar{p}}{m} \frac{\partial \bar{p}}{\partial t} + \frac{\partial U}{\partial t} \\ &= \frac{\partial}{\partial t} \left[\frac{\bar{p}^2(q, t)}{2m} + U(q, t) \right] = \frac{d}{dt}\bar{E}(t) \end{aligned} \quad (34)$$

which is the desired result. In obtaining Eq. 34 we have made repeated use of the identities $\partial_q S = 2\bar{p}$ and $v = -\partial_t S / \partial_q S$ (Eqs. 11 and 12).

C. C. Local dynamical invariance of $J(q, p, t)$

$H_{\text{FF}}(z, t)$ generates the equations of motion

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -U' + ma = -U' + mv'v + m\frac{\partial v}{\partial t} \quad (35)$$

Consider the quantity

$$J(q, p, t) = I(q, p - mv(q, t), t) \quad (36)$$

and let $\dot{J}(z, t)$ denote the instantaneous rate of change of J along a trajectory that passes through the point $z = (q, p)$ at time t . We have, by direct substitution,

$$\begin{aligned} \dot{J}(z, t) &= \frac{\partial I}{\partial q} \dot{q} + \frac{\partial I}{\partial p} \left(\dot{p} - mv' \dot{q} - m \frac{\partial v}{\partial t} \right) + \frac{\partial I}{\partial t} \\ &= \frac{\partial I}{\partial q} \frac{p}{m} - \frac{\partial I}{\partial p} U' - \frac{\partial I}{\partial p} v'(p - mv) + \frac{\partial I}{\partial t} \end{aligned} \quad (37)$$

where the derivatives of I are evaluated at $(q, p - mv(q, t), t)$.

In general $\dot{J}(z, t) \neq 0$. However, let us now restrict our attention to a point z that satisfies

$J(z, t) = I_0$ at a particular time t . At such a point, we have

$$p = \pm \bar{p}(q, t) + mv(q, t) \quad (38)$$

with $\bar{p} = [2m(\bar{E} - U)]^{1/2}$ as in the main text. Taking $p = \bar{p} + mv$ for specificity (the case $p = -\bar{p} + mv$ gives the same result) we get

$$\begin{aligned} \dot{J}(z, t) &= \frac{\partial I}{\partial q} \left(\frac{\bar{p}}{m} + v \right) - \frac{\partial I}{\partial p} U' - \frac{\partial I}{\partial p} v' \bar{p} + \frac{\partial I}{\partial t} \\ &= \{I, H\} + \{I, K\} + \frac{\partial I}{\partial t} \end{aligned} \quad (39)$$

where all quantities on the right side are evaluated at $(q, \bar{p}) \in \mathcal{E}(t)$. From Eqs. 4 and 15 we conclude that the right side of the above equation is zero, hence

$$J(z, t) = I_0 \quad \Rightarrow \quad \dot{J}(z, t) = 0 \quad (40)$$

where the symbol \Rightarrow is short for “implies that”.

Eq. 40 establishes that $J(z, t)$ is a local dynamical invariant, in the following sense. Along trajectories z_t evolving under $H_{\text{FF}}(z, t)$ from initial conditions $z_0 \in \mathcal{E}(0)$, the value of J remains constant:

$$J(z_t, t) = I_0 \quad (41)$$

D. D. Evolution of the microcanonical measure under H_{FF}

As mentioned in the main text, initial conditions that are sampled from a microcanonical distribution on $\mathcal{E}(0)$ generally evolve (under H_{FF}) to final conditions that are *not* distributed microcanonically on $\mathcal{E}(\tau)$, as illustrated in Figs. 2(a) and 2(c). To understand this point, let

$$\Phi_{\text{FF}} : z_0 \rightarrow z_\tau \quad (42)$$

denote evolution under $H_{\text{FF}}(z, t)$ from $t = 0$ to $t = \tau$. Φ_{FF} maps initial points $z_0 \in \mathcal{E}(0)$ to final points $z_\tau \in \mathcal{E}(\tau)$. Now consider an initial phase space distribution $\rho(z, 0)$ that is

uniform in the thin annular region \mathcal{R} between the energy shells $\mathcal{E}(0)$ and

$$\mathcal{E}_{dE}(0) \equiv \{z | H(z, 0) = \bar{E}(0) + dE\} \quad (43)$$

and zero elsewhere. In the limit $dE \rightarrow 0$, this distribution converges to a microcanonical distribution on $\mathcal{E}(0)$.

For finite dE , $\rho(z, 0)$ evolves to a distribution $\rho(z, \tau)$ that is uniform (by Liouville's theorem) in the region $\mathcal{R}' = \Phi_{\text{FF}}(\mathcal{R})$ between the *images* of $\mathcal{E}(0)$ and $\mathcal{E}_{dE}(0)$ under Φ_{FF} . Although Φ_{FF} maps $\mathcal{E}(0)$ to $\mathcal{E}(\tau)$, in general it does not map $\mathcal{E}_{dE}(0)$ to an energy shell of $H(z, t)$. As a result, in the limit $dE \rightarrow 0$, $\rho(z, \tau)$ converges to a distribution on $\mathcal{E}(\tau)$ that is not microcanonical. Thus the clustering of points in Fig. 2(c) traces back to the fact that $V_{\text{FF}}(q, t)$ depends on the choice of I_0 .

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