©2017 American Physical Society. Access to this work was provided by the University of Maryland, Baltimore County (UMBC) ScholarWorks@UMBC digital repository on the Maryland Shared Open Access (MD-SOAR) platform.

## Please provide feedback

Please support the ScholarWorks@UMBC repository by emailing scholarworks-group@umbc.edu and telling us what having access to this work means to you and why it's important to you. Thank you.

# Fast forward to the classical adiabatic invariant 

Christopher Jarzynski<br>Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742, USA; Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742, USA and Department of Physics, University of Maryland, College Park, Maryland 20742, USA

Sebastian Deffner<br>Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA and Department of Physics, University of Maryland Baltimore County, Baltimore, Maryland 21250, USA

Ayoti Patra
Department of Physics, University of Maryland, College Park, Maryland 20742, USA
Yiğit Subaşı
Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742, USA and Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
(Received 24 May 2016; revised manuscript received 9 February 2017; published 10 March 2017)


#### Abstract

We show how the classical action, an adiabatic invariant, can be preserved under nonadiabatic conditions. Specifically, for a time-dependent Hamiltonian $H=p^{2} / 2 m+U(q, t)$ in one degree of freedom, and for an arbitrary choice of action $I_{0}$, we construct a so-called fast-forward potential energy function $V_{\mathrm{FF}}(q, t)$ 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.


DOI: 10.1103/PhysRevE. 95.032122

For a classical system in one degree of freedom, the action variable $I=\oint p d q$ 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 $\omega$ change with time, but their ratio $E / \omega$, 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 following question: How can the adiabatic invariant be preserved under nonadiabatic driving conditions? We consider a Hamiltonian $H(q, p, t)=p^{2} / 2 m+U(q, t)$ 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 nonadiabatic 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 $\tau$, 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 $V_{\mathrm{FF}}(q, t)$ with the following property. Under the dynamics generated by the Hamiltonian $H_{\mathrm{FF}}=H+V_{\mathrm{FF}}$, all trajectories that begin with action $I_{0}$ at $t=0$ will end with 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 selfcontained 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

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

$H$ varies with time during the interval $0 \leqslant t \leqslant \tau$, but is constant outside this interval. We assume that $H$ is twice continuously differentiable with respect to time, and 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

$$
\begin{equation*}
\Omega(E, t)=\int d z \theta[E-H(z, t)]=\oint_{E} p d q \tag{2}
\end{equation*}
$$



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 $I=\oint p d q$. Trajectories were generated using $H(q, p, t)$ given by Eq. (22), setting $\tau=10.0$ to achieve slow driving.
is the volume of phase space enclosed by the energy shell $E$ of $H(z, t)$, and the action,

$$
\begin{equation*}
I(z, t)=\Omega[H(z, t), t], \tag{3}
\end{equation*}
$$

is the volume enclosed by the energy shell that contains the point $z$. Equation (3) implies

$$
\begin{equation*}
\{I, H\} \equiv \frac{\partial I}{\partial q} \frac{\partial H}{\partial p}-\frac{\partial I}{\partial p} \frac{\partial H}{\partial q}=0 \tag{4}
\end{equation*}
$$

which will prove useful.
Let us choose an arbitrary action value $I_{0}>0$ and define the adiabatic energy $\bar{E}(t)$ by the condition

$$
\begin{equation*}
\Omega[\bar{E}(t), t]=I_{0} \tag{5}
\end{equation*}
$$

The adiabatic energy shell $\mathcal{E}(t)=\{z \mid H(z, t)=\bar{E}(t)\}$ 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,

$$
\begin{equation*}
\mathcal{L}(t)=\left\{z=z_{t}\left(z_{0}\right) \mid z_{0} \in \mathcal{E}(0)\right\} \tag{6}
\end{equation*}
$$

where $z_{t}\left(z_{0}\right)$ 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 $V_{\mathrm{FF}}(q, t)$, let $z_{t}^{\mathrm{FF}}\left(z_{0}\right)$ indicate evolution under $H_{\mathrm{FF}}=H+V_{\mathrm{FF}}$, and consider the loop

$$
\begin{equation*}
\mathcal{L}_{\mathrm{FF}}(t)=\left\{z=z_{t}^{\mathrm{FF}}\left(z_{0}\right) \mid z_{0} \in \mathcal{E}(0)\right\} \tag{7}
\end{equation*}
$$

that evolves under $H_{\mathrm{FF}}$ from the initial conditions defined by $\mathcal{E}(0)$. Our aim is to construct $V_{\mathrm{FF}}(q, t)$ such that $\mathcal{L}_{\mathrm{FF}}(\tau)=\mathcal{E}(\tau)$ : 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 $V_{\mathrm{FF}}$ 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 $V_{\mathrm{FF}}(q, t)$ with this property.

Imagine a set of line segments at locations $q_{1}(t), \ldots, q_{N-1}(t)$ 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 $a(q, t)$ :

$$
\begin{equation*}
\frac{d q_{n}}{d t}=v\left(q_{n}, t\right), \quad \frac{d^{2} q_{n}}{d t^{2}}=a\left(q_{n}, t\right)=\frac{\partial v}{\partial q} v+\frac{\partial v}{\partial t} . \tag{8}
\end{equation*}
$$

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

$$
\begin{equation*}
v(q, 0)=v(q, \tau)=0, \quad a(q, 0)=a(q, \tau)=0 \tag{9}
\end{equation*}
$$

We now claim that the desired fast-forward potential satisfies

$$
\begin{equation*}
-\frac{\partial V_{\mathrm{FF}}}{\partial q}=m a \tag{10a}
\end{equation*}
$$



FIG. 2. The region of phase space enclosed by the adiabatic energy shell $\mathcal{E}(t)$ is divided by line segments at $\left\{q_{n}(t)\right\}$ into vertical strips of equal phase space volume. The motion of these lines is described by velocity and acceleration fields $v(q, t)$ and $a(q, t)$.
and therefore it is given by ${ }^{1}$

$$
\begin{equation*}
V_{\mathrm{FF}}(q, t)=-\int_{q_{0}(t)}^{q} d q^{\prime} m a\left(q^{\prime}, t\right) \tag{10b}
\end{equation*}
$$

By Eq. (9), $V_{\mathrm{FF}}(q, t)$ 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 $V_{\mathrm{FF}}(q, t)$. 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 $q \in\left[q_{0}, q_{N}\right]$, is given by

$$
\begin{equation*}
S(q, t)=2 \int_{q_{0}(t)}^{q} d q^{\prime} \bar{p}\left(q^{\prime}, t\right) \tag{11}
\end{equation*}
$$

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

$$
\begin{equation*}
v(q, t)=\left.\frac{d q}{d t}\right|_{S}=-\frac{\partial_{t} S}{\partial_{q} S} \tag{12}
\end{equation*}
$$

Now consider a point in phase space, $\left[q_{n}(t), p_{n}(t)\right]$, attached to the top of the $n$th line segment: $p_{n}=\bar{p}\left(q_{n}, t\right)$ (see Fig. 2). As the shape of the energy shell and the locations of the line segments vary parametrically with time, this point $\left(q_{n}, p_{n}\right)$ moves in phase space, surfing the upper branch of the energy shell. This motion is described by the equations

$$
\begin{equation*}
\dot{q}_{n}=v\left(q_{n}, t\right), \quad \dot{p}_{n}=-p_{n} v^{\prime}\left(q_{n}, t\right), \tag{13}
\end{equation*}
$$

where the equation for $\dot{p}_{n}$ is obtained by demanding that the phase space volume of the strip between neighboring vertical lines, $\delta S_{n} \equiv 2 p_{n}\left(q_{n+1}-q_{n}\right)$, remain constant. In Eq. (13) and throughout the paper, dots and primes denote derivatives with respect to $t$ and $q$, respectively. Equation (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

$$
\begin{equation*}
K(q, p, t)=p v(q, t) \tag{14}
\end{equation*}
$$

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 $\delta t$, 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,

[^0]we have
\[

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

\]

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

$$
\begin{equation*}
\dot{q}=\frac{p}{m}+v(q, t), \quad \dot{p}=-U^{\prime}(q, t)-p v^{\prime}(q, t) . \tag{16}
\end{equation*}
$$

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

$$
\begin{equation*}
\dot{I}=\frac{d}{d t} I[z(t), t]=\frac{\partial I}{\partial t}+\{I, H\}+\{I, K\} \tag{17}
\end{equation*}
$$

Equations (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 $\delta t$, 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 $V_{\mathrm{FF}}(q, t)$ that we seek.

Consider the evolution of the observables

$$
\begin{equation*}
Q(q, p, t)=q, \quad P(q, p, t)=p+m v(q, t), \tag{18}
\end{equation*}
$$

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

$$
\begin{equation*}
\frac{d Q}{d t}=\frac{P}{m}, \quad \frac{d P}{d t}=-U^{\prime}(Q, t)+m a(Q, t) \tag{19}
\end{equation*}
$$

using Eq. (8). Equation (19) is generated by the Hamiltonian

$$
\begin{equation*}
H_{\mathrm{FF}}(Z, t)=H(Z, t)+V_{\mathrm{FF}}(Q, t), \tag{20}
\end{equation*}
$$

where $Z=(Q, P)$ and $V_{\mathrm{FF}}$ 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 $H_{\mathrm{FF}}(Z, t)$. 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 $H_{\mathrm{FF}}$ ) is displaced along the momentum axis by an amount $m v(q, t)$ [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 $\mathcal{L}_{\mathrm{FF}}(t)$ to denote a loop in phase space evolving under $H_{\mathrm{FF}}$. The results of the previous paragraph can be written compactly as follows:

$$
\begin{equation*}
\mathcal{M}_{t}: \mathcal{E}(t) \rightarrow \mathcal{L}_{\mathrm{FF}}(t) \tag{21}
\end{equation*}
$$

At any time $t, \mathcal{L}_{\mathrm{FF}}(t)$ is the image of $\mathcal{E}(t)$ under the transformation defined by Eq. (18) (see Fig. 4 below). This result implies that the function $J(q, p, t) \equiv I[q, p-m v(q, t), t]$ is


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 $H_{\mathrm{FF}}=H+V_{\mathrm{FF}}$, with $\tau=1.0$. The solid black curves show the adiabatic energy shell $\mathcal{E}(t)$ at initial and final times.
a local dynamical invariant. That is, if a trajectory $z(t)$ is launched from the energy shell $\mathcal{E}(0)$ and then evolves under $H_{\mathrm{FF}}$, 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 $d J / d t=0$ for any point $z \in \mathcal{L}_{\mathrm{FF}}$ (see Appendix C).

To illustrate our results, we chose the dimensionless Hamiltonian

$$
\begin{equation*}
H(z, t)=\frac{p^{2}}{2}+q^{4}-16 q^{2}+\alpha(t) q \tag{22a}
\end{equation*}
$$

with

$$
\begin{equation*}
\alpha(t)=4 \cos (\pi t / \tau)[5-\cos (2 \pi t / \tau)] \tag{22b}
\end{equation*}
$$

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 nonadiabatic 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 $V_{\mathrm{FF}}(q, t)$ 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 $H_{\mathrm{FF}}=$ $H+V_{\mathrm{FF}}$. In the absence of the fast-forward potential $V_{\mathrm{FF}}$, 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 $V_{\mathrm{FF}}$ 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 measure, this is not the case for the final conditions in Fig. 3(c). As discussed in the Appendix D, this nonuniformity is due to the fact that $V_{\mathrm{FF}}(q, t)$ depends on the choice of $I_{0}$.

We also performed simulations with a shorter duration, $\tau=0.2$. After constructing $V_{\mathrm{FF}}(q, t)$ for this faster protocol, we simulated 50 trajectories evolving under $H_{\mathrm{FF}}=H+V_{\mathrm{FF}}$, using the initial conditions in Fig. 3(a). Figure 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 $H_{\mathrm{FF}}=H+V_{\mathrm{FF}}$ are located on a loop $\mathcal{L}_{\mathrm{FF}}(t)$ that is obtained by shearing the instantaneous energy shell $\mathcal{E}(t)$ along the momentum axis, by an amount $m v(q, t)$.

For so-called scale-invariant driving [11], the time dependence of $U(q, t)$ is described by scaling and translation parameters $\gamma(t)$ and $f(t)$ :

$$
\begin{equation*}
U(q, t)=\frac{1}{\gamma^{2}} U_{0}\left(\frac{q-f}{\gamma}\right) \tag{23}
\end{equation*}
$$

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

$$
\begin{equation*}
V_{\mathrm{FF}}(q, t)=-\frac{m}{2} \frac{\ddot{\gamma}}{\gamma}(q-f)^{2}-m \ddot{f} q \tag{24}
\end{equation*}
$$



FIG. 4. A snapshot, at $t=\tau / 2$, of 50 trajectories evolving under $H_{\mathrm{FF}}(z, t)$ 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 $m v(q, t)$ along the $p$ axis. As predicted by Eq. (21), the trajectories coincide with the red loop.
which does not depend on $I_{0}$. [11] In this rather special case, every trajectory evolving under $H_{\mathrm{FF}}$ 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 analog, introduced by Masuda and Nakamura [3,4]: Given a Hamiltonian

$$
\begin{equation*}
\hat{H}(t)=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial q^{2}}+U(q, t) \tag{25}
\end{equation*}
$$

construct $V_{\mathrm{FF}}^{(n)}(q, t)$ such that evolution under $\hat{H}+V_{\mathrm{FF}}^{(n)}$ causes a selected eigenstate $\varphi_{n}(q, 0) \equiv\langle q \mid n(0)\rangle$ 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]), and hence a well-behaved $V_{\mathrm{FF}}^{(n)}(q, t)$ cannot generally be constructed for $n>0 .{ }^{2}$ Our result offers an alternative approach: For the corresponding classical Hamiltonian $H(z, t)=p^{2} / 2 m+U(q, t)$, choose $I_{0}=2 \pi \hbar[n+(1 / 2)]$ and construct the fast-forward potential $V_{\mathrm{FF}}^{(n)}(q, t)$ using the method developed in this paper. This potential is free from singularities, and for large $n$ the correspondence principle suggests that evolution under $\hat{H}+V_{\mathrm{FF}}^{(n)}$ 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 counterdiabatic 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 momentum-dependent term $H_{\mathrm{CD}}(z, t)$ rather than a potential $V_{\mathrm{FF}}(q, t)$, to the Hamiltonian. For scale-invariant driving [11], $H_{\mathrm{CD}}$ coincides with our term $K$ [Eq. (14)], but more generally $H_{\mathrm{CD}}$ 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 nonadiabatic conditions has gained attention only recently. Here we have shown how to construct a potential $V_{\mathrm{FF}}(q, t)$ that guides trajectories launched

[^1]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.

## ACKNOWLEDGMENTS

We acknowledge financial support from the US National Science Foundation under Grant No. DMR-1506969 (C.J.), the US Department of Energy through a LANL Directors Funded Fellowship (S.D.), and from the U.S. Army Research Laboratory and the U.S. Army Research Office under Contract No. W911NF-13-1-0390 (A.P., Y.S.).

## APPENDIX A: CONTINUITY CONDITIONS ON $\boldsymbol{H}(z, t)$

In the main text, we specified that $H(z, t)$ is constant in time for $t<0$, then varies between $t=0$ and $t=\tau$, and then remains constant in time for $t>\tau$. As a result, $H$ cannot be an entirely smooth function of time: For some $n \geqslant 0$, the derivative $\partial^{n} H / \partial t^{n}$ must be discontinuous. We explicitly assumed that this discontinuity occurs at $n \geqslant 3$, giving us

$$
\begin{align*}
\frac{\partial H}{\partial t}(z, 0) & =\frac{\partial H}{\partial t}(z, \tau)=0  \tag{A1a}\\
\frac{\partial^{2} H}{\partial t^{2}}(z, 0) & =\frac{\partial^{2} H}{\partial t^{2}}(z, \tau)=0 \tag{Alb}
\end{align*}
$$

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. (A1) 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 abovementioned discontinuity occurs at $n=2$, i.e., Eq. (A1a) holds but Eq. (A1b) 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. (A1b) simply implies that $V_{\mathrm{FF}}(q, t)$ is turned on and/or off suddenly rather than continuously.

Now consider the case in which the discontinuity occurs at $n=1$; hence Eq. (A1a) is violated. Specifically, suppose the time dependence of the Hamiltonian is turned on abruptly: $\partial H / \partial t \neq 0$ at $t=0^{+}$, and hence

$$
\begin{equation*}
v_{0}(q) \equiv v\left(q, 0^{+}\right) \neq 0 \tag{A2}
\end{equation*}
$$

The velocity field changes suddenly from $v\left(q, 0^{-}\right)=0$ to $v\left(q, 0^{+}\right)=v_{0}(q)$. 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 $V_{\mathrm{FF}}$ that is proportional to $\delta(t)$, which produces an impulsive force field
at $t=0$ :

$$
\begin{equation*}
-\frac{\partial V_{\mathrm{FF}}}{\partial q}(q, t)=m v_{0}(q) \delta(t)+[\text { other terms }] . \tag{A3}
\end{equation*}
$$

The effect of this impulse is simple to state: A trajectory located at $(q, p)$ at time $t=0^{-}$is instantaneously boosted to [ $q, p+$ $\left.m v_{0}(q)\right]$ at time $t=0^{+}$as it evolves under $H_{\mathrm{FF}}$.

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

$$
\begin{equation*}
v_{\tau}(q) \equiv v\left(q, \tau^{-}\right) \neq 0, \tag{A4}
\end{equation*}
$$

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

$$
\begin{equation*}
-m v_{\tau}(q) \delta(t-\tau) \tag{A5}
\end{equation*}
$$

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 $\mathcal{L}_{\mathrm{FF}}(t)$ describe the evolution of these trajectories, under $H_{\mathrm{FF}}(z, t)$. At $t=0$, the impulsive force in Eq. (A3) boosts these trajectories from $\mathcal{L}_{\mathrm{FF}}\left(0^{-}\right)=\mathcal{E}(0)$ to a loop $\mathcal{L}_{\mathrm{FF}}\left(0^{+}\right)$that is displaced along the momentum axis by an amount $m v_{0}(q)$. Subsequently, this loop evolves exactly as described in the main text: For $0<t<\tau$, $\mathcal{L}_{\mathrm{FF}}(t)$ is displaced from the adiabatic energy shell $\mathcal{E}(t)$ by an amount $m v(q, t)$ [Eq. (21)]. In particular, at $t=\tau^{-}$this loop is displaced from $\mathcal{E}(\tau)$ by $m v_{\tau}(q)$. The final impulse at $t=\tau$ [Eq. (A5)] instantaneously brings the collection of trajectories from $\mathcal{L}_{\mathrm{FF}}\left(\tau^{-}\right)$to $\mathcal{L}_{\mathrm{FF}}\left(\tau^{+}\right)=\mathcal{E}(\tau)$.

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

## APPENDIX B: FLOW UNDER G PRESERVES THE ADIABATIC ENERGY SHELL

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

$$
\begin{equation*}
\dot{q}=\frac{p}{m}+v(q, t), \quad \dot{p}=-\frac{\partial U}{\partial q}(q, t)-p \frac{\partial v}{\partial q}(q, t) . \tag{B1}
\end{equation*}
$$

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:

$$
\begin{align*}
\dot{H}(q, p, t) & \equiv \frac{\partial H}{\partial q} \dot{q}+\frac{\partial H}{\partial p} \dot{p}+\frac{\partial H}{\partial t} \\
& =\frac{\partial U}{\partial q} v-\frac{p^{2}}{m} \frac{\partial v}{\partial q}+\frac{\partial U}{\partial t} . \tag{B2}
\end{align*}
$$

To establish that the flow given by Eq. (B1) preserves the adiabatic energy shell, we must show that

$$
\begin{equation*}
\dot{H}(q, p, t)=\frac{d}{d t} \bar{E}(t) \quad \text { when } \quad(q, p) \in \mathcal{E}(t) \tag{B3}
\end{equation*}
$$

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

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

$$
\begin{align*}
& =\frac{\partial_{q} S}{\partial_{t} S} \frac{\partial}{\partial q}\left[\frac{\bar{p}^{2}}{2 m}\left(\frac{\partial_{t} S}{\partial_{q} S}\right)^{2}\right]+\frac{\partial U}{\partial t} \\
& =\frac{\bar{p}}{2 m} \partial_{q} \partial_{t} S+\frac{\partial U}{\partial t}=\frac{\bar{p}}{m} \frac{\partial \bar{p}}{\partial t}+\frac{\partial U}{\partial t} \\
& =\frac{\partial}{\partial t}\left[\frac{\bar{p}^{2}(q, t)}{2 m}+U(q, t)\right]=\frac{d}{d t} \bar{E}(t), \tag{B4}
\end{align*}
$$

which is the desired result. In obtaining Eq. (B4) 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)].

## APPENDIX C: LOCAL DYNAMICAL INVARIANCE OF $J(q, p, t)$

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

$$
\begin{equation*}
\dot{q}=\frac{p}{m}, \quad \dot{p}=-U^{\prime}+m a=-U^{\prime}+m v^{\prime} v+m \frac{\partial v}{\partial t} \tag{C1}
\end{equation*}
$$

Consider the quantity

$$
\begin{equation*}
J(q, p, t)=I[q, p-m v(q, t), t] \tag{C2}
\end{equation*}
$$

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,

$$
\begin{align*}
\dot{J}(z, t) & =\frac{\partial I}{\partial q} \dot{q}+\frac{\partial I}{\partial p}\left(\dot{p}-m v^{\prime} \dot{q}-m \frac{\partial v}{\partial t}\right)+\frac{\partial I}{\partial t} \\
& =\frac{\partial I}{\partial q} \frac{p}{m}-\frac{\partial I}{\partial p} U^{\prime}-\frac{\partial I}{\partial p} v^{\prime}(p-m v)+\frac{\partial I}{\partial t} \tag{C3}
\end{align*}
$$

where the derivatives of $I$ are evaluated at $[q, p-m v(q, t), t]$.
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

$$
\begin{equation*}
p= \pm \bar{p}(q, t)+m v(q, t) \tag{C4}
\end{equation*}
$$

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

$$
\begin{align*}
\dot{J}(z, t) & =\frac{\partial I}{\partial q}\left(\frac{\bar{p}}{m}+v\right)-\frac{\partial I}{\partial p} U^{\prime}-\frac{\partial I}{\partial p} v^{\prime} \bar{p}+\frac{\partial I}{\partial t} \\
& =\{I, H\}+\{I, K\}+\frac{\partial I}{\partial t} \tag{C5}
\end{align*}
$$

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, and hence

$$
\begin{equation*}
J(z, t)=I_{0} \quad \Rightarrow \quad \dot{J}(z, t)=0 \tag{C6}
\end{equation*}
$$

where the symbol $\Rightarrow$ is short for "implies that."
Equation (C6) establishes that $J(z, t)$ is a local dynamical invariant, in the following sense. Along trajectories $z_{t}$ evolving under $H_{\mathrm{FF}}(z, t)$ from initial conditions $z_{0} \in \mathcal{E}(0)$, the value of $J$ remains constant:

$$
\begin{equation*}
J\left(z_{t}, t\right)=I_{0} \tag{C7}
\end{equation*}
$$

## APPENDIX D: EVOLUTION OF THE MICROCANONICAL MEASURE UNDER $\boldsymbol{H}_{\mathrm{FF}}$

As mentioned in the main text, initial conditions that are sampled from a microcanonical distribution on $\mathcal{E}(0)$ generally evolve (under $H_{\mathrm{FF}}$ ) 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

$$
\begin{equation*}
\Phi_{\mathrm{FF}}: z_{0} \rightarrow z_{\tau} \tag{D1}
\end{equation*}
$$

denote evolution under $H_{\mathrm{FF}}(z, t)$ from $t=0$ to $t=\tau$. $\Phi_{\mathrm{FF}}$ 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

$$
\begin{equation*}
\mathcal{E}_{\mathrm{d} E}(0) \equiv\{z \mid H(z, 0)=\bar{E}(0)+d E\} \tag{D2}
\end{equation*}
$$

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

For finite $d E, \rho(z, 0)$ evolves to a distribution $\rho(z, \tau)$ that is uniform (by Liouville's theorem) in the region $\mathcal{R}^{\prime}=\Phi_{\mathrm{FF}}(\mathcal{R})$ between the images of $\mathcal{E}(0)$ and $\mathcal{E}_{\mathrm{d} E}(0)$ under $\Phi_{\mathrm{FF}}$. Although $\Phi_{\mathrm{FF}}$ maps $\mathcal{E}(0)$ to $\mathcal{E}(\tau)$, in general it does not map $\mathcal{E}_{\mathrm{d} E}(0)$ to an energy shell of $H(z, t)$. As a result, in the limit $\mathrm{d} E \rightarrow 0, \rho(z, \tau)$ 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 $V_{\mathrm{FF}}(q, t)$ depends on the choice of $I_{0}$.
[1] H. Goldstein, Classical Mechanics, 2nd ed. (Addison-Wesley, Reading, MA, 1980).
[2] E. Torrontegui, S. S. Ibáñez, S. Martínez-Garaot, M. Modugno, A. del Campo, D. Guéry-Odelin, A. Ruschhaupt, X. Chen, and J. G. Muga, Adv. At. Mol. Opt. Phys. 62, 117 (2013).
[3] S. Masuda and K. Nakamura, Proc. R. Soc. London, Ser. A 466, 1135 (2010).
[4] S. Masuda and K. Nakamura, Phys. Rev. A 84, 043434 (2011).
[5] E. Torrontegui, S. Martínez-Garaot, A. Ruschhaupt, and J. G. Muga, Phys. Rev. A 86, 013601 (2012).
[6] E. Torrontegui, X. Chen, M. Modugno, S. Schmidt, A. Rauschhaupt, and J. G. Muga, New J. Phys. 14, 013031 (2012).
[7] S. Masuda, K. Nakamura, and A. del Campo, Phys. Rev. Lett. 113, 063003 (2014).
[8] A. Kiely, J. P. L. McGuinness, J. G. Muga, and A. Rauschhaupt, J. Phys. B: At. Mol. Opt. Phys. 48, 075503 (2015).
[9] K. Takahashi, Phys. Rev. A 91, 042115 (2015).
[10] S. Deffner, New J. Phys. 18, 012001 (2016).
[11] S. Deffner, C. Jarzynski, and A. del Campo, Phys. Rev. X 4, 021013 (2014).
[12] H. R. Lewis, J. Math. Phys. 9, 1976 (1968).
[13] H. R. Lewis and W. B. Riesenfeld, J. Math. Phys. 10, 1458 (1969).
[14] A. Patra and C. Jarzynski (unpublished).
[15] M. Demirplak and S. A. Rice, J. Chem. Phys. A 107, 9937 (2003).
[16] M. Berry, J. Phys. A: Math. Theor. 42, 365303 (2009).
[17] C. Jarzynski, Phys. Rev. A 88, 040101(R) (2013).
[18] J. Deng, Q. Wang, Z. Liu, P. Hänggi, and J. Gong, Phys. Rev. E 88, 062122 (2013).
[19] A. Patra and C. Jarzynski, J. Phys. Chem. B (2016), doi:10.1021/acs.jpcb.6b08769.
[20] I. Bloch, Nat. Phys. 1, 23 (2005).
[21] M. Berry, AIP Conference Proceedings Vol. 46, edited by S. Jorna (AIP, New York, 1978), p. 16.
[22] P. Navarro and E. Pérez, Arch. Hist. Exact Sci. 60, 209 (2006).
[23] V. I. Arnold, Mathematical Methods of Classical Mechanics (Springer, New York, 1978).


[^0]:    ${ }^{1}$ The choice of setting the lower bound of integration at $q_{0}(t)$ is arbitrary. A different choice would modify $V_{\mathrm{FF}}(q, t)$ by an additive function $\phi(t)$, having no effect on the dynamics.

[^1]:    ${ }^{2}$ The special case of scale-invariant driving is an exception to this statement.

