Nonadiabatic tunneling in ponderomotive barriers

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Localized regions of intense large-scale radiofrequency field are known to act like effective ("ponderomotive") potential barriers, which scatter particles elastically and in the direction determined by the particle initial velocity rather than phase. In smaller-scale fields, transmission through a ponderomotive barrier is probabilistic and resembles tunneling of a quantum particle through a static potential. We derive asymptotic expressions for the phase-averaged transmission coefficient T as a function of the particle energy \mathcal{E}_0 . We show that, unlike for a truly quantum particle, $T(\mathcal{E}_0)$ is of algebraic form and has a threshold, below which transmission does not occur. We also find a threshold in \mathcal{E}_0 , above which all particles are transmitted regardless of their initial phase.

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I. INTRODUCTION

Charged particle interaction with intense radio-frequency (rf) field is one of the key problems in plasma and accelerator physics. In weak fields, when the particle energy is far above the oscillating potential, linear or quasilinear models are sufficient to describe the interaction. However, studying particle dynamics at larger amplitudes requires fully nonlinear treatment capturing particle reflection and transmission by rf field inhomogeneities. We draw a distinction between two kinds of nonlinear rf barriers, the large-amplitude multiperiod wave packets and the oscillating fields with stationary spatial profiles, or what we call stationary ponderomotive barriers (SPBs). Both in the case of a wave packet $\mathbf{E}_{rf}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})\sin(\omega t - \mathbf{k} \cdot \mathbf{r})$ and the SPB-type field (\mathbf{k} =0), the particle dynamics can often be approximately described in terms of the effective ("ponderomotive") potential

$$\Phi = \frac{e^2 E^2}{4m(\omega - \mathbf{k} \cdot \mathbf{v})^2},\tag{1}$$

which a particle sees in average over its fast oscillations, assuming that the spatial scale L of the envelope $\mathbf{E}(\mathbf{r})$ is sufficiently large [1-4]. (Here *e* and *m* are the mass and the charge of the particle.) Despite the apparent similarity though, the particle dynamics in a SPB is qualitatively different from that in a multiperiod wave packet $(kL \gg 1)$. In the latter, reflection and transmission of a particle are generally determined by particle trapping and detrapping by the wave [5-8]. At $kL \leq 1$, however, trapping is impossible, so scattering in SPBs does not follow the traditional models developed for multiperiod wave packets, at least with comparable L. Particle scattering off a two-scale SPB (e.g., a standing wave) is more similar to that with a wave packet, yet still exhibits peculiar features [9]. The reason for this is that, given the requirement of stationary envelope $\mathbf{E}(\mathbf{r})$, there is no coordinate transformation converting a wave packet into a SPB. Thus the physics of SPBs is irreducible to that of wave packets with finite **k** and must be studied separately (see also our previous publications [10–15]).

SPBs appear in many contexts, for example, in ion traps [16,17], at interaction of rf waves with overcritical plasmas, between pair electrodes closely immersed in a plasma [18,19], near high-frequency probes and antennas [20,21],

and in other situations. They can be used for isotope separation [22], current drive [10–12], and low-frequency modes stabilization in magnetized plasmas [23–26]. SPBs could also serve as a promising means of edge plasma control in fusion reactors, including that for reducing the heat flow on divertors [27–31]. To study the interaction of charged particles with SPBs, particularly the effects of nonlinear transmission and reflection, is the purpose of this paper.

In Ref. [14], we showed that rf-driven particle dynamics may not fit into the simplified effective-potential model [Eq. (1)] and can be similar to that of a quantum object in a potential field. In particular, transmission through a ponderomotive barrier can be probabilistic, i.e., depend not only on the particle energy but also the initial phase (see also Ref. [32]), and hence resemble quantum tunneling. Here we derive asymptotic expressions for the phase-averaged transmission coefficient *T* as a function of the particle energy \mathcal{E}_0 for one-dimensional (1D) SPBs. We show that, unlike for a truly quantum particle, $T(\mathcal{E}_0)$ is of algebraic form and has a threshold, below which transmission does not occur. We also find a threshold in \mathcal{E}_0 , above which all particles are transmitted regardless of their initial phase.

The work is organized as follows. In Sec. II, we restate the ponderomotive potential concept. In Sec. III, we derive the phase-dependent "tunneling" effect. In Sec. IV, we summarize our main ideas. Supplementary calculations are given in the Appendixes, where we also revise the traditional adiabatic theory of particle interaction with SPBs [1,2].

II. BASIC EQUATIONS

Consider 1D charged particle motion governed by

$$m\ddot{z} = -e\phi'(z)\sin\omega t,$$
(2)

where $\phi(z)$ is the envelope of the oscillating electrostatic potential, $E(z)=-\phi'(z)$ is the electric field profile, $E=E_0f(z/L_0)$, and f(x) is a localized function of unit peak and unit width [Fig. 1(a)]. Suppose that the particle approaches the field from infinity, so the initial conditions are $z(t_0)=z_0 \rightarrow -\infty$ and $\dot{z}(t_0)=v_0$ at $t_0 \rightarrow -\infty$. There are two dimensionless parameters in the system then, except for the phase $\varphi_0=\omega t_0$. The first one, $\epsilon_0=v_0/\omega L_0$, determines how



FIG. 1. Particle scattering off smooth ponderomotive barriers: (a) symmetric barrier; (b) asymmetric barrier.

small the particle average displacement on the field period is compared to L_0 . The second parameter, $\sigma_0 = e^2 E_0 / m\omega^2 L_0$, is the ratio of the particle oscillations amplitude to the field scale. We will assume that both ϵ_0 and σ_0 are small compared to unity, so we can separate the particle motion z(t)into the slow drift motion $\overline{z}(t)$ and the oscillatory motion $z_{\sim}(\overline{z}, t)$ and Taylor-expand E(z) around \overline{z} in Eq. (2). An asymptotic series can be constructed for z_{\sim} then and reads

$$\frac{z_{\sim}}{L_0} = -\sigma_0 f \sin \omega t - \frac{\sigma_0^2}{8} f f' \cos 2\omega t$$
$$- \frac{\sigma_0^3}{16} \bigg[(f f'^2 + 6f^2 f'') \sin \omega t$$
$$- \frac{1}{9} (f f'^2 + 2f^2 f'') \sin 3\omega t \bigg] + \cdots, \qquad (3)$$

where f is taken at \overline{z}/L_0 . After substituting Eq. (3) into Eq. (2) one gets

$$m\bar{\bar{z}} = -\bar{\Phi}'(\bar{z}), \qquad (4)$$

where $\bar{\Phi} \approx \Phi = e^2 E^2 / 4m\omega^2$ [Eq. (1)], or, more precisely,

$$\bar{\Phi} = \Phi \left[1 + \frac{\sigma_0^2}{4} \left(f f'' + \frac{f'^2}{4} \right) + \cdots \right].$$
 (5)

The variable transformation $z \rightarrow \overline{z}$ is essentially the Lie transformation to the "oscillation center" coordinates, also considered, e.g., in Refs. [33–36]. It allows removing the fast oscillations from the particle motion equation, so the resulting equation (4) is time-independent and has an integral

$$\mathfrak{E} = \frac{1}{2m}\bar{p}^2 + \bar{\Phi}(\bar{z}),\tag{6}$$

which we further term as the particle quasienergy because it can be considered as the energy conservation for the oscillation center traveling with momentum $\bar{p} = m\dot{z}$ in the "ponderomotive" potential $\bar{\Phi}(\bar{z})$. Equation (4) itself though is only an asymptotic approximation of Eq. (2); the expansions (3), (5) are generally divergent, so the actual particle motion does not have an exact integral. We then define the quasienergy as an integral with finite uncertainty, which depends on the local field scale *L*, and consider Eq. (6) as an asymptotic approximation for \mathfrak{E} . As the quasienergy can also be interpreted as an adiabatic invariant (Appendix A), we further use the same term to denote effects, which are adequately described within the approximation of fixed \mathfrak{E} . The quasienergy local uncertainty $\delta \mathfrak{E}$ is exponential in *L* for it is not captured by the power expansion (6). It must be distinguished from the precisely defined quasienergy change $\Delta \mathfrak{E}$ between the regions of uniform or zero field [the series (3), (5) converge in those regions, and $\delta \mathfrak{E}=0$]. Whereas $\Delta \mathfrak{E}$ is determined by ϵ_0 (Appendix B), the quasienergy uncertainty $\delta \mathfrak{E}$ depends on a similar yet local parameter $\epsilon = \overline{z}/\omega L$ (Appendix A). Analogously, σ_0 and $\sigma = eE/m\omega^2 L$ define, correspondingly, the characteristic and local accuracy of the asymptotic approximation (6), i.e., determine how many terms can be kept in Eqs. (3) and (5) [37]. Hence the oscillation-center approximation applies with different precision at different *z*. Below we use this fact to study how ponderomotive barriers scatter incident particles under very general assumptions on field profiles.

III. TUNNELING AND REFLECTION

Like a static potential with the same height Φ_{max} , an adiabatic ponderomotive barrier (i.e., one with $L_0 \rightarrow \infty$) transmits all particles with initial energy $\mathcal{E}_0 > \bar{\Phi}_{\text{max}}$ and reflects those with $\mathcal{E}_0 < \bar{\Phi}_{\text{max}}$, resulting in a steplike transmission coefficient, $T(\mathcal{E}_0) = \Theta(\mathcal{E}_0 - \bar{\Phi}_{\text{max}})$. For a SPB with finite L_0 , though, one could expect the transmission to depend on both energy and phase, so the phase-averaged $T(\mathcal{E}_0)$ would be a continuous function. An analogy with quantum tunneling through a static potential can be drawn in this case [14]; yet $T(\mathcal{E}_0)$ is of algebraic form here rather than exponential, as we show below.

Given a sufficiently small ϵ_0 , each particle with \mathcal{E}_0 close enough to $\overline{\Phi}_{max}$ would reach the peak-field region $|z| \ll L_0$. As the drift velocity there is small compared to v_0 , the local parameter of adiabaticity ϵ is much smaller than ϵ_0 . Therefore one can attribute nonadiabatic effects entirely to the slope region $|z| \sim L_0$ but describe the trajectory adiabatically near the field maximum. Then the particle quasienergy remains well defined near z=0 yet generally different from the initial value \mathcal{E}_0 :

$$\mathfrak{E} = \mathcal{E}_0 + \Delta \mathfrak{E}(\mathcal{E}_0, \varphi_0), \tag{7}$$

where $\Delta \mathfrak{E}$ is the previously gained nonadiabatic variation, constant for given \mathcal{E}_0 and φ_0 . Importantly, $\Delta \mathfrak{E}$ is large compared to the local uncertainty of \mathfrak{E} due to small $\boldsymbol{\epsilon}$. Simultaneously, $\Delta \mathfrak{E}$ is also large compared to the error of the asymptotic approximation (6) at $|z| \ll L_0$, because the former is determined by the field largest gradient at the slope, whereas the latter is due to a smaller gradient at $z \rightarrow 0$ [38]. Hence near the field maximum one can combine Eq. (7) with the adiabatic conservation law (6); one finds then that transmission through the peak field occurs if

$$\Delta \mathfrak{E} + \mathcal{E}_0 - \Phi_{\max} > 0, \qquad (8)$$

and reflection occurs otherwise. Further deviations from the adiabatic approximation are possible at $|z| \sim L_0$. Those, however, can result only in small variations of the drift kinetic energy, whereas the latter again becomes of the order of $\mathcal{E}_0 \gg \Delta \mathfrak{E}$ by then. It means that the particle drift velocity cannot get close to zero, i.e., such a particle cannot be reflected away from the field maximum. Therefore Eq. (8) guarantees particle transmission through the whole barrier, while the opposite condition similarly leads to reflection from the whole barrier.

It is difficult to calculate $\Delta \mathfrak{E}$ analytically with appropriate accuracy to obtain the actual value of $T(\mathcal{E}_0)$; yet knowing the basic features of $\Delta \mathfrak{E}(\mathcal{E}_0, \varphi_0)$ is sufficient to determine the general properties of the transmission coefficient. First of all, transmission through SPB is a threshold effect. From the derivation of Eq. (6) it follows that, for all particles with energies below a certain limit, one has $|\Delta \mathfrak{E}| < \hat{\varepsilon}$, where $\hat{\varepsilon}$ is a constant small compared to \mathcal{E}_0 . Equation (8) predicts then that all particles are reflected, regardless of phase, if \mathcal{E}_0 $<\Phi_{\rm max}-\hat{\varepsilon}$; similarly, reflection does not occur at $\mathcal{E}_0>\Phi_{\rm max}$ $+\hat{\varepsilon}$. A more detailed analysis can be developed as follows. Since the system is periodic in φ_0 and ϵ_0 is small enough, $\Delta \mathfrak{E}(\mathcal{E}_0, \varphi_0)$ can be approximated with the first harmonic of the Fourier series: $\Delta \mathfrak{E} \approx \varepsilon \sin(\varphi_0 - \overline{\varphi})$, where ε is positive and $\overline{\varphi}$ is an insignificant phase shift. The fraction of transmitted particles in a beam uniformly distributed in φ_0 is then given by $T = \Delta \varphi_0 / 2\pi$, where $\Delta \varphi_0$ is the phase interval, on which

$$\varepsilon \sin(\varphi_0 - \bar{\varphi}) + \mathcal{E}_0 - \bar{\Phi}_{\max} > 0. \tag{9}$$

Hence $T \equiv 0$ for $\mathcal{E}_0 < \mathcal{E}_{\min}$, and $T \equiv 1$ for $\mathcal{E}_0 > \mathcal{E}_{\max}$, where \mathcal{E}_{\min} and \mathcal{E}_{\max} are defined as

$$\mathcal{E}_{\min} = \bar{\Phi}_{\max} - \varepsilon(\mathcal{E}_{\min}), \qquad (10a)$$

$$\mathcal{E}_{\max} = \bar{\Phi}_{\max} + \varepsilon(\mathcal{E}_{\max}),$$
 (10b)

whereas on the interval $\mathcal{E}_{min} < \mathcal{E}_0 < \mathcal{E}_{max}$ the transmission coefficient equals

$$T \approx \frac{1}{2} - \frac{1}{\pi} \arcsin \frac{\bar{\Phi}_{\max} - \mathcal{E}_0}{\varepsilon}.$$
 (11)

As ε approaches zero at $\sigma_0 \rightarrow 0$, one recovers the adiabatic formula $T \approx \Theta(\mathcal{E}_0 - \overline{\Phi}_{\max})$, where $\Theta(x)$ is the step function. If ε is non-negligible though, it can be treated as a constant on the whole interval $(\mathcal{E}_{\min}, \mathcal{E}_{\max})$ (Fig. 2) or, even more precisely, approximated with constants ε_1 and ε_2 on small energy intervals near $\mathcal{E}_0 = \mathcal{E}_{\min}$ and $\mathcal{E}_0 = \mathcal{E}_{\max}$ correspondingly. For \mathcal{E}_0 close to \mathcal{E}_{\min} , the transmission coefficient equals then

$$T \approx \frac{1}{\pi} \sqrt{\frac{2(\mathcal{E}_0 - \mathcal{E}_{\min})}{\varepsilon_1}} \Theta(\mathcal{E}_0 - \mathcal{E}_{\min}), \qquad (12)$$

and for \mathcal{E}_0 close to \mathcal{E}_{max} , one gets, respectively,

$$T \approx 1 - \frac{1}{\pi} \sqrt{\frac{2(\mathcal{E}_{\max} - \mathcal{E}_0)}{\varepsilon_2}} \Theta(\mathcal{E}_{\max} - \mathcal{E}_0)$$
(13)

(Fig. 3). Because ε depends on the detailed structure of E(z) along the particle trajectory, it would be different for particles approaching z=0 from the right and from the left, if E(z) is not symmetric. Unlike for adiabatic transmission de-



FIG. 2. Transmission coefficient $T(\mathcal{E}_0)$ for a particle scattering off a smooth ponderomotive barrier depicted in Fig. 1(a), with $E(z)=E_0 \exp(-z^2/L_0^2)$, $\sigma_0=0.1$, $\Phi_{\max}=e^2E_0^2/4m\omega^2$: numerical (solid gray) and analytical [Eq. (11), using a fitting parameter $\varepsilon \approx 5.1$ $\times 10^{-5}\Phi_{\max}$] results (dashed); also shown is the "adiabatic" stepfunction approximation (solid black).

termined by the particle energy only, $T(v_0)$ is generally not equal to $T(-v_0)$ here (Fig. 4). Such asymmetric barriers can produce electric current in isotropic media [10–12] and experience a nonzero recoil force as a result.

Scalings similar to Eq. (12) hold also for abrupt barriers [Figs. 5(a) and 5(b)], in which nonadiabatic effects pertain mostly to the peak field. In this case the approximation (8) is invalid, so a different model must be applied. Suppose that E(z) has an adiabatic slope on the left, from where particles approach, and drops to zero abruptly at z=0: $E(z>0)\equiv 0$. If, at some $t, z(t)=\overline{z}+z_{\sim}$ is larger than zero, no force is imposed on the particle afterwards, so it travels freely to $z=+\infty$. Assuming uniform distribution in phase ωt of particles with given energy close to z=0, the transmission coefficient equals $T=\omega \Delta t/2\pi$, where Δt is the time interval, on which z(t)>0, assuming $\Delta t < 2\pi/\omega$. To the leading approximation, $z_{\sim} \approx -A_0 \sin \omega t$, where $A_0 = e^2 E_0/m\omega^2$. Therefore $\Delta t \equiv 0$ for



FIG. 3. Transmission coefficient *T* vs initial energy \mathcal{E}_0 (measured in units $\Phi_{\text{max}} = e^2 E_0^2 / 4m\omega^2$) for a particle scattering off a smooth ponderomotive barrier depicted in Fig. 1(a), with $E(z) = E_0 \exp(-z^2/L_0^2)$: $\sigma_0 = 0.4$, 0.5, 0.6. The numerical results shown comply with the asymptotic scalings (12) and (13), where \mathcal{E}_{min} , \mathcal{E}_{max} , ε_1 , and ε_2 are treated as unknown fitting parameters.



FIG. 4. Transmission coefficient *T* vs initial energy \mathcal{E}_0 (measured in units $\Phi_{\text{max}} = e^2 E_0^2 / 4m\omega^2$) for a particle scattering off a smooth asymmetric ponderomotive barrier depicted in Fig. 1(b), with $E(z) = \frac{1}{2} E_0 [1 - \tanh(5z/L_0)] \exp(-z^2/L_0^2)$, $\sigma_0 = 0.5$: $v_0 > 0$ (solid, T_+) and $v_0 < 0$ (dashed, T_-). $T(v_0)$ is not equal to $T(-v_0)$, unlike for adiabatic transmission determined by the particle energy only.

trajectories, which do not approach z=0 at least at a distance A_0 , and T=0 for the corresponding energies $\mathcal{E}_0 < \mathcal{E}_{\min}$.

The value of \mathcal{E}_{\min} and $T(\mathcal{E}_0 > \mathcal{E}_{\min})$ depends on the structure of the SPB at the abrupt peak. For a barrier with nonzero E'(0) at the left slope [Fig. 5(a)], one can use the approximation

$$z(t) = z_* - \frac{1}{2} |a| (t - \tau - t_0)^2 - A_0 \sin \omega t, \qquad (14)$$

where $z_*(\mathcal{E}_0)$ is the adiabatic turning point (assuming $\mathcal{E}_0 < \bar{\Phi}_{\max}$), $a = -\bar{\Phi}'(0)/m$ is the acceleration in the peak field, and τ is the (phase-independent) time of adiabatic travel from the initial location z_0 to z_* . Since local maxima of z(t) are close to $t_n = -\pi/2 + 2\pi n$, with *n* being an integer, transmission occurs for those t_0 , which satisfy

$$z_* - \frac{1}{2} |a| (t_n - \tau - t_0)^2 + A_0 > 0.$$
(15)

At partial transmission (T < 1), there is only one period of oscillations, at which the inequality (15) *can* hold, hence $n = n_*$ is fixed. Equation (15) predicts then that particles are transmitted if and only if



FIG. 5. Particle scattering off abrupt ponderomotive barriers: (a) E'(0) > 0; (b) E''(0) = 0.



FIG. 6. Transmission coefficient *T* vs initial energy \mathcal{E}_0 (measured in units $\Phi_{\text{max}} = e^2 E_0^2 / 4m\omega^2$) for a particle scattering off an abrupt ponderomotive barrier depicted in Fig. 5(a), with $E(z) = E_0 \exp(z/L_0)\Theta(-z)$ (numerical results). The lowest-order analytical approximation (17) fits precisely into the numerical curves if multiplied by a factor $\chi = 1 + \mathcal{O}(\sigma_0)$, namely $\chi = 1.15$, 1.18, 1.24 for $\sigma_0 = 0.075$, 0.1, 0.15 correspondingly.

$$|t_0 - \tau - t_{n_*}| < \sqrt{2\frac{A_0 - |z_*|}{|a|}}.$$
(16)

Since $|z_*| \approx (\bar{\Phi}_{\max} - \mathcal{E}_0) / \bar{\Phi}'(0)$, one gets

$$T \approx \frac{1}{\pi \sigma_0} \sqrt{\frac{2(\mathcal{E}_0 - \mathcal{E}_{\min})}{\bar{\Phi}_{\max}}} \Theta(\mathcal{E}_0 - \mathcal{E}_{\min}), \qquad (17)$$

where σ_0 is calculated with $L_0 = E(0)/E'(0)$, and $\mathcal{E}_{\min} = \overline{\Phi}(-A_0)$. Equation (17) holds for \mathcal{E}_0 such that $T(\mathcal{E}_0) < 1$; for higher energies, $T \equiv 1$ must be taken, as follows from the derivation (Fig. 6).

Consider now an abrupt barrier with E'(0)=0 [Fig. 5(b)]. The approximation (14) would be inaccurate for this case; a more precise calculation of the particle trajectory near the adiabatic reflection point z_* yields

$$z(t) = z_* \cosh\left[\sqrt{\frac{|\bar{\Phi}''(0)|}{m}}(t - \tau - t_0)\right] - A_0 \sin \omega t.$$
(18)

Deriving the transmission coefficient in a similar way than above, one gets

$$T \approx \frac{1}{\pi \sigma_0^2} \sqrt{\frac{\mathcal{E}_0 - \mathcal{E}_{\min}}{2\bar{\Phi}_{\max}}} \Theta(\mathcal{E}_0 - \mathcal{E}_{\min}), \qquad (19)$$

where σ_0 is calculated with $L_0^2 = 2E(0)/|E''(0)|$, and $\mathcal{E}_{\min} = \overline{\Phi}(-A_0)$. Like for Eq. (17), Eq. (19) holds for \mathcal{E}_0 such that $T(\mathcal{E}_0) < 1$; for higher energies, $T \equiv 1$ must be taken (Fig. 7).

IV. CONCLUSIONS

We show that classical particle transmission through a stationary ponderomotive barrier, or SPB, resembles tunneling of a quantum particle through a static potential. Adiabatic scattering corresponds to the quasiclassical limit: in this case,



FIG. 7. Transmission coefficient *T* vs initial energy \mathcal{E}_0 (measured in units $\Phi_{\text{max}} = e^2 E_0^2 / 4m\omega^2$) for a particle scattering off an abrupt ponderomotive barrier depicted in Fig. 5(b), with $E(z) = E_0 \exp(-z^2/L_0^2)\Theta(-z)$ [solid: numerical results; dashed: analytical results, using Eq. (19)]: (a) $\sigma_0 = 0.075$; (b) $\sigma_0 = 0.1$.

all particles with energies $\mathcal{E}_0 < \bar{\Phi}_{max}$ are reflected, and all particles with $\mathcal{E}_0 > \bar{\Phi}_{max}$ are transmitted, regardless of their initial phases, so the phase-averaged transmission coefficient *T* is a step function of energy: $T(\mathcal{E}_0) = \Theta(\mathcal{E}_0 - \bar{\Phi}_{max})$. On the contrary, nonadiabatic scattering is phase dependent, so $T(\mathcal{E}_0)$ becomes a continuous function, like in the quantum tunneling problem. We show, however, that, unlike for a quantum particle, $T(\mathcal{E}_0)$ is not exponential here but algebraic and can be different for particles approaching the barrier from different sides. We find a threshold in the particle energy, \mathcal{E}_{min} , below which transmission does not occur, and derive the asymptotic form of *T* for \mathcal{E}_0 close to \mathcal{E}_{min} : for all types of SPBs contemplated, $T(\mathcal{E}_0) \propto \sqrt{\mathcal{E}_0 - \mathcal{E}_{min}}\Theta(\mathcal{E}_0 - \mathcal{E}_{min})$. We also find a threshold in \mathcal{E}_0 , above which all particles are transmitted regardless of their initial phase.

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APPENDIX A: ADIABATIC INVARIANT

Consider 1D particle motion governed by the Hamiltonian

$$H(z,p;t) = \frac{1}{2m}p^2 + e\phi(z)\sin\omega t.$$
 (A1)

Suppose that the local amplitude of the particle oscillations $A = eE^2/m\omega^2$ [here $E = -\phi'(z)$] is much less than the local field scale L = A/A', so that $\sigma \equiv A'(z)$ is a small parameter. This system is nearly integrable, with a parameter ϕ slowly varying with z. However, since z is the canonical rather than the independent variable in Eq. (A1), the action $\oint pdz$ is not a traditional adiabatic invariant [39,40] here. To find the true action I, which would be an approximate invariant, we must

find a variable transformation $(z,p) \rightarrow (I,\theta)$, which allows writing the Hamiltonian in the canonical form [4]:

$$\mathcal{H} = \mathcal{H}_0(I;\tau) + \epsilon \mathcal{H}_{\sim}(I,\theta;\tau), \tag{A2}$$

where τ is the independent variable (not necessarily the time *t*) and ϵ is the parameter of adiabaticity. Such a transformation can be performed in different ways [4–7,15]; below we will use a particular method, which allows us to find the explicit and precise analytical form of \mathcal{H} for particle scattering off a stationary ponderomotive barrier.

Let us treat the energy $\mathcal{E}=H(z,p;t)$ as the canonical momentum with *t* being the conjugate coordinate, and consider *z* and *p*, respectively, as the independent variable and the Hamiltonian $H_1=p(t,\mathcal{E};z)$:

$$H_1(t,\mathcal{E};z) = \sqrt{2m[\mathcal{E} - e\phi(z)\sin\omega t]}.$$
 (A3)

[The function (A3) has two branches corresponding to positive and negative p, so the algebraic (signed) square root must be considered.] Let us now make a canonical transformation to the new variables (φ, J) , where $J = \frac{1}{2\pi} \oint \mathcal{E} dt$ is the integral taken over the periodic trajectory with fixed z, and φ is yet to be defined. At fixed z, one has $\mathcal{E}=e\phi \sin \omega t + \text{const}$, so

$$J = (\mathcal{E} - e\phi \sin \omega t)/\omega, \qquad (A4)$$

or $J=p^2/2m\omega$, as follows from Eq. (A1). To have J be the canonical momentum, consider the generating function $F_1 = \int \mathcal{E}dt$, with the integral again taken at fixed z:

$$F_1(t,J;z) = J\omega t - \frac{e\phi(z)}{\omega}\cos\omega t.$$
 (A5)

This gives $\varphi = \partial F_1 / \partial J = \omega t$, so the new Hamiltonian $H_2 = H_1 + \partial F_1 / \partial z$ equals

$$H_2(\varphi, J; z) = \sqrt{2m\omega J + m\omega A(z)\cos\varphi}.$$
 (A6)

Introduce now a new canonical pair (θ, I) , where $I = \frac{1}{2\pi} \oint J d\varphi$, or $I = \langle p^2 \rangle_z / 2m\omega$, with $\langle \cdots \rangle_z$ denoting average over the field period at fixed z. Solving for J at fixed z, one gets

$$J = I + \frac{\Phi}{\omega} \cos 2\varphi - A\sqrt{2m(\omega I - \Phi)} \cos \varphi, \qquad (A7)$$

where $\Phi = e^2 E^2 / 4m\omega^2$ is the ponderomotive potential given by Eq. (1). Consider now the generating function $F_2 = \int Jdt$:

$$F_2(\varphi, I; z) = I\varphi + \frac{\Phi}{2\omega}\sin 2\varphi - A\sqrt{2m(\omega I - \Phi)}\sin\varphi.$$
(A8)

The new canonical variable is given by $\theta = \partial F_2 / \partial I$, or

$$\theta = \varphi - \nu \sin \varphi, \tag{A9}$$

where $\nu = \mathcal{P}_{\sim}/\mathcal{P}$, with $\mathcal{P}_{\sim} = m\omega A$ and $\mathcal{P} = \sqrt{2m(\omega I - \Phi)}$. (Precisely, $p = \mathcal{P} - \mathcal{P}_{\sim} \cos \varphi$; hence to the leading order in σ , \mathcal{P}_{\sim} equals the amplitude of the particle oscillatory momentum p_{\sim} , and \mathcal{P} approximates the average momentum $\langle p \rangle$.) The new Hamiltonian $\mathcal{H} = H_2 + \partial F_2/\partial z$ then equals

$$\mathcal{H} = \mathcal{P} + \frac{\Phi'}{2\omega} \sin 2\varphi + \mathcal{P}A' \left(\frac{\nu^2}{2} - 1\right) \sin \varphi, \quad (A10)$$

and, to put it in the form (A2), one must express φ in terms of the canonical coordinate θ .

Denote $\sin \varphi$ with $\mathcal{S}^{(1)}$. From Eq. (A9), it follows that $\mathcal{S}^{(1)} = \sin(\theta + \nu \mathcal{S}^{(1)})$; therefore $\mathcal{S}^{(1)}[\varphi(\theta + 2\pi)] = \mathcal{S}^{(1)}[\varphi(\theta)]$, hence $\mathcal{S}^{(1)}$ is a periodic function of θ with period 2π . Using this, one proves similarly that the same applies to $\mathcal{C}^{(1)} \equiv \cos \varphi$ and thus to $\mathcal{S}^{(2)} \equiv \sin 2\varphi = 2\mathcal{S}^{(1)}\mathcal{C}^{(1)}$. Hence one can write each of these functions as a Fourier series in θ :

$$\mathcal{F} = \sum_{n=-\infty}^{\infty} \mathcal{F}_n \exp(in\theta), \qquad (A11)$$

where \mathcal{F} stands for $\mathcal{C}^{(1)}$, $\mathcal{S}^{(1)}$, or $\mathcal{S}^{(2)}$, and

$$\mathcal{F}_n = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathcal{F}(\varphi) e^{-in(\varphi - \nu \sin \varphi)} (1 - \nu \cos \varphi) d\varphi.$$
(A12)

A straightforward calculation of $S_n^{(1)}$ and $S_n^{(2)}$ allows rewriting Eq. (A10) as

$$\mathcal{H}(\theta, I; z) = \mathcal{P}\left[1 - \sigma \sum_{n=1}^{\infty} \frac{2J'_n(n\nu)}{n^2} \sin n\theta\right], \quad (A13)$$

where J'_n are the derivatives of the Bessel functions of the order *n* with respect to the whole argument $n\nu$.

The Hamiltonian (A13) is of the form of that for a nonlinear pendulum, with "frequency" $\kappa_0 = (\partial \mathcal{H} / \partial I)_{\sigma=0}$ slowly varying with "time" *z*. The parameter ϵ , which denotes the slowness of "frequency" variations, equals the inverse product of $\kappa_0 = m\omega/\mathcal{P}$ and its local scale *L* [40]:

$$\boldsymbol{\epsilon} = \mathcal{P}/m\omega L, \tag{A14}$$

or $\epsilon = \sigma/\nu$. [Having $\epsilon_0 \ll 1$ for a particle scattering off a SPB automatically guarantees that σ is also small along the whole trajectory. (Here $\epsilon_0 = v_0/\omega L_0$, with v_0 being the initial velocity, and L_0 being the characteristic field scale.) As follows from Eq. (6), an initially adiabatic particle will be reflected at $\sigma \leq \epsilon_0 \sqrt{2}$, i.e., before it even enters the nonadiabatic region, whereas for a transiting adiabatic particle $\sigma \leq \epsilon_0 \sqrt{2} \ll 1$ by definition.] The required form (A2) of the Hamiltonian (A13), is then

$$\mathcal{H}(\theta, I; z) = \mathcal{P} - \epsilon \mathcal{P}_{\sim} \sum_{n=1}^{\infty} \frac{2J'_n(n\nu)}{n^2} \sin n\theta.$$
(A15)

Since $\tau \equiv z$ here [see Eq. (A2)], the pendulum (A15) is somewhat similar to that described by the stationary Schrödinger equation, which governs the quantum particle motion in a static potential. This explains the analogy between ponderomotive and quantum dynamics, which we reported in Ref. [14].

Consider now the Hamiltonian equations, which flow from Eq. (A15):

$$\frac{dI}{dz} = \epsilon \mathcal{P}_{\sim} \sum_{n=1}^{\infty} \frac{2J'_n(n\nu)}{n} \cos n\theta, \qquad (A16a)$$

$$\frac{d\theta}{dz} = \frac{m\omega}{\mathcal{P}} \left\{ 1 + \epsilon \nu^3 \sum_{n=1}^{\infty} \left[\frac{2J'_n(n\nu)}{n\nu} \right]' \sin n\theta \right\}$$
(A16b)

(with the derivatives in the right-hand side taken with respect to $n\nu$), or, in a noncanonical form,

$$\frac{dI}{dz} = \sigma \left(\frac{1}{2} \mathcal{P}_{\sim} + \mathcal{P} \cos \varphi \right), \qquad (A17a)$$

$$\frac{d\theta}{dz} = \frac{m\omega}{\mathcal{P}} \left(1 - \sigma \sin \varphi + \frac{1}{2} \sigma \nu \sin 2\varphi \right), \quad (A17b)$$

which one gets, e.g., by calculating $C_n^{(1)}$ using Eq. (A12). As seen from Eqs. (A17), regardless of the initial phase, dI/dz is everywhere finite and $\theta(z)$ oscillates rapidly enough at $\epsilon \ll 1$. Therefore Eqs. (A16) predict that

$$d\langle\langle I\rangle\rangle/dz = o[\epsilon(z)], \tag{A18}$$

where $\langle \langle \cdots \rangle \rangle$ stands for averaging over θ on the period 2π . Suppose that a particle has small ϵ as it enters the field. It will provide then that *I* does not change significantly in the beginning of the interaction, so one can approximate $\epsilon(z)$ by taking *I*=const. In this case, $\epsilon(z) < \epsilon_0$; thus having a sufficiently small ϵ_0 guarantees the smallness of the adiabaticity parameter along the whole trajectory and therefore the existence of an approximate integral.

The conservation law for *I* can be written as the energy conservation for the particle oscillation center traveling in the effective potential $\langle p_{\sim}^2 \rangle_z / 2m \approx \Phi(z)$:

$$\frac{1}{2m} \langle p \rangle^2 + \Phi(z) \approx \text{const.}$$
(A19)

Since variations of *I* scale linearly with ϵ though [see Eq. (A17a)], Eq. (A19) is accurate only in the zeroth-order approximation. Nevertheless, there exists a *true* adiabatic invariant $\overline{I} \equiv \mathfrak{E}/\omega$ defined with exponential accuracy (Appendix B); an asymptotic (generally divergent) series for that can be derived from elaborating a solution for *I* [Eqs. (A16)] to higher orders in ϵ :

$$I = \overline{I} + \epsilon \frac{\mathcal{PP}_{\sim}}{m\omega} \sum_{n=1}^{\infty} \frac{2J'_n(n\nu)}{n^2} \sin n\theta + \cdots .$$
 (A20)

APPENDIX B: ENERGY CHANGE

Assuming a localized field $[E(\pm \infty)=0]$, the overall change of the quasienergy \mathfrak{E} exactly equals the kinetic energy change $\Delta \mathcal{E}$, which can be calculated as

$$\Delta \mathcal{E} = e \omega \int_{-\infty}^{+\infty} \phi[z(t)] \cos \omega t dt.$$
 (B1)

One can prove, by induction, that the oscillatory displacement $z_{-}=z-\overline{z}$ as a function of time contains terms proportional only to sines of odd and cosines of even frequencies (in units of ω), with coefficients being smooth ("adiabatic") functions of \overline{z} . Hence the expansion of $\phi[z(t)]$ does not contain terms proportional to $\cos \omega t$ in any order of the adiabaticity parameter $\epsilon_0 = v_0 / \omega L_0$ (Appendix A). It means that $\Delta \mathcal{E}$ is not representable in powers of ϵ_0 , since smooth expansion coefficients integrated with rapidly oscillating sines and cosines will result only in exponential contribution to $\Delta \mathcal{E}$. Keeping the leading term only, one can write then

$$\Delta \mathcal{E} \approx e \omega \int_{-\infty}^{+\infty} \phi[\bar{z}(t)] \cos \omega t dt, \qquad (B2)$$

where we calculate $\overline{z}(t)$ approximately, using Eq. (A19). Since the motion equation for $\overline{z}(t)$ is autonomous by definition, Eq. (B2) predicts that $\Delta \mathcal{E}$ will be an oscillatory function of the initial phase $\varphi_0 = \omega t_0$. Denoting it with $\Delta \mathcal{E}_{\sim}$ and averaging over φ_0 with $\langle \langle \cdots \rangle \rangle_0$, the phase-averaged energy change can be obtained from [41]

$$\langle\langle\Delta\mathcal{E}\rangle\rangle_0 \approx \frac{1}{2} \frac{\partial}{\partial\mathcal{E}_0} \langle\langle\Delta\mathcal{E}_{\sim}^2\rangle\rangle_0.$$
 (B3)

As an example, consider two cases when the expression (B2) can be further simplified. Suppose, at first, that $\mathcal{E}_0 \gg e\phi$, so a particle is transmitted through the SPB without substantial energy change, and $\overline{z} \approx v_0(t-t_0)$. Taking $\phi = \phi_0 h(z/L_0)$, where *h* is a function of unit peak and unit width, one gets

$$\Delta \mathcal{E}_{\sim} = \frac{e \phi_0}{\epsilon_0} \operatorname{Re} \left[e^{i \omega t_0} \overline{h}(\epsilon_0^{-1}) \right], \tag{B4}$$

where $\bar{h}(k) = \int h(x)e^{ikx}dk$ is the spectrum of *h*. If the potential is a smooth function, $\bar{h}(k)$ decays exponentially at large *k*, so $\Delta \mathcal{E}^{\alpha} \exp(-\alpha/\epsilon^q)$, with α and *q* being positive numbers.

Consider now a particle reflection from $\phi(z) = \phi_0 \exp(z/L_0)$. The adiabatic trajectory calculated using Eq. (A19) is given by

$$\overline{z}(t) = z_* - L_0 \ln \left\{ \cosh \left[\frac{v_0}{L_0} (t - t_0) \right] \right\}, \tag{B5}$$

where t_0 is the time when the particle arrives at the turning point $z_* = \frac{1}{2}L_0 \ln[\mathcal{E}_0/\Phi(0)]$. After substitution into Eq. (B2), one gets

$$\Delta \mathcal{E}_{\sim} = \mathcal{E}_0 \frac{4\pi\sqrt{2}}{\epsilon_0^2} \exp\left(-\frac{\pi}{2\epsilon_0}\right) \cos \omega t_0.$$
 (B6)

The above calculations show that the overall variations $\Delta \mathfrak{E} = \Delta \mathcal{E}$ are generally nonzero, so there is no exact integral in the system. On the other hand, those variations are exponentially small with respect to ϵ_0 for any smooth field, meaning that the information about the particle initial energy is preserved in \mathfrak{E} with the same accuracy throughout the interaction. Therefore one can consider \mathfrak{E} as an approximate integral with an assigned uncertainty. Depending on the local adiabaticity parameter ϵ (Appendix A), this uncertainty may vary, yet it always remains exponentially small, which is consistent with the fact that variations of \mathfrak{E} are not captured by the asymptotic power expansion (6).

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