Paradoxical reflection in quantum mechanics

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Abstract

We discuss a phenomenon of elementary quantum mechanics that is counterintuitive, non-classical, and apparently not widely known: the reflection of a particle at a downward potential step. In contrast, classically, particles are reflected only at upward steps. The conditions for this effect are that the wavelength be much greater than the width of the potential step, and the kinetic energy of the particle be much smaller than the depth of the potential step. The phenomenon is suggested by non-normalizable solutions to the time-independent Schrödinger equation. We present numerical and mathematical evidence that it is also predicted by the time-dependent Schrödinger equation. The paradoxical reflection effect suggests, and we confirm mathematically, that a particle can be trapped for a long time (though not indefinitely) in a region surrounded by downward potential steps, that is, on a plateau.

I. INTRODUCTION

Suppose a particle moves toward a sudden drop of potential as in Fig. 1, with the particle arriving from the left. Will it accelerate or be reflected? Classically, the particle is certain to accelerate, but quantum mechanically, the particle has a chance to be reflected. That sounds paradoxical because the particle turns around and returns to the left under a force pointing to the right. Under suitable conditions, reflection even becomes close to certain. We call this non-classical, counterintuitive phenomenon "paradoxical reflection," or when a region is surrounded by downward potential steps, "paradoxical confinement," where paradoxical is understood as counterintuitive, not illogical. It can be derived easily using the following simple reasoning.

Suppose the particle moves in one dimension, and the potential is a rectangular step as in Fig. 1,

$$V(x) = -\Delta\,\Theta(x) \tag{1}$$

with Θ the Heaviside function and $\Delta \geq 0$. A wave packet coming from the left is partially reflected at the step and partially transmitted. The size of the reflected and the transmitted packets can be determined by the standard method of stationary analysis (see, for example, Refs. 1 and 2), where the wave packet is replaced by a plane wave of energy E and the stationary Schrödinger equation is solved. The transmitted and reflected probability currents, divided by the incoming current, yield the reflection and transmission coefficients $R \geq 0$ and $T \geq 0$ with $R + T = 1$. We give the results in Sec. II and observe that $R \neq 0$, implying that partial reflection occurs although the potential step is downward, and R converges to 1, so that reflection becomes nearly certain, as the ratio E/Δ goes to zero. Thus, paradoxical reflection can be made arbitrarily strong by a suitable choice of parameters.

If it sounds remarkable that a particle can be repelled by a downward potential step, the following fact may add to the amazement. As derived in Ref. 2, p. 76, the reflection coefficient does not depend on whether the incoming wave comes from the left or from the right (provided the total energy and the potential are not changed). Thus, a downward step yields the same reflection coefficient as an upward step. (But keep in mind that at an upward step, energies below the height of the step are also possible for the incoming particle, a case in which reflection is certain, $R = 1$.)

To provide some perspective, we point to some parallels with tunneling, where the probability of a particle passing through a potential barrier is positive even in cases in which this is impossible classically. Paradoxical reflection is similar to what could be called *anti-tunneling*, the effect that a particle can have a nonzero probability of being reflected by a barrier so small that classically the particle would be certain to cross it. Paradoxical reflection is less surprising when we think of a wave being reflected from a potential step, and more surprising from the particle point of view. It is sometimes mentioned in textbooks (see Refs. 3 and 4).

The goal of this article is to address the following questions: Is paradoxical reflection a real physical phenomenon or an artifact of mathematical over-simplifications? How does it depend on the width L (see Fig. 2), the depth Δ of the potential step, the wavelength λ, and the width σ of the incoming wave packet? Why does this phenomenon not occur classically? That is, how can it be that classical mechanics is a limit of quantum mechanics if paradoxical reflection occurs in the latter but not the former? Can this phenomenon be used in principle for constructing a particle trap? These questions gave rise to lively and contentious discussions between a number of physics researchers visiting the Institut des Hautes Études Scientifiques near Paris, France in spring 2005. These discussions inspired the present article.

II. STATIONARY ANALYSIS OF THE RECTANGULAR STEP

We first provide more details about the stationary analysis of the rectangular step in Eq. (1), and consider the time-independent Schrödinger equation

$$E\psi(x) = -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x), \tag{2}$$

where m is the mass. Equation (2) can be solved in the usual way. For $x < 0$, let ψ be a superposition of an incoming wave $\mathrm{e}^{\mathrm{i}k_1 x}$ and a reflected wave $B\mathrm{e}^{-\mathrm{i}k_1 x}$, and for $x > 0$, let ψ be the transmitted wave $A\mathrm{e}^{\mathrm{i}k_2 x}$, with a possibly different wave number k_2. From Eq. (2) we obtain

$$k_1 = \sqrt{2mE}/\hbar \text{ and } k_2 = \sqrt{2m(E+\Delta)}/\hbar\,. \tag{3}$$

The value $E \geq 0$ is the kinetic energy associated with the incoming wave. The coefficients A and B are determined by requiring the continuity of ψ and its derivative ψ' at $x = 0$:

$$A = \frac{2k_1}{k_1 + k_2} \text{ and } B = \frac{k_1 - k_2}{k_1 + k_2}\,. \tag{4}$$

The reflection and transmission coefficients R and T are defined as the ratio of the probability current $j = (\hbar/m)\,\mathrm{Im}(\psi^*\psi')$ associated with the reflected respectively transmitted wave to the current associated with the incoming wave,

$$R = \frac{|j_{\rm ref}|}{j_{\rm in}} \text{ and } T = \frac{j_{\rm tr}}{j_{\rm in}}\,. \tag{5}$$

We note that $j_{\rm tr} = \hbar k_2|A|^2/m$, $j_{\rm ref} = -\hbar k_1|B|^2/m$, $j_{\rm in} = \hbar k_1/m$, and we find that

$$R = |B|^2 = 1 - \frac{k_2}{k_1}|A|^2 \text{ and } T = \frac{k_2}{k_1}|A|^2\,. \tag{6}$$

The values of both R and T are in the interval $[0, 1]$, and $R + T = 1$. By inserting Eq. (4) into Eq. (6), we obtain

$$R = \frac{(k_1 + k_2)^2 - 4k_1k_2}{(k_1 + k_2)^2} = \frac{(k_2 - k_1)^2}{(k_1 + k_2)^2}. \tag{7}$$

We observe that $R \neq 0$, implying that reflection occurs, if $k_1 \neq k_2$, which is the case if $\Delta \neq 0$. Also, R converges to 1, so that reflection becomes nearly certain, as the ratio $r \equiv E/\Delta \to 0$ because

$$R = \left(\frac{k_2 - k_1}{k_2 + k_1}\right)^2 = \left(\frac{\sqrt{E+\Delta} - \sqrt{E}}{\sqrt{E+\Delta} + \sqrt{E}}\right)^2 = \left(\frac{\sqrt{r+1} - \sqrt{r}}{\sqrt{r+1} + \sqrt{r}}\right)^2 \to 1\,, \tag{8}$$

and both the numerator and the denominator approach 1. This derivation is the simplest way to obtain paradoxical reflection.

The effect possesses an analog in wave optics. The refractive index, which may vary with the position x, plays a role similar to the potential (for example, it influences the speed of wave propagation), and changes suddenly at a surface between different media. Light can be reflected at the surface on both sides. In particular, at a surface between water and air, light coming from the water (the high-index region) can be reflected back into the water.

III. SOFT STEP

For a deeper analysis of the effect we will consider increasingly more realistic models. In this section we consider a soft (a smooth, that is, differentiable) potential step, as in Fig. 2, for which the drop in the potential is not infinitely rapid but takes place over some distance L. The result is that paradoxical reflection exists also for soft steps, so that the effect is not just a feature of rectangular steps which cannot occur in nature. We also find how the effect depends on the width L of the step.

It is useful to consider the function

$$V(x) = -\frac{\Delta}{2}\left(1 + \tanh\frac{x}{L}\right), \tag{9}$$

depicted in Fig. 2. Recall that $\tanh(x)$ converges to ± 1 as $x \to \pm\infty$. The reflection coefficient for this potential can be calculated by a stationary analysis, obtaining solutions $\psi(x)$ to Eq. (2) which are asymptotic to $\mathrm{e}^{\mathrm{i}k_1 x} + B\mathrm{e}^{-\mathrm{i}k_1 x}$ as $x \to -\infty$ and asymptotic to $A\mathrm{e}^{\mathrm{i}k_2 x}$ as $x \to \infty$, that is, $\lim_{x\to\infty}(\psi(x) - A\mathrm{e}^{\mathrm{i}k_2 x}) = 0$. The calculation is given in Ref. 2, p. 78. The values of k_1 and k_2 are given by Eq. (3), and the reflection coefficient turns out to be

$$R = \left(\frac{\sinh\left(\frac{\pi}{2}(k_2 - k_1)L\right)}{\sinh\left(\frac{\pi}{2}(k_2 + k_1)L\right)}\right)^2. \tag{10}$$

From Eqs. (10) and (3) we can read off that $R \neq 0$ for $\Delta \neq 0$, and $R \to 1$ as $E \to 0$ while Δ and L are fixed because then $k_1 \to 0$, $k_2 \to \sqrt{2m\Delta}/\hbar$, so that both the numerator and the denominator approach $\sinh(\pi\sqrt{2m\Delta}L/2\hbar)$. As $\Delta \to \infty$ while E and L are fixed, $R \to \exp(-2\pi\sqrt{2mE}L/\hbar)$ because $\sinh x \approx \frac{1}{2}\exp x$ for $x \gg 1$.

In addition, we can keep E and Δ fixed and see how R varies with L. In the limit $L \to 0$, Eq. (10) converges to Eq. (7) because $\sinh(\alpha L) \approx \alpha L$ for $L \ll 1$ and fixed α, which is what we would expect when the step becomes sharper and Eq. (9) converges to Eq. (1). In the limit $L \to \infty$, R converges to 0 because for fixed $\beta > \alpha > 0$ we have

$$\frac{\sinh(\alpha L)}{\sinh(\beta L)} = \frac{\mathrm{e}^{\alpha L} - \mathrm{e}^{-\alpha L}}{\mathrm{e}^{\beta L} - \mathrm{e}^{-\beta L}} = \frac{\mathrm{e}^{(\alpha-\beta)L} - \mathrm{e}^{(-\alpha-\beta)L}}{1 - \mathrm{e}^{-2\beta L}} \to 0, \tag{11}$$

because the numerator approaches 0 and the denominator approaches 1. Thus, paradoxical reflection disappears for large L, in other words, it is crucial for the effect that the drop in the potential is sudden.

R in Eq. (10) is a decreasing function of L, which means that reflection will be more probable the more sudden the drop in the potential. To see this behavior, we check that for $\beta > \alpha > 0$ and $L > 0$ the function $f(L) = \sinh(\alpha L)/\sinh(\beta L)$ is decreasing:

$$\frac{\mathrm{d}f}{\mathrm{d}L} = \frac{\alpha\cosh(\alpha L)\sinh(\beta L) - \beta\sinh(\alpha L)\cosh(\beta L)}{\sinh^2(\beta L)} < 0, \tag{12}$$

because $x/\tanh x$ is an increasing function of x for $x > 0$ and thus

$$\frac{\alpha}{\tanh\alpha} < \frac{\beta}{\tanh\beta}. \tag{13}$$

How about soft steps with shapes other than that of the tanh function? Suppose that the potential $V(x)$ is a continuous, monotonically decreasing function such that $V(x) \to 0$ as $x \to -\infty$ and $V(x) \to -\Delta$ as $x \to +\infty$. We note that the fact that the reflection coefficient is the same for particles coming from the left or from the right, still holds true for a general potential (see Ref. 2, p. 76). This fact suggests that paradoxical reflection occurs also for general potential steps. However, we do not know of a general result on lower bounds for the reflection coefficient R that could be used to establish paradoxical reflection in this generality. An upper bound is known, see Ref. 5, according to which R is less than or equal to the reflection coefficient in Eq. (7) for the rectangular step. This result agrees with our observation that reflection is more likely the sharper the step.

IV. WAVE PACKETS

Another way to make our treatment more realistic is to assume that the wave function is not an infinitely-extended plane wave $\mathrm{e}^{\mathrm{i}k_1 x}$, but is a wave packet of finite width σ, for example, a Gaussian wave packet

$$\psi_{\mathrm{in}}(x) = G_{\mu,\sigma}(x)^{1/2}\, \mathrm{e}^{\mathrm{i}k_1 x} \tag{14}$$

with $G_{\mu,\sigma}$ a Gaussian with mean μ and variance σ^2,

$$G_{\mu,\sigma}(x) = \frac{1}{\sqrt{2\pi}\sigma}\mathrm{e}^{-(x-\mu)^2/2\sigma^2}\,. \tag{15}$$

Suppose this packet arrives from the left and evolves in the potential $V(x)$ according to the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t) + V(x)\,\psi(x,t)\,. \tag{16}$$

As $t \to \infty$, there will be a reflected packet ψ_{ref} in the region $x < 0$ moving to the left and a transmitted packet ψ_{tr} in the region $x > 0$ moving to the right, and thus the reflection and transmission probabilities are

$$R = \|\psi_{\mathrm{ref}}\|^2 \text{ and } T = \|\psi_{\mathrm{tr}}\|^2\,, \tag{17}$$

with $\|\psi\|^2 = \int_{-\infty}^{\infty} |\psi(x)|^2\,\mathrm{d}x$.

Because of the paradoxical feel of paradoxical reflection, we might suspect that the effect does not exist for wave packets but is an artifact of the stationary analysis. We thus address the question as to how wave packets behave, and whether the reflection probability (17) agrees with the reflection coefficient of Eq.s (7) or (10). We begin with the numerical evidence which confirms paradoxical reflection.

A. Numerical simulation

A simulation of a wave packet partly reflected from a (hard) downward step is shown in Fig. 3. The simulation starts with a Gaussian wave packet moving to the right and initially located on the left of the potential step. After passing the step, there remain two wave packets, no longer exactly Gaussian, one continuing to move to the right and the other, reflected and returning to the left. For the choice of parameters in this simulation, the transmitted and reflected packet are of comparable size, thus providing evidence that there can be a substantial probability of reflection at a downward step (even for wave packets of finite width). Hence, the simulation confirms the prediction of the stationary analysis.

B. Is it for real?

We now discuss how rigorous mathematics confirms paradoxical reflection as a consequence of the Schrödinger equation. We thus exclude the possibility that it is merely a numerical error that led to the appearance of paradoxical reflection for wave packets.

Do not think the concern that numerical errors may lead to the incorrect behavior of a wave packet is paranoid. There are cases in which this problem occurs. For example, when we did a simulation of the evolution of a wave packet in a soft step potential (that is, the same situation as in Fig. 3, but with the hard step of Eq. (1) replaced by the soft step of Eq. (9)), we obtained wrong outcomes for the reflection probabilities (see Fig. 4).

The rigorous analysis of scattering problems of this type is a complex and subtle topic. The main techniques and results (also for higher dimensional problems) are described in Refs. 7 and 8, and the results relevant to step type potentials of can be found in Ref. 9. The reflection probability R of Eq. (17) is given in terms of the plane wave reflection coefficients $R(k_1)$ by the following relation, which expresses what would be expected:

$$R = \int_0^\infty \mathrm{d}k_1 \, R(k_1) |\widehat{\psi}_{\mathrm{in}}(k_1)|^2 \,. \tag{18}$$

The same expression holds with all Rs replaced by Ts. In Eq. (18), $R(k_1)$ is given by the stationary analysis, as in Eqs. (7) or (10), with $k_2 = \sqrt{k_1^2 + 2m\Delta/\hbar^2}$, and $\widehat{\psi}_{\text{in}}(k_1)$ the Fourier transform of the incoming wave packet $\psi_{\text{in}}(x)$. [To be precise, the incoming packet $\psi_{\text{in}}(x,t)$ is defined as the free asymptote of $\psi(x,t)$ for $t \to -\infty$, that is, $\psi_{\text{in}}(x,t)$ evolves without the potential,

$$\mathrm{i}\hbar \frac{\partial \psi_{\text{in}}}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi_{\text{in}}}{\partial x^2}(x,t)\,, \tag{19}$$

and

$$\lim_{t\to-\infty} \|\psi_{\text{in}}(\cdot,t) - \psi(\cdot,t)\| = 0\,. \tag{20}$$

Similarly, $\psi_{\text{ref}} + \psi_{\text{tr}}$ is the free asymptote of ψ for $t \to +\infty$. When we write $\psi_{\text{in}}(x)$, we implicitly have set $t = 0$. Note that the right-hand side of Eq. (18) does not depend on t because by Eq. (19), $\widehat{\psi}_{\text{in}}(k,t) = \exp(-it\hbar k^2/2m)\,\widehat{\psi}_{\text{in}}(k,0)$ and thus $|\widehat{\psi}_{\text{in}}(k,t)|^2 = |\widehat{\psi}_{\text{in}}(k,0)|^2$. Because we assumed that the incoming wave packet comes from the left, ψ_{in} is a "right-moving" wave packet consisting only of Fourier components with $k \geq 0$.]

From Eq. (18) we can read off the following: If the incoming wave packet consists only of Fourier components k_1 for which $R(k_1) > 1 - \varepsilon$ for some (small) $\varepsilon > 0$, then $R > 1 - \varepsilon$. More generally, if the incoming wave packet consists mainly of Fourier components with $R(k_1) > 1 - \varepsilon$, that is, if the proportion of Fourier components with $R(k_1) > 1 - \varepsilon$ is

$$\int_0^\infty \mathrm{d}k_1 \Theta\big(R(k_1) - (1-\varepsilon)\big) |\widehat{\psi}_{\text{in}}(k_1)|^2 = 1 - \delta\,, \tag{21}$$

then $R > 1 - \varepsilon - \delta$ because

$$\begin{aligned}
\int_0^\infty \mathrm{d}k_1 R(k_1) |\widehat{\psi}_{\text{in}}(k_1)|^2 &\geq \int_0^\infty \mathrm{d}k_1 R(k_1) \Theta\big(R(k_1) - (1-\varepsilon)\big) |\widehat{\psi}_{\text{in}}(k_1)|^2 && \text{(22a)}\\
&\geq \int_0^\infty \mathrm{d}k_1 (1-\varepsilon) \Theta\big(R(k_1) - (1-\varepsilon)\big) |\widehat{\psi}_{\text{in}}(k_1)|^2 && \text{(22b)}\\
&= (1-\varepsilon)(1-\delta) > 1 - \varepsilon - \delta\,. && \text{(22c)}
\end{aligned}$$

Therefore, whenever the stationary analysis predicts paradoxical reflection for certain parameters and values of k_1, then wave packets consisting of these Fourier components also are subject to paradoxical reflection.

V. PARAMETER DEPENDENCE

Let us summarize and be explicit about how the reflection probability R from a downward potential step depends on the mean wave number k_1 and the width σ of the incoming wave packet, and the depth Δ and width L of the potential step. We claim that R is close to 1 in the parameter region given by

$$\frac{1}{k_1} \gg L \tag{23a}$$

$$\Delta \gg \frac{\hbar^2 k_1^2}{2m} = E \tag{23b}$$

$$\sigma \gg \frac{1}{k_1}\,. \tag{23c}$$

Note that $1/k_1$ is (up to the factor 2π) the (mean) wavelength λ.

To derive this claim from Eqs. (10) and (18), consider first the case $\sigma \to \infty$ of a very very wide packet. For such a packet, its Fourier transform is very sharply peaked at k_1. The reflection coefficient R given by Eq. (10) depends on the parameters k_1, L, Δ, and m only in the dimensionless combinations

$$u = \frac{\pi}{2} k_1 L \text{ and } v = \frac{\pi}{2}\sqrt{2m\Delta}L/\hbar\,, \tag{24}$$

that is,

$$R = R(u,v) = \left[\frac{\sinh(\sqrt{u^2+v^2}-u)}{\sinh(\sqrt{u^2+v^2}+u)}\right]^2. \tag{25}$$

Fig. 5 shows the region in the u-v plane in which $R > 0.99$. As can be read off from the figure, for (u, v) to lie in that region, it is sufficient, for example, that

$$u < 10^{-3} \text{ and } v > 10^3 u\,. \tag{26}$$

More generally, for $R(u, v)$ to be very close to 1 it is sufficient that $u \ll 1$ and $v \gg u$, which are Eqs. (23a) and (23b). To see these conditions, note that

$$\begin{aligned}\sinh(\sqrt{u^2+v^2}-u) \;&=\; \sinh(\sqrt{u^2+v^2}+u-2u) = \sinh(\sqrt{u^2+v^2}+u)\cosh(2u)\\ &\quad - \cosh(\sqrt{u^2+v^2}+u)\sinh(2u),\end{aligned} \tag{27}$$

so that

$$\sqrt{R(u,v)} = \frac{\sinh(\sqrt{u^2+v^2}-u)}{\sinh(\sqrt{u^2+v^2}+u)} = \cosh(2u) - \frac{\sinh(2u)}{\tanh(\sqrt{u^2+v^2}+u)}\,. \tag{28}$$

Suppose that $u \ll 1$. Then a Taylor expansion to first order in u yields

$$\sqrt{R(u,v)} \approx 1 - \frac{2u}{\tanh v}\,. \tag{29}$$

If v is of order 1, the right-hand side of Eq. (29) is close to 1 because $u \ll 1$. If, however, v is small, then $\tanh v$ is of order v, and the right-hand side of Eq. (29) is close to 1 when

$u/v \ll 1$. Thus, when conditions (23a) and (23b) are satisfied, then $\sqrt{R}$ is close to 1, and thus so is R.

Now consider a wave packet that is less sharply peaked in the momentum representation. If it has width σ in position space, then by the Heisenberg uncertainty relation, it has width of order $1/\sigma$ in Fourier space. For the reflection probability to be close to one, the wave packet should consist almost exclusively of Fourier modes that have reflection coefficients close to one. Thus, every wave number $\tilde{k}_1$ in the interval, say, $[k_1 - 10/\sigma, k_1 + 10/\sigma]$ should satisfy Eqs. (23a) and (23b), as is the case if $10/\sigma$ is small compared to k_1, or $\sigma \gg 1/k_1$. Thus, Eq. (23c), which is what is required for the right-hand side of Eq. (14) to be a good wave packet, that is, an approximate plane wave, is a natural condition on σ for keeping R close to 1.

VI. THE CLASSICAL LIMIT

If paradoxical reflection exists, why do we not see it in the classical limit? On the basis of Eq. (23) we can understand why. Classical mechanics is a good approximation to quantum mechanics in the regime in which a wave packet moves in a potential that varies very slowly in space, so that the force varies appreciably only over distances much larger than the wavelength. For paradoxical reflection, in contrast, it is essential that the length scale of the drop in the potential be smaller than the wavelength. For further discussion of the classical limit of quantum mechanics, see Ref. 10.

VII. A PLATEAU AS A TRAP

Given that a particle will likely be reflected from a suitable downward potential step, it is obvious that it could be trapped, more or less, in a region surrounded by such potential steps. In other words, potential plateaus, and not only potential valleys, can be confining. To explore this possibility of “paradoxical confinement,” we consider the potential plateau

$$V(x) = -\Delta\big[\Theta(x-a) + \Theta(-x-a)\big]\,, \tag{30}$$

as depicted in Fig. 6.

A particle starting on the plateau could remain there — at least with high probability — for a very long time, much longer than the maximal time τ_{cl} that a classical particle with energy E would remain on the plateau, which is

$$\tau_{\rm cl} = a\sqrt{\frac{2m}{E}}\,, \tag{31}$$

independently of the height of the plateau. The following theorem, which will be proved in Appendix B using the results of Secs. VIII, IX, and Appendix A, guarantees that paradoxical confinement actually works for sufficiently high plateaus.

Theorem I. Let $a > 0$ *and choose an initial wave function* ψ_0 *that satisfies* $\psi_0(x) = 0$ *for* $|x| > a$ *and is normalized but otherwise arbitrary for* $|x| \leq a$*. For every constant* $\Delta > 0$*, consider the potential* V*, as in Eq.* (30) *and in Fig. 6, and the time-evolved wave function* $\psi_t = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi_0$ *(with* H *denoting the unique self-adjoint extension of* $-(\hbar^2/2m)\partial^2/\partial x^2 + V$*); we write* $\psi_t = \psi_t^\Delta$ *to make explicit the dependence on* Δ*. During an arbitrarily long time interval* $[0, t_0]$ *and with arbitrarily small error* $\varepsilon > 0$*,* ψ_t^Δ *stays concentrated in the plateau region* $[-a, a]$*, that is,*

$$\int_{-a}^{a} \left|\psi_t^\Delta(x)\right|^2 \mathrm{d}x > 1 - \varepsilon \textit{ for all } t \in [0, t_0], \tag{32}$$

provided that Δ *is large enough,* $\Delta \geq \Delta_0(\psi_0, t_0, \varepsilon)$*.*

Given a fixed Δ, the particle does not stay forever in the plateau region. The time it likely remains there is of the order $\sqrt{\Delta/E}\,\tau_{\rm cl}$, which is much larger than $\tau_{\rm cl}$ if the height Δ is large enough. As we shall prove, a particle starting in the plateau region will leave it, if Δ is large enough, at the rate $\tau_{\rm qu}^{-1}$ with the decay time

$$\tau_{\rm qu} = a\frac{\sqrt{2m\Delta}}{4E} = \frac{1}{4}\sqrt{\frac{\Delta}{E}}\,\tau_{\rm cl}\,. \tag{33}$$

The lifetime (33) can be obtained semi-classically. Imagine a particle traveling along the plateau with the speed $\sqrt{2E/m}$ corresponding to energy E, which is reflected at the edge with probability R given by Eq. (7), then travels back with the same speed, is reflected at the other edge with probability R, and so on. Because the transmission probability $T = 1 - R$ corresponding to Eq. (7) is

$$4\sqrt{E/\Delta} + \text{higher powers of } E/\Delta\,, \tag{34}$$

a number of reflections of order $(\sqrt{E/\Delta})^{-1}$ will typically be required before transmission occurs, in qualitative agreement with Eq. (33). The transmission probability $T = 4\sqrt{E/\Delta}$, when small, corresponds to a decay rate $T/\tau_{\rm cl}$ and hence to the decay time $\tau_{\rm cl}/T$ given by Eq. (33).

We must be careful with this reasoning, because applied carelessly, it would lead to the same lifetime for the potential well depicted in Fig. 7 as for the potential plateau because the reflection probability at an upward potential step is the same as that at a downward potential step. However, the potential well possesses bound states for which the lifetime is infinite. In this regard it is important to bear in mind that the symmetry in the reflection coefficient derived in Ref. 2 always involves incoming waves at the same total energy $E > 0$. For a potential well the symmetry argument would thus say nothing about bound states, which have $E < 0$.

A basic difference between confinement in a potential well and paradoxical confinement on a potential plateau is that in the well the particle has a probability to stay forever. The potential well has bound states (that is, eigenfunctions in the Hilbert space $L^2(\mathbb{R})$ of square-integrable functions), but the potential plateau does not. For the potential well the initial wave packet will typically be a superposition $\psi = \psi_{\rm bound} + \psi_{\rm scattering}$ of a bound state (a superposition of one or more square-integrable eigenfunctions) and a scattering state (orthogonal to all bound states). Then $\|\psi_{\rm bound}\|^2$ is the probability that the particle remains in (the neighborhood of) the well forever. In contrast, because of paradoxical reflection, the potential plateau has metastable states, which remain on the plateau for a long time but not forever, namely, with lifetime (33).

Let us give a cartoon of how we might expect these metastable states to behave, as described in terms of the probability density function $\rho_t(x)$ at time t. Let P_t denote the probability that the particle is in the plateau region at time t, $P_t = \int_{-a}^{a} \rho_t(x)\, dx$, and suppose that the particle is there initially, $P_0 = 1$. Assuming that the particle leaves the plateau at the rate $\tau = \tau_{\rm qu}$, we have $P_t = e^{-t/\tau}$. For simplicity, we assume that the distribution in the plateau region is flat, $\rho_t(x) = P_t/2a$ for $-a < x < a$. After leaving the plateau, the particle moves away from the plateau, say at speed v. Then $\rho_t(x) = 0$ for $|x| > a + vt$ because this value of x cannot be reached by time t, and the probability between x and $x + dx$ (with $a < x < a + vt$) at time t, $\rho_t(x)\, dx$, is what flowed off at $x = a$ between $\tilde{t} = t - (x - a)/v$ and $\tilde{t} - d\tilde{t} = t - (x + dx - a)/v$, which is half of the decrease in P_t between $\tilde{t} - d\tilde{t}$ and $\tilde{t}$ (half because the other half was lost at $x = -a$). That is,

$$\rho_t(x)dx = \frac{1}{2}\left|\frac{dP_{\tilde{t}}}{d\tilde{t}}\right| d\tilde{t} = \frac{1}{2\tau} e^{-\tilde{t}/\tau}\, d\tilde{t} = \frac{1}{2v\tau} e^{-t/\tau} e^{(x-a)/v\tau}\, dx\,. \tag{35}$$

Likewise, for $-a - vt < x < -a$, $\rho_t(x) = (1/2v\tau)e^{-t/\tau}e^{(|x|-a)/v\tau}$. This simplified model of $\rho_t(x)$ conveys an impression of what kind of behavior to expect. Some of its features, notably the exponential increase with $|x|$ outside the plateau region, will be encountered again in the following.

In Sec. IX we investigate how a wave packet initially in the plateau region will behave. In Sec. VIII we calculate the lifetime and confirm Eq. (33). Our tool will be a method similar to the stationary analysis of Sec. II, using special states lying outside the Hilbert space $L^2(\mathbb{R})$ (as do the stationary states of Sec. II). And again like the stationary states of Sec. II, the special states are similar to eigenfunctions of the Hamiltonian in that they are solutions of Eq. (2), but with complex "energy."

VIII. EIGENFUNCTIONS WITH COMPLEX ENERGY

We now derive Eq. (33) for the lifetime $\tau = \tau_{\rm qu}$ from the behavior of solutions to Eq. (2), but with complex eigenvalues. To avoid confusion, we call the eigenvalue Z instead of E, and thus Eq. (2) becomes

$$Z\psi(x) = -\frac{\hbar^2}{2m}\psi''(x) + V(x)\,\psi(x)\,, \tag{36}$$

where V is the plateau potential as in Eq. (30). Such eigenfunctions of complex energy were first considered by Gamow[11,12] for the theoretical treatment of radioactive alpha decay.

The fact that the eigenvalue is complex might be confusing, because the Hamiltonian is a self-adjoint operator, and the eigenvalues of a self-adjoint operator are known to be real. However, in the standard terminology for self-adjoint operators in Hilbert spaces, the words "eigenvalue" and "eigenfunction" are reserved for such solutions of Eq. (36) where ψ is square-integrable (normalizable), that is, $\psi \in L^2(\mathbb{R})$. In this sense all eigenvalues must be real. This condition means that any solution ψ of Eq. (36) for $Z \in \mathbb{C} \setminus \mathbb{R}$ (where $\setminus$ denotes the set difference, that is, we require that $\operatorname{Im} Z \neq 0$) is not square-integrable. Even the eigenfunctions with real eigenvalue E considered in Eq. (2) are not square-integrable, which means that they do not count as eigenfunctions and do not make the number E

an eigenvalue. Instead, E is called an *element of the spectrum* of the Hamiltonian. Still, the spectrum of any self-adjoint operator consists of real numbers, and thus $Z \in \mathbb{C} \setminus \mathbb{R}$ cannot belong to the spectrum of the Hamiltonian. Therefore, the eigenvalues Z we are considering are neither eigenvalues in the standard sense, nor even elements of the spectrum. Nevertheless, we continue to call them "eigenvalues," because they satisfy Eq. (36) for some nonzero function.

Let us explain how these complex eigenvalues can be useful in describing the time evolution of wave functions. Consider an eigenfunction ψ with a complex eigenvalue Z. It generates a solution to the time-dependent Schrödinger equation by defining

$$\psi(x,t) = \mathrm{e}^{-\mathrm{i}Zt/\hbar}\psi(x,0)\,. \tag{37}$$

The function grows or shrinks exponentially with time, with rate given by the imaginary part of Z. More precisely,

$$|\psi(x,t)|^2 = \mathrm{e}^{2\,\mathrm{Im}\,Zt/\hbar}|\psi(x,0)|^2\,, \tag{38}$$

so that $2\,\mathrm{Im}\,Z/\hbar$ is the rate of growth of the density $|\psi(x,t)|^2$. For the eigenfunctions relevant to our purposes, the imaginary part of Z is always negative, so that ψ shrinks with time. In particular, the amount of $|\psi|^2$ in the high-potential region decays with the exponential factor in Eq. (38). If we assume that $|\psi|^2$ is proportional to the probability density at least in some region around the plateau (though not on the entire real line) for a sufficiently long time, and use the fact that the lifetime τ for which the particle remains on the plateau is the reciprocal of the decay rate of the probability in the plateau region, we have

$$\tau = -\frac{\hbar}{2\mathrm{Im}\,Z}\,. \tag{39}$$

From Eq. (37) we can read off that the phase of $\psi(x,t)$ at any fixed x rotates with frequency $\mathrm{Re}\,Z/\hbar$, while for eigenfunctions with real eigenvalue E it does so with frequency $E/\hbar$, which motivates us to call $\mathrm{Re}\,Z$ the energy and denote it by E. Thus,

$$Z = E - \mathrm{i}\frac{\hbar}{2\tau}\,. \tag{40}$$

Later, we will determine τ by determining the relevant eigenvalues Z, that is, those corresponding to decay eigenfunctions, see Eq. (43).

The eigenfunctions ψ differ from physical wave functions, among other respects, in that $|\psi|^2$ shrinks everywhere. Because a local conservation law holds for $|\psi|^2$, this decrease corresponds to a loss of $|\psi|^2$ at $x = \pm\infty$. What do these eigenfunctions have to do with physical wave functions? In the situation we want to consider, the physical wave function ϕ_t is such that the amount of $|\phi_t|^2$ in the plateau region continuously shrinks due to a flow of $|\phi|^2$ away from the plateau. On any large but finite interval $[-b, b]$ containing the plateau $[-a, a]$, ϕ_t may approach an eigenfunction ψ_t, and thus become a quasi-steady-state; that is, stationary up to an exponential shrinking due to outward flux through $x = \pm b$ (like the density $\rho_t(x)$ described around Eq. (35) for $t > (b - a)/v$). This picture will be confirmed to some extent in Theorem II. It also suggests that, like ρ_t, ψ should grow exponentially as $x \to \pm\infty$, and hence the density at great distance from the plateau would be expected to agree with the flow off the plateau in the distant past, which was exponentially larger than in the present if the wave function in the plateau region shrinks exponentially with time. As we will see in Eqs. (41)–(43), the eigenfunctions do grow exponentially with $|x|$ outside the plateau.

We now specify the eigenfunctions, starting with the general solution of Eq. (36) without any requirements on the behavior at $\pm a$ (such as continuity of ψ and ψ'). For $Z \in \mathbb{C}$ except $Z = 0$ or $Z = -\Delta$ we have[13]

$$\psi(x) = \begin{cases} B_- e^{-i\tilde{k}x} + C_- e^{i\tilde{k}x} & \text{if } x < -a \\ A_+ e^{ikx} + A_- e^{-ikx} & \text{if } -a < x < a \\ B_+ e^{i\tilde{k}x} + C_+ e^{-i\tilde{k}x} & \text{if } x > a, \end{cases} \tag{41}$$

where

$$k = \sqrt{2mZ}/\hbar \text{ and } \tilde{k} = \sqrt{2m(Z + \Delta)}/\hbar \tag{42}$$

with the usual definition of the complex square root. That is, for a complex number ζ other than one that is real and ≤ 0, $\sqrt{\zeta}$ denotes the square root with positive real part, $\mathrm{Re}\sqrt{\zeta} > 0$. For $\zeta \leq 0$, we let $\sqrt{\zeta} = i\sqrt{|\zeta|}$. (Because Eq. (41) is invariant under changes in the signs of k and $\tilde{k}$, choosing the positive branch for the square roots is not a restriction on the solutions.)

We remind readers that a term such as $B_+ e^{i\tilde{k}x}$ is not a plane wave because $\tilde{k}$ is not real but complex. It is the product of a plane wave and an exponential growth factor governed by the imaginary part of $\tilde{k}$.

We are interested only in those solutions for Z with $\mathrm{Re}\, Z = E > 0$, because these are the ones that should be relevant to the behavior of states starting out on the plateau (with positive energy). Nevertheless, for simplicity, we will also allow $\mathrm{Re}\, Z \leq 0$, but exclude any

Z that is real and negative or zero. For any $Z \in \mathbb{C} \setminus (-\infty, 0]$ we have that $\mathrm{Re}\,\tilde{k} > 0$, so that the probability current j associated with $\exp(\mathrm{i}\tilde{k}x)$ is positive, namely $j = (\hbar/m)|\psi|^2 \mathrm{Re}\,\tilde{k}$. Because we do not want to consider any contribution with a current from infinity to the plateau, we assume that

$$C_+ = C_- = 0\,. \tag{43}$$

Thus, the relevant kind of eigenfunction is what we define to be a *decay eigenfunction* or *Gamow eigenfunction*, which is a nonzero function ψ with the form given by Eq. (41) with k and $\tilde{k}$ given by Eq. (42) and $C_\pm = 0$, satisfying Eq. (36) except at $x = \pm a$ (where ψ'' does not exist) for some $Z \in \mathbb{C} \setminus (-\infty, 0]$, such that both ψ and ψ' are continuous at $\pm a$. Those Z corresponding to a decay eigenfunction we call *decay eigenvalues* or *Gamow eigenvalues.*[14]

The remaining coefficients $A_\pm$ and $B_\pm$, as well as the possible values of Z, k, and $\tilde{k}$ are determined (up to an overall factor for $A_\pm, B_\pm$) from Eqs. (41), (42), and (43) by the requirement that both ψ and its derivative ψ' be continuous at $\pm a$, the ends of the plateau. We have collected the details of the calculations in Appendix A, and report the results here. To express them, we use the natural unit of energy in this setting, which is the energy whose de Broglie wavelength is equal to the length $2a$ of the plateau,

$$W \equiv \frac{\pi^2 \hbar^2}{2ma^2}. \tag{44}$$

For paradoxical confinement to occur, Δ should be large compared to W. The eigenvalues Z relevant to paradoxical confinement are those whose real part, the energy $\mathrm{Re}\,Z = E$, is positive (because we want to look at states starting on top of the plateau) and small (because only states of small energy are affected by paradoxical reflection), and whose imaginary part, $\mathrm{Im}\,Z = -\hbar/2\tau$, is negative (because eigenfunctions with $\mathrm{Im}\,Z > 0$ would grow with t, rather than shrink, due to influx from $x = \pm\infty$), and small (because they have large lifetime τ). In particular, we are not interested in eigenvalues Z far away from zero.

Theorem II. Suppose $\Delta \geq 100W$*. Then the number* N *of decay eigenvalues* Z *of Eq.* (36) *with* $|Z| \leq \Delta/4$ *lies in the range* $\sqrt{\Delta/W} - 2 < N \leq \sqrt{\Delta/W} + 2$*. There is a natural way of numbering these eigenvalues as* $Z_1, \ldots, Z_N$*. (There is no expression for* Z_n*, but it can be defined implicitly.) With each* Z_n *is associated a unique (up to a factor) eigenfunction* ψ_n*, and* $|\psi_n(x)|$ *is exponentially increasing as* $x \to \pm\infty$ *(that is,* $\mathrm{Im}\,\tilde{k} < 0$ *for* ψ_n*). Furthermore, for* $n \ll \sqrt{\Delta/W}$*,*

$$Z_n \approx \left(\frac{W}{4} - \mathrm{i}\frac{W^{3/2}}{2\pi\sqrt{\Delta}} \right) n^2\,. \tag{45}$$

The proof is given in Appendix A, and to our knowledge, the values in Eq. (45) are not in the literature. The precise meaning of approximate equality $x \approx y$ is $\lim x/y = 1$ as $\Delta \to \infty$ and a, n are fixed.

What can we read off about the lifetime τ? In the regime $\Delta \gg W$, the nth complex eigenvalue Z_n with $n \ll \sqrt{\Delta/W}$ is such that

$$\mathrm{Re}\, Z_n \approx \frac{\hbar^2 \pi^2 n^2}{8ma^2} \text{ and } \mathrm{Im}\, Z_n \approx -\frac{2\hbar}{a\sqrt{2m\Delta}} \mathrm{Re}\, Z_n \,. \tag{46}$$

Readers familiar with the infinite well potential, which corresponds to the limit $\Delta \to \infty$ of very deep wells of the type shown in Fig. 7, will notice that $\mathrm{Re}\, Z_n$ coincides with the eigenvalues of the infinite well potential of length $2a$. If we use Eq. (39) and $E = \mathrm{Re}\, Z$, we find that

$$\tau \approx a\frac{\sqrt{2m\Delta}}{4E} = \frac{1}{4}\sqrt{\frac{\Delta}{E}}\tau_{\mathrm{cl}} = \tau_{\mathrm{qu}} \,, \tag{47}$$

which is the same value as specified in Eq. (33). We have completed our derivation of the lifetime Eq. (33) from complex eigenvalues.

As we did for the potential step, we now also determine whether wave packets behave in the same way as the eigenfunctions, that is, whether a wave packet can remain in the plateau region for the time span (33).

IX. WAVE PACKETS ON THE PLATEAU

We will now use the eigenfunctions to draw conclusions about the behavior of normalized (square-integrable) wave packets (see Ref. 17 for similar considerations about radioactive decay). We will first show that, for large Δ, there exist normalized wave packets, initially concentrated in the plateau interval and leaking out at an exponential, but slow rate. The wave packets approach a quasi-steady-state situation in an expanding region surrounding the plateau – one that differs from a genuine steady state in that there is a global uniform overall exponential decay in time. This picture is similar to the behavior of the model $\rho_t(x)$ described around Eq. (35). Within the expanding region, the wave function is approximately given by an eigenfunction with a complex eigenvalue as described in Sec. VIII. An example of a normalized wave packet that behaves in this way is given by cutting off an eigenfunction outside the plateau interval, as described in Theorem III. These results can partially be generalized for other compactly supported potentials, not just for the plateau potential considered here. This generalization requires more advanced mathematical tools: see Refs. 15, 16 and 17.

We write ψ_n for the eigenfunction with eigenvalue Z_n, $\psi_{n,t} = \mathrm{e}^{-iZ_nt/\hbar}\psi_n$ for the time-dependent eigenfunction, $\tau_n = -\hbar/2\mathrm{Im}\, Z_n$ for the corresponding decay time, and

$$v_n = \frac{\hbar}{m}\mathrm{Re}\,\tilde{k}_n \tag{48}$$

for the speed at which an escaping particle moves away from the plateau.

Theorem III. Let n be a fixed positive integer; keep the plateau length $2a$ fixed and consider the regime $\Delta \gg W$. The initial wave function

$$\varphi_0(x) = \begin{cases} A_n\psi_n(x) & -a \leq x \leq a \\ 0 & \textit{otherwise,} \end{cases} \tag{49}$$

with normalization constant A_n, evolves with time in such a way that, for $0 < t < \tau_n$, φ_t is close to $A_n\psi_{n,t}$ on the interval $[-a - v_nt, a + v_nt]$ growing at speed v_n. Explicitly, for $0 < t < \tau_n$, we have

$$\int_{-a-v_nt}^{a+v_nt} \left|\varphi_t(x) - A_n\psi_{n,t}(x)\right|^2 \mathrm{d}x \ll 1\,. \tag{50}$$

The proof is included in Appendix B. Theorem III is used in the proof of Theorem I.

Theorem III provides a deeper justification of Eq. (33) for the decay time τ_{qu} by showing that $1/\tau_{\mathrm{qu}}$ is not merely the decay rate of eigenfunctions ψ_n, but also the decay rate of certain normalized wave packets φ_t. The probability in $[-a, a]$ decreases at the rate $1/\tau_{\mathrm{qu}} = 1/\tau_n$, at least up to time τ_n. In particular, the particle has probability $\approx 1/\mathrm{e} = 0.3679$ to stay in the plateau region until τ_n.

It may seem that Theorem III concerns only a specially chosen wave packet φ_0, but by forming linear combinations we can obtain the slow decay for any wave packet of low energy:

Corollary. Let $\Delta \gg W$. For any initial wave function ψ on the plateau with contributions only from eigenfunctions ψ_n with low n, that is,

$$\psi(x) = \begin{cases} \displaystyle\sum_{n=1}^{n_{\max}} c_n\,\psi_n(x) & -a \leq x \leq a, \\ 0 & \textit{otherwise,} \end{cases} \tag{51}$$

with Δ independent $n_{\max}$ and coefficients c_n, the time-evolved wave function $\psi_t = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi$ is close to $\sum_n c_n\,\psi_{n,t}$ on the interval $[-a-vt, a+vt]$ growing at speed $v = \min(v_1, \ldots, v_{n_{\max}})$, *at least up to time* $\min(\tau_1,\ldots,\tau_{n_{\max}})$. *That is,*

$$\int_{-a-vt}^{a+vt}\Big|\psi_t(x)-\sum_n c_n\,\psi_{n,t}(x)\Big|^2 \mathrm{d}x \ll 1 \tag{52}$$

for $t\leq \min(\tau_1,\ldots,\tau_{n_{\max}})$.

The corollary means that any such wave packet ψ will have a long decay time on the plateau, namely, at least $\min(\tau_1,\ldots,\tau_{n_{\max}})$ [with each τ_n given by Eq. (33) and not by the classical expression (31)]. Equation (52) suggests that the decay time of ψ is of the order of the largest τ_n with $1\leq n\leq n_{\max}$ and significant $|c_n|^2$.

We note that the decay results described here, both qualitative and quantitative, presumably apply as well to the standard tunneling situation in which a particle is confined inside a region by a potential barrier (a wall) that is high but not infinitely high, separating the inside from the outside. For this situation, more detailed results were obtained in Ref. 18 by other methods based on analytic continuation.

X. CONCLUSIONS

We have argued that paradoxical reflection and paradoxical confinement are real phenomena and not artifacts of the stationary analysis. The effect is a robust prediction of the Schrödinger equation, and persists when the potential step is not assumed to be rectangular but soft, and when the incoming wave is a packet of finite width. We have provided numerical evidence and identified the relevant conditions on the parameters. We have explained why it is not a counterargument to note that paradoxical reflection is impossible classically. We conclude that paradoxical reflection is real and not an artifact. Finally, we have shown that a state (of sufficiently low energy) on a potential plateau as in Fig. 6 has a long decay time, no less than τ_{qu} given by Eq. (33). We conclude that a plateau potential can, for suitable parameters, be confining. Thus, the effect could be used for constructing a (metastable) particle trap.

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APPENDIX A: SOLVING THE PLATEAU EIGENVALUE EQUATION

We now prove Theorem II by determining all the decay eigenfunctions of Eq. (36), as defined after Eq. (43). The continuity of ψ requires that

$$A_+ \mathrm{e}^{\mathrm{i}ka} + A_- \mathrm{e}^{-\mathrm{i}ka} = B_+ \mathrm{e}^{\mathrm{i}\tilde{k}a} \tag{A1}$$

$$A_+ \mathrm{e}^{-\mathrm{i}ka} + A_- \mathrm{e}^{\mathrm{i}ka} = B_- \mathrm{e}^{\mathrm{i}\tilde{k}a}\,, \tag{A2}$$

and continuity of ψ' requires

$$k\left(A_+ \mathrm{e}^{\mathrm{i}ka} - A_- \mathrm{e}^{-\mathrm{i}ka}\right) = \tilde{k} B_+ \mathrm{e}^{\mathrm{i}\tilde{k}a} \tag{A3}$$

$$k\left(A_+ \mathrm{e}^{-\mathrm{i}ka} - A_- \mathrm{e}^{\mathrm{i}ka}\right) = -\tilde{k} B_- \mathrm{e}^{\mathrm{i}\tilde{k}a}. \tag{A4}$$

Both k and $\tilde{k}$ may be complex. Because we assume $\Delta > 0$, and by Eq. (36), $\tilde{k}^2 = k^2 + 2m\Delta/\hbar^2$, we have that $k \pm \tilde{k} \neq 0$, and these equations are readily solved. First, we find the relations

$$A_- = \mathrm{e}^{\mathrm{i}2ak} \frac{k-\tilde{k}}{k+\tilde{k}} A_+, \tag{A5}$$

$$B_+ = \mathrm{e}^{\mathrm{i}a(k-\tilde{k})} \frac{2k}{k+\tilde{k}} A_+, \tag{A6}$$

$$B_- = \mathrm{e}^{-\mathrm{i}a(k+\tilde{k})} \frac{2k}{k-\tilde{k}} A_+, \tag{A7}$$

with the additional requirement that, because $A_+ \neq 0$ for decay eigenfunctions:

$$\left(\frac{k+\tilde{k}}{k-\tilde{k}}\right)^2 = \mathrm{e}^{\mathrm{i}4ak}. \tag{A8}$$

Let

$$\lambda_0 = \frac{2\pi\hbar}{\sqrt{2m\Delta}} \text{ and } \alpha = \frac{a}{\pi\hbar}\sqrt{2m\Delta} = \frac{2a}{\lambda_0}. \tag{A9}$$

λ_0 is the de Broglie wavelength corresponding to the height Δ of the potential plateau, and α is the width of the plateau in units of λ_0. Thus in terms of W defined in Eq. (44) we have $\alpha = \sqrt{\Delta/W}$. To express k in natural units, let

$$\kappa \equiv \frac{\lambda_0 k}{2\pi}\,. \tag{A10}$$

Then

$$k = \frac{2\pi}{\lambda_0}\kappa \text{ and } \tilde{k} = \frac{2\pi}{\lambda_0}\sqrt{1+\kappa^2}\,, \tag{A11}$$

and we have

$$\frac{k+\tilde{k}}{k-\tilde{k}} = \frac{\kappa+\sqrt{1+\kappa^2}}{\kappa-\sqrt{1+\kappa^2}} = -\left(\kappa+\sqrt{1+\kappa^2}\right)^2. \tag{A12}$$

Thus Eq. (A8) is equivalent to

$$\left(\kappa+\sqrt{1+\kappa^2}\right)^4 = \mathrm{e}^{\mathrm{i}4\pi\kappa\alpha}. \tag{A13}$$

The solutions of Eq. (A13) coincide with those of the equation

$$\ln(\kappa+\sqrt{1+\kappa^2}) = \mathrm{i}\pi\kappa\alpha - \mathrm{i}\frac{\pi n}{2} \tag{A14}$$

where $n \in \mathbb{Z}$ is arbitrary and ln denotes the principal branch of the complex logarithm.[19]

Thus, with every decay eigenfunction ψ is associated a solution κ of Eq. (A14) (with $\operatorname{Re}\kappa > 0$, because $\operatorname{Re} k > 0$ by the definition of k in Eq. (42)) and an integer n. Furthermore, $n \geq -1$, because $\operatorname{Re}\kappa > 0$ and the imaginary part of the left-hand side of Eq. (A14) must lie between $-\pi$ and π. Conversely, with every solution κ of Eq. (A14) with $\operatorname{Re}\kappa > 0$ there is associated a decay eigenvalue

$$Z = \kappa^2\Delta, \tag{A15}$$

and an eigenfunction ψ that is unique up to a factor. Equations (A10) and (A11) provide the values of k and $\tilde{k}$ and imply Eqs. (A15) and (A8); $\operatorname{Re}\kappa > 0$ implies $Z \notin (-\infty, 0]$, as well as $\operatorname{Re} k > 0$, so that $k = \sqrt{2mZ}/\hbar$; $k \pm \tilde{k} \neq 0$; A_+ can be chosen arbitrarily in $\mathbb{C}\setminus\{0\}$, and if A_- and $B_\pm$ are chosen according to Eqs. (A5)–(A7), then ψ is nonzero (as, for example, $B_+ \neq 0$ when $k \neq 0$ and $A_+ \neq 0$) and a decay eigenfunction. Note that the condition $\operatorname{Re}\kappa > 0$ is automatically satisfied when $n \geq 2$, as we can see from the imaginary part of Eq. (A14) using that ln has an imaginary part in $(-\pi, \pi]$.

To determine ψ explicitly, note that $\mathrm{e}^{\mathrm{i}2ak}(k-\tilde{k})/(k+\tilde{k}) = (-1)^{n+1}$, and thus $A_- = (-1)^{n+1}A_+$, $B_- = (-1)^{n+1}B_+$. If we set $A_+ = 1/2$ and introduce the notation

$$B \equiv B_+ \mathrm{e}^{\mathrm{i}a\tilde{k}} = \mathrm{e}^{\mathrm{i}ak}\frac{k}{k+\tilde{k}} = \mathrm{e}^{\mathrm{i}\pi\kappa\alpha}\frac{\kappa}{\sqrt{1+\kappa^2}+\kappa} = \mathrm{i}^n\kappa\,, \tag{A16}$$

we obtain that for odd n

$$\psi(x) = B\left[\chi(x>a)\mathrm{e}^{\mathrm{i}\tilde{k}(x-a)} + \chi(x<-a)\mathrm{e}^{-\mathrm{i}\tilde{k}(x+a)}\right] + \chi(-a \le x \le a)\cos(kx)\,, \tag{A17}$$

and for even n

$$\psi(x) = B\left[\chi(x>a)\mathrm{e}^{\mathrm{i}\tilde{k}(x-a)} - \chi(x<-a)\mathrm{e}^{-\mathrm{i}\tilde{k}(x+a)}\right] + \chi(-a \le x \le a)\sin(kx)\,, \tag{A18}$$

where $\chi(Q)$ is defined by

$$\chi(Q) = \begin{cases} 1 & \text{if } Q \text{ is true,} \\ 0 & \text{otherwise.} \end{cases} \tag{A19}$$

To sum up what we have so far, the decay eigenvalues are characterized, via Eq. (A15), through the solutions κ of Eq. (A14) with $\mathrm{Re}\,\kappa > 0$. To study existence, uniqueness, and the asymptotics for $\alpha \to \infty$ of these solutions, we now assume, as in Theorem II, that $\alpha \ge 10$ and $|Z| \le \Delta/4$. By virtue of Eq. (A15), the latter assumption is equivalent to $|\kappa| \le 1/2$.

We first show that solutions with $|\kappa| \le 1/2$ must have $|n| \le \alpha + 2$. Because ln has an imaginary part in $(-\pi, \pi]$, Eq. (A14) implies that $\mathrm{Re}\,\kappa \in (\frac{n-2}{2\alpha}, \frac{n+2}{2\alpha}]$, and hence

$$\frac{1}{2} \ge |\kappa| \ge |\mathrm{Re}\,\kappa| \ge \frac{|n|-2}{2\alpha}\,, \tag{A20}$$

or $|n| \le \alpha + 2$. Next recall that for decay eigenvalues, $n \ge -1$, and therefore we obtain at this stage that the number of values that n can assume is at most $\alpha + 4$, because the possible values are $-1, 0, 1, 2, \ldots \le \alpha + 2$. We will later exclude $n = 0$ and $n = -1$.

We now show that there exists a unique solution κ of Eq. (A14) for every n with $|n| \le \alpha + 2$. Let

$$F(\kappa) = \frac{n}{2\alpha} - \frac{\mathrm{i}}{\pi\alpha}\ln\left(\kappa + \sqrt{1+\kappa^2}\right)\,, \tag{A21}$$

so that Eq. (A14) can equivalently be rewritten as the fixed point equation

$$F(\kappa) = \kappa\,. \tag{A22}$$

We use the Banach fixed point theorem[20] to conclude the existence and uniqueness of κ. Because

$$F'(\kappa) = -\frac{\mathrm{i}}{\pi\alpha}\frac{1}{\sqrt{1+\kappa^2}}\,, \tag{A23}$$

we have, by the triangle inequality, that

$$|F'(\kappa)| = \frac{1}{\pi\alpha|1+\kappa^2|^{1/2}} \le \frac{1}{\pi\alpha|1-|\kappa|^2|^{1/2}}\,. \tag{A24}$$

Consider for a moment, instead of $|\kappa| \le 1/2$, the disk $|\kappa| \le r$ for any radius $0 < r < \sqrt{1-1/\pi^2\alpha^2}$. There we have that $|F'(\kappa)| \le 1/(\pi\alpha\sqrt{1-r^2}) \equiv K < 1$. Thus, for any κ, κ' in the closed disk of radius r, $|F(\kappa') - F(\kappa)| \le K|\kappa' - \kappa|$, and, using $|F(0)| = |n|/2\alpha$, we have

$$|F(\kappa)| \le |F(\kappa) - F(0)| + |F(0)| \le rK + \frac{|n|}{2\alpha} \le r\,, \tag{A25}$$

provided that

$$|n| \le 2\alpha r(1-K)\,. \tag{A26}$$

Thus, in this case, F is a contraction in the ball of radius r, with a contraction constant of at most K. By the Banach fixed point theorem there is a unique solution to the equation $F(\kappa) = \kappa$ in the ball $|\kappa| \le r$. Even though we are ultimately interested in the radius $1/2$, we set $r = 1/\sqrt{2}$, which satisfies $r < \sqrt{1-1/\pi^2\alpha^2}$ as $\alpha \ge 10$. Also Eq. (A26) is satisfied because $|n| \le \alpha + 2$ and $\alpha \ge 10 > 2(1+1/\pi)/(\sqrt{2}-1) \approx 6.37$. Hence, for every n with $|n| \le \alpha + 2$, there is a unique solution κ_n with $|\kappa_n| \le 1/\sqrt{2}$.

Returning to the ball of radius $1/2$, although some of the κ_n may have moduli greater than $1/2$, we can at least conclude that there is at most one solution with modulus $\le 1/2$ for every n with $|n| \le \alpha+2$. In addition, by setting $r = 1/2$, we obtain from Eq. (A26) that $|\kappa_n| \le 1/2$ for every n with $|n| \le \alpha - 1$. If $n = 0$, then $F(0) = 0$ and $\kappa_0 = 0$ is the unique solution, which would lead to $\psi = 0$. Thus, $n = 0$ is excluded. Which of the solutions have $\operatorname{Re}\kappa_n > 0$, as required for decaying eigenvalues? For any n with $|n| \le \alpha + 2$, let $\kappa_n^{(j)}$ be defined recursively by $\kappa_n^{(j+1)} = F(\kappa_n^{(j)})$ with $\kappa_n^{(0)} = 0$. Then, again by the Banach fixed point theorem for $r = 1/\sqrt{2}$, we have $\kappa_n^{(j)} \to \kappa_n$ as $j \to \infty$, and

$$|\kappa_n - \kappa_n^{(j)}| \le \frac{K^j}{1-K}|\kappa_n^{(1)} - \kappa_n^{(0)}| \le |n|\alpha^{-(j+1)}\,. \tag{A27}$$

For $n = -1$ and $j = 1$, Eq. (A27) gives that $|\kappa_{-1} - \kappa_{-1}^{(1)}| \le \alpha^{-2}$, and with $\kappa_{-1}^{(1)} = -1/2\alpha$ and $\alpha \ge 10$, we can conclude that $\operatorname{Re}\kappa_{-1} < 0$. Thus, $n = -1$ is excluded. For $n > 0$, in contrast, the fact that $|\kappa_n - \kappa_n^{(1)}| \leq |n|\alpha^{-2}$ allows us to conclude, with $\kappa_n^{(1)} = n/2\alpha$ and $\alpha \geq 10$, that $\operatorname{Re}\kappa_n > 0$. Hence, the decay eigenvalues with $|Z| \leq \Delta/4$ are in one-to-one correspondence with those κ_n, $0 < n \leq \alpha + 2$, that have $|\kappa_n| \leq 1/2$; the number of these κ_n must be greater than $\alpha - 2$ and less than or equal to $\alpha + 2$.

Furthermore, we can now check that for these κ_n, $\operatorname{Im}\kappa_n < 0$. The explicit calculation of $\kappa_n^{(2)}$ yields

$$\kappa_n^{(2)} = \nu - \mathrm{i}\frac{1}{\pi\alpha}\ln\left(\nu + \sqrt{1+\nu^2}\right), \tag{A28}$$

with $\nu = n/2\alpha$. Using Eq. (A27) as before, the result follows if we can show that $\operatorname{Im}\kappa_n^{(2)} < -n\alpha^{-3}$. We claim that for all $x \geq 0$,

$$\frac{1}{\sqrt{1+x^2}}x \leq \ln(x + \sqrt{1+x^2}) \leq x\,. \tag{A29}$$

Because $0 < \nu \leq (\alpha+2)/2\alpha \leq 0.6$ by the assumption $\alpha \geq 10$, for such ν and α we have $-\operatorname{Im}\kappa_n^{(2)} \geq (1/\sqrt{2}\pi\alpha)\nu > n\alpha^{-3}$, and thus $\operatorname{Im}\kappa_n < 0$.

The inequalities in Eq. (A29) can be derived as follows. Consider the function $f(x) = \ln(x+\sqrt{1+x^2})-x$, for which $f(0) = 0$ and $f'(x) = (1/\sqrt{1+x^2})-1$. Thus $f(x) = \int_0^x \mathrm{d}y\, f'(y)$, and $-1 + 1/\sqrt{1+x^2} \leq f'(y) \leq 0$ for all $0 \leq y \leq x$, which immediately yields the bounds in Eq. (A29).

As a consequence of $\operatorname{Im}\kappa_n < 0$ (and $\operatorname{Re}\kappa_n > 0$), $\operatorname{Im}\tilde{k} < 0$, so that $|\psi(x)|$ grows exponentially as $x \to \pm\infty$. By $|\kappa_n - \kappa_n^{(2)}| \leq n/\alpha^3$ and the previous estimates for $\operatorname{Im}\kappa_n^{(2)}$, we also have the following explicit bounds for the real and imaginary parts of κ_n,

$$\frac{n}{2\alpha}\left(1 - \frac{2}{\alpha^2}\right) \leq \operatorname{Re}\kappa_n \leq \frac{n}{2\alpha}\left(1 + \frac{2}{\alpha^2}\right) \tag{A30}$$

$$\frac{n}{2\pi\alpha^2}\left(1 - \frac{2\pi}{\alpha} - \frac{n^2}{4\alpha^2}\right) \leq -\operatorname{Im}\kappa_n \leq \frac{n}{2\pi\alpha^2}\left(1 + \frac{2\pi}{\alpha}\right), \tag{A31}$$

where in Eq. (A31), we have simplified the result using the bound $1/\sqrt{1+\nu^2} \geq 1/(1+\nu^2) \geq 1 - \nu^2$.

Now let us consider the asymptotics for $n \ll \alpha$. From Eq. (A27) we have that κ_n is given by the right-hand side of Eq. (A28) up to an error of order $O(n\alpha^{-3})$. Therefore, for integers n with $0 < n \ll \alpha$ we have that

$$k_n \approx \frac{\pi n}{2a} - \mathrm{i}\frac{n}{2a\alpha} \quad \text{and} \quad \tilde{k}_n \approx \frac{\pi\alpha}{a} - i\frac{n^2}{4a\alpha^2} \tag{A32}$$

$$Z_n = \kappa_n^2\Delta \approx \frac{n^2\Delta}{4\alpha^2}\left(1 - i\frac{2}{\pi\alpha}\right). \tag{A33}$$

The previous estimates, in particular Eqs. (A30) and (A31), can be used to estimate the accuracy of these approximations. For instance,

$$\left|k_n - \frac{\pi n}{2a}\right| = \frac{2\pi}{\lambda_0}|\kappa_n - \kappa_n^{(1)}| \leq \frac{2\pi}{\lambda_0}\frac{n}{\alpha^2} = \frac{\pi n}{a\alpha}\,. \tag{A34}$$

Also, because $-\mathrm{Im}\, Z_n = 2\Delta\, \mathrm{Re}\, \kappa_n(-\mathrm{Im}\kappa_n)$, the lifetimes τ_n satisfy

$$C_1\frac{\pi\alpha^3\hbar}{n^2\Delta} \leq \tau_n \leq C_2\frac{\pi\alpha^3\hbar}{n^2\Delta}\,, \tag{A35}$$

for all $0 < n \leq \alpha$, and with some numerical constants $C_1, C_2 > 0$. Using the definition of α, $\pi\alpha^3\hbar/(n^2\Delta) = (ma^2/\pi\hbar)\alpha n^{-2}$. Thus if we consider the limit $\Delta \to \infty$ while keeping all other parameters fixed, we have $\alpha \to \infty$ and can choose $C_1 = 1 - O(\alpha^{-1})$ and $C_2 = 1 + O(\alpha^{-1})$. Therefore, $\tau_n/\alpha \to (ma^2/\pi\hbar)n^{-2}$ for any fixed n. In particular, $\tau_n \to \infty$.

APPENDIX B: DERIVATION OF THE LIFETIME ESTIMATES FOR THE METASTABLE STATES IN THE PLATEAU REGION

Proof of Theorem III. We construct an auxiliary function $f(x,t)$ that does not obey the Schrödinger equation, but remains close to the time-evolved eigenfunction in a growing region around the plateau. We then prove that $f(x,t)$ forms an excellent approximation of $\varphi_t(x)$. We will define $f(x,t)$ by cutting off the time-evolved eigenfunction $\mathrm{e}^{-\mathrm{i}tZ_n/\hbar}\psi_n$ in a continuous way using Gaussians with time-dependent parameters.

We begin by estimating the normalization constant A_n. We define for all $|x| \leq a$ and integers $n \geq 1$, $\phi_n(x) = \cos[(\pi n/2a)x]$, if $n \geq 1$ is odd, and $\phi_n(x) = \sin[(\pi n/2a)x]$, if $n \geq 2$ is even. A short calculation shows that $\phi_n(x) = \pm\sin[(\pi n/2a)(x+a)]$, and thus the collection of functions (ϕ_n) is up to a constant equal the sine-basis of square integrable functions on $[-a,a]$. We also define $\phi_n(x) = 0$ for $|x| > a$. Because $\int_{-a}^{a}|\phi_n(x)|^2 = a$, their normalization constants are independent of n, and are all equal to $a^{-1/2}$. By Eq. (A34) for any n the difference $z_n = k_n - (\pi n/2a)$ satisfies $|z_n| \leq \pi n/a\alpha$. Therefore, by expanding the appropriate cosine or sine, we find for all $|x| \leq a$,

$$\left|\psi_n(x) - \phi_n(x)\right| \leq |1 - \cos(z_n x)| + |\sin(z_n x)| \leq (|z_n x|^2 + |z_n x|)\mathrm{e}^{|z_n x|}\,, \tag{B1}$$

where $|z_n x| \leq \pi n/\alpha \leq \pi(1 + 2/\alpha)$. Thus there is a pure constant c such that

$$\int_{-a}^{a}\left|\psi_n(x) - \phi_n(x)\right|^2 \leq ac^2\frac{n^2}{\alpha^2}\,. \tag{B2}$$

($c = 2\pi$ will suffice if n/α is small enough.) By the triangle inequality and the definition of the normalization constant $A_n > 0$, the left-hand side has a lower bound $|A_n^{-1} - \sqrt{a}|^2$. Thus $A_n = a^{-1/2} + O(n/\alpha)$, and if $n \leq \alpha/(2c)$, we have $\frac{2}{3} \leq \sqrt{a}A_n \leq 2$. Therefore, in this case the normalization constant remains bounded away from both zero and infinity, uniformly in n and α. As a consequence of these estimates, we also have $\left\|\varphi_{n,0} - a^{-1/2}\phi_n\right\| \leq 2cn/\alpha$.

To define $f(x,t)$ we first introduce the abbreviation

$$\beta = -\mathrm{Im}\,\tilde{k} \approx \frac{n^2}{4a\alpha^2}, \tag{B3}$$

and recall

$$v = \frac{\hbar}{m}\mathrm{Re}\,\tilde{k} \approx \frac{\hbar\pi\alpha}{ma}. \tag{B4}$$

Hence, $\tilde{k} = (m/\hbar)v - \mathrm{i}\beta$ with $v, \beta > 0$. We further define

$$R(t) = a + vt \text{ and } b(t) = \sigma^2 + \mathrm{i}\frac{\hbar}{2m}t, \tag{B5}$$

where the initial Gaussian spread $\sigma > 0$ is left arbitrary for the moment (a convenient choice will be $\sigma = a$). The Gaussians will be attached symmetrically to $x = \pm R(t)$ with the "variance" $b(t)$, which yields

$$f(x,t) = A_n \mathrm{e}^{-\mathrm{i}tZ_n/\hbar} \times \begin{cases} \pm B\mathrm{e}^{\mathrm{i}\tilde{k}(-x-a) - \dfrac{1}{4b(t)}(-x-R(t))^2}, & \text{if } x < -R(t), \\ B\mathrm{e}^{\mathrm{i}\tilde{k}(x-a) - \dfrac{1}{4b(t)}(x-R(t))^2}, & \text{if } x > R(t), \\ \psi_n(x), & \text{if } |x| \leq R(t). \end{cases} \tag{B6}$$

Note that for all $t \geq 0$, $f(\cdot,t)$ is normalizable but not normalized, and that $f(x,t)$ is continuously differentiable in x because ψ_n is, and because the unnormalized Gaussian $\exp(-(x-\mu)^2/4b)$ has, at its mean μ, value 1 and derivative 0. It is a short calculation[21] to check that for all $t > 0$

$$(H - Z)f(x,t) = -\frac{\hbar^2}{2m}\partial_x^2 f(x,t) + (V(x) - Z)f(x,t) \tag{B7}$$

$$= -\frac{\hbar^2}{2m}\left[g_1(x - R(t), t) \pm g_1(-x - R(t), t)\right] f(x,t), \tag{B8}$$

with [using the notation $\chi(\cdots)$ as in Eq. (A19)]

$$g_1(y,t) = \chi(y > 0)\left(\frac{y^2}{4b(t)^2} - \frac{1}{2b(t)} - \mathrm{i}\tilde{k}\frac{y}{b(t)}\right). \tag{B9}$$

In addition, we have

$$\mathrm{i}\hbar\partial_t f(x,t) = Zf(x,t) - \frac{\hbar^2}{2m}\left[g_2(x-R(t),t) \pm g_2(-x-R(t),t)\right] f(x,t), \tag{B10}$$

with $g_2 = g_1 + g_3$, where

$$g_3(y,t) = \chi(y>0)\frac{1+2\beta y}{2b(t)}. \tag{B11}$$

Because, for a fixed t, the function $f(x,t)$ is square integrable, we can define a mapping

$$t \mapsto F(t) = \mathrm{e}^{\mathrm{i}tH/\hbar} f(\cdot,t) - \varphi_0, \tag{B12}$$

with $F(t) \in L^2$ for all $t \geq 0$, and

$$\|F(0)\|^2 = \|f(\cdot,0) - \varphi_0\|^2 = \int_a^\infty \left|f(x,0)\right|^2 \mathrm{d}x + \int_{-\infty}^{-a} \left|f(x,0)\right|^2 \mathrm{d}x\,. \tag{B13}$$

For any $t \geq 0$ and $|x| > R(t)$, the definition of f yields

$$|f(x,t)|^2 = |A_n|^2|B|^2 \exp\left(2\,\mathrm{Re}\left[-\mathrm{i}\frac{t}{\hbar}Z + \mathrm{i}\tilde{k}(y+vt) - \frac{1}{4b(t)}y^2\right]\right)\,, \tag{B14}$$

with $y = |x| - R(t)$. Here the argument of the exponential can be simplified using $Z = (\hbar^2/2m)\tilde{k}^2 - \Delta$ to

$$2\beta y - \frac{\sigma^2}{2|b_t|^2}y^2 = \frac{1}{2}c_t^2 - \frac{1}{2}\left[\frac{2\beta}{c_t}y - c_t\right]^2, \tag{B15}$$

with $c_t = 2\beta|b(t)|\sigma^{-1}$. Thus for $t=0$, we have $c_0 = 2\beta\sigma$ and $R(0) = a$, and by changing the integration variable to $y' = (|x|-a)2\beta/c_0$, we find the bound

$$\|F(0)\|^2 \leq 2|A_n|^2|B|^2\mathrm{e}^{c_0^2/2}\frac{c_0}{2\beta}\int_0^\infty \mathrm{d}y'\,\mathrm{e}^{-(y'-c_0)^2/2} \leq 2\sigma|A_n|^2|B|^2\mathrm{e}^{c_0^2/2}\sqrt{2\pi}\,. \tag{B16}$$

Here $c_0 \approx (\sigma/a)n^2/(2\alpha^2)$, $A_n^2 \approx 1/a$, and $|B|^2 = |\kappa_n|^2 = O(n^2\alpha^{-2})$. Thus if we choose $\sigma = a$, there is a pure constant c' such that $\|F(0)\| \leq c'n/\alpha$ for all sufficiently small n/α.

F is differentiable and by the previous estimates for all $t > 0$,

$$\partial_t F(t) = \mathrm{e}^{\mathrm{i}tH/\hbar}\left[\frac{\mathrm{i}}{\hbar}Hf(\cdot,t) + \partial_t f(\cdot,t)\right] = \mathrm{e}^{\mathrm{i}tH/\hbar}g(\cdot,t), \tag{B17}$$

where

$$g(x,t) = \mathrm{i}\frac{\hbar}{2m}\left[g_3(x-R(t),t) \pm g_3(-x-R(t),t)\right] f(x,t). \tag{B18}$$

Because the derivative is continuous (in the L^2-norm) in t, it can be integrated to yield $F(t) = F(0) + \int_0^t \mathrm{d}s\,\partial_s F(s)$. Then, by the unitarity of the time evolution, we find that

$$\|f(\cdot,t) - \varphi_t\| = \|F(t)\| \leq \|F(0)\| + \int_0^t \mathrm{d}s\,\,\|\partial_s F(s)\| \leq c'n\alpha^{-1} + \int_0^t \mathrm{d}s\,\,\|g(\cdot,s)\|\,. \tag{B19}$$

Thus we need only to estimate the magnitude of $\int_0^t \mathrm{d}s\, \|g(\cdot, s)\|$. As before,

$$\|g(\cdot,t)\|^2 = \left(\frac{\hbar}{2m}\right)^2 2\int_0^\infty \mathrm{d}y\, |f(y+R(t),t)|^2 |g_3(y,t)|^2 \tag{B20}$$

$$= \left(\frac{\hbar|A_n||B|}{2m|b_t|}\right)^2 \frac{1}{2}\int_0^\infty \mathrm{d}y\, (1+2\beta y)^2 \exp\left(2\beta y - \frac{\sigma^2}{2|b_t|^2}y^2\right) \tag{B21}$$

$$= \left(\frac{\hbar\beta|A_n||B|}{m\sigma c_t}\right)^2 \frac{c_t}{4\beta}\mathrm{e}^{\frac{1}{2}c_t^2}\int_{-c_t}^\infty \mathrm{d}x\, (1+c_t^2+c_t x)^2 \mathrm{e}^{-\frac{1}{2}x^2} \tag{B22}$$

$$\leq \left(\frac{\hbar\beta|A_n||B|}{m\sigma c_t}\right)^2 \frac{c_t}{4\beta}\mathrm{e}^{\frac{1}{2}c_t^2}\int_{-\infty}^\infty \mathrm{d}x\, ((1+c_t^2)^2 + c_t^2 x^2) \mathrm{e}^{-\frac{1}{2}x^2} \tag{B23}$$

$$= \left(\frac{\hbar\sqrt{\beta}|A_n||B|}{2m\sigma}\right)^2 \frac{1}{c_t}\mathrm{e}^{\frac{1}{2}c_t^2}\sqrt{2\pi}((1+c_t^2)^2 + c_t^2). \tag{B24}$$

For sufficiently large α and all $0 \leq t \leq \tau \approx (2ma^2/\hbar\pi n^2)\alpha$,

$$c_t \leq c_\tau = 2\beta|b(\tau)|\sigma^{-1} = \frac{2}{\sigma}\beta\sqrt{\sigma^4 + \left(\frac{\hbar}{2m}\right)^2\tau^2} \tag{B25}$$

$$\approx \frac{2}{\sigma}\frac{n^2}{4a\alpha^2}\sqrt{\sigma^4 + \left(\frac{a^2}{\pi n^2}\right)^2\alpha^2} \leq \frac{a}{\pi\sigma}\frac{1}{\alpha}\,, \tag{B26}$$

and therefore

$$\|g(\cdot,t)\| \leq \frac{\hbar\sqrt{\beta}|A_n||B|}{2m\sigma}\frac{2}{\sqrt{c_t}}\,. \tag{B27}$$

Because

$$c_s = \sqrt{(2\beta\sigma)^2 + (s\beta\hbar/(m\sigma))^2} \geq s\frac{\beta\hbar}{m\sigma}, \tag{B28}$$

we can estimate the integral over s by

$$\int_0^t \mathrm{d}s \frac{1}{\sqrt{c_s}} \leq \int_0^t \mathrm{d}s \sqrt{\frac{m\sigma}{\beta\hbar s}} = 2\sqrt{\frac{m\sigma t}{\beta\hbar}}. \tag{B29}$$

This bound proves that for all $0 \leq t \leq \tau$, and sufficiently small n/α

$$\|f(\cdot,t) - \varphi_t\|^2 \leq 2\|F(0)\|^2 + 8|A_n|^2|B|^2\frac{\hbar}{m\sigma}t \leq 2(c')^2\frac{n^2}{\alpha^2} + \frac{4a}{\pi\sigma}\frac{t}{\tau}\frac{1}{\alpha} \ll 1\,, \tag{B30}$$

where we have used $(|z|+|z'|)^2 \leq 2(|z|^2+|z'|^2)$, valid for all $z, z' \in \mathbb{C}$ by Hölder's inequality. Because on the interval $[-a-vt, a+vt]$, $f(x,t) = A_n\psi_{n,t}(x)$, we have that

$$\int_{-a-vt}^{a+vt} |\varphi_t(x) - A_n\psi_{n,t}(x)|^2 \mathrm{d}x \leq \int_{-\infty}^\infty |\varphi_t(x) - f(x,t)|^2 \mathrm{d}x = \|f(\cdot,t) - \varphi_t\|^2 \ll 1\,, \tag{B31}$$

which is what we wanted to show.

Proof of Corollary. The Corollary follows easily from Theorem III. We write $\varphi_{n,0}$ for the wave function in Eq. (49) and have that

$$\psi(x) = \sum_{n=1}^{n_{\max}} \frac{c_n}{A_n} \varphi_{n,0}(x) \, . \tag{B32}$$

From Eq. (B32) we obtain that, provided $0 < t < \tau_n$ for each n,

$$\begin{aligned} &\left\| \Big(\psi_t - \sum_n c_n \psi_{n,t} \Big) \chi(-a - vt \le x \le a + vt) \right\| \\ &\le \sum_n \left| \frac{c_n}{A_n} \right| \left\| \Big(\varphi_{n,t} - A_n \psi_{n,t} \Big) \chi(-a - vt \le x \le a + vt) \right\| \ll 1, \end{aligned} \tag{B33}$$

with the notation $\chi(\cdots)$ as in Eq. (A19). Thus, Eq. (52) is proven.

Proof of Theorem I. As we proved, for all small enough n/α the vectors $\varphi_{n,0}$ can be approximated by $e_n(x) = \pm a^{-1/2} \sin[(\pi n/2a)(x + a)]$ with the error bounded by cn/α and c a numerical constant. The functions e_n are up to a sign equal to the sine-basis of square integrable functions on $[-a, a]$, and therefore they form an orthonormal basis. Let a_n denote the expansion constants of ψ_0 in this basis; that is, they are the unique constants for which $\psi_0 = \sum_{n=1}^{\infty} a_n e_n$. Because a_n are obtained by projecting ψ_0 to e_n, they depend only on ψ_0, a, and n.

Now $\sum_n |a_n|^2 = \|\psi_0\|^2 = 1$, and for any given ε, there is an α-independent constant $n_{\max}(\varepsilon) < \infty$, such that

$$\left\| \psi_0 - \sum_{n=1}^{n_{\max}(\varepsilon)} a_n e_n \right\| \le \frac{1}{4} \varepsilon \, . \tag{B34}$$

Also, necessarily $\sum_{n=1}^{n_{\max}(\varepsilon)} |a_n|^2 \ge 1 - \varepsilon^2/16$. Therefore,

$$\left\| \psi_0 - \sum_{n=1}^{n_{\max}(\varepsilon)} a_n \varphi_{n,0} \right\| \le \frac{1}{4} \varepsilon + \frac{c n_{\max}(\varepsilon)^2}{\alpha} \, . \tag{B35}$$

As we proved in Appendix A, for any fixed n, $\tau_n \to \infty$ in the limit $\alpha \to \infty$. Therefore, for all sufficiently large α, we have $t_0 \le \tau_n$, for all $1 \le n \le n_{\max}(\varepsilon)$. Thus by the explicit estimate in Eq. (B30), the time-evolved vectors in Hilbert space satisfy for such large α and any $0 \le t \le t_0$

$$\Big\|\chi(|x|\le a)\Big(\psi_t - \sum_{n=1}^{n_{\max}(\varepsilon)} a_n A_n \psi_{n,t}\Big)\Big\| \tag{B36}$$

$$\le \Big\|\psi_t - \sum_{n=1}^{n_{\max}(\varepsilon)} a_n \varphi_{n,t}\Big\| + \sum_{n=1}^{n_{\max}(\varepsilon)} |a_n| \Big\|\chi(|x|\le a)\Big(\varphi_{n,t} - A_n\psi_{n,t}\Big)\Big\| \tag{B37}$$

$$\le \frac{1}{4}\varepsilon + \frac{c n_{\max}(\varepsilon)^2}{\alpha} + c'\frac{n_{\max}(\varepsilon)^3}{\alpha^2}, \tag{B38}$$

with some numerical constant c'. For sufficiently large α, the right-hand side is bounded by $\varepsilon/2$.

Because $A_n\psi_{n,t}(x)\chi(|x|\le a) = \mathrm{e}^{-\mathrm{i}Z_n t/\hbar}\varphi_{n,0}(x)$ and $\lim_{\alpha\to\infty} Z_n = \hbar^2\pi^2 n^2/8ma^2$, we have $A_n\psi_{n,t}(x)\chi(|x|\le a) \to \mathrm{e}^{-\mathrm{i}\frac{\hbar\pi^2 n^2}{8ma^2}t} e_n(x)$ in norm when $\alpha\to\infty$, in fact uniformly in $t\in[0,t_0]$. As a consequence,

$$\lim_{\alpha\to\infty}\Big\|\chi(|x|\le a)\sum_{n=1}^{n_{\max}(\varepsilon)} a_n A_n\psi_{n,t}\Big\|^2 = \sum_{n=1}^{n_{\max}(\varepsilon)} |a_n|^2 \ge 1 - \frac{\varepsilon^2}{16} \tag{B39}$$

uniformly in $t\in[0,t_0]$, and thus

$$\Big\|\chi(|x|\le a)\sum_{n=1}^{n_{\max}(\varepsilon)} a_n A_n\psi_{n,t}\Big\|^2 \ge 1 - \frac{\varepsilon^2}{8} \tag{B40}$$

for all $t\in[0,t_0]$, provided α is big enough. By the triangle inequality, $\|\chi(|x|\le a)\psi_t\| \ge \sqrt{1-\varepsilon^2/8} - \varepsilon/2$. As $\|\psi_t\| = 1$, then necessarily $\|\chi(|x|>a)\psi_t\|^2 \le 1 - (\sqrt{1-\varepsilon^2/8}-\varepsilon/2)^2 < \varepsilon$, which concludes the proof of Theorem I.

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[14] Here is a look at the negative Z's that we excluded in this definition: for $Z \in (-\infty, 0] \setminus \{-\Delta\}$ there exist no nonzero functions with $C_\pm = 0$ satisfying the eigenvalue equation (36) for all $x \neq \pm a$ such that ψ and ψ' are continuous. We have not included the proof in this paper. For $Z = -\Delta$, the coefficients $C_\pm$ are not defined, so the condition (43) makes no sense.

[15] E. Skibsted, "Truncated Gamow functions, α-decay and the exponential law," Commun. Math. Phys. **104**, 591–604 (1986).

[16] O. Costin and M. Huang, "Gamow vectors and Borel summability," `<arxiv.org/abs/0902.0654>`.

[17] D. Dürr, R. Grummt, and M. Kolb, "On the time-dependent analysis of Gamow decay," `<arxiv.org/abs/1011.6084>`.

[18] R. M. Cavalcanti and C. A. A. de Carvalho, "On the effectiveness of Gamow's method for

calculating decay rates," Revista Brasileira de Ensino de Física **21(4)**, 464–468 (1999), `<arxiv.org/abs/quant-ph/9711037>`.

[19] For $\zeta \in \mathbb{C} \setminus \{0\}$, the equation $\mathrm{e}^z = \zeta$ has infinitely many solutions z, all of which have real part $\ln|\zeta|$; the imaginary parts differ by integer multiples of 2π; by $\ln \zeta$ we denote that z which has $-\pi < \operatorname{Im} z \leq \pi$.

[20] Banach fixed point theorem, `<en.wikipedia.org/wiki/Banach_fixed_point_theorem>`.

[21] The computation can be given the following mathematical justification: Because the potential V is bounded, by an application of the Kato-Rellich theorem, Ref. 22, Theorem X.15, the Hamiltonian $H = -(\hbar^2/2m)\partial_x^2 + V$ is self-adjoint on the domain of $-\partial_x^2$. It can be easily checked that for any t the derivative $\partial_x f(x,t)$ is absolutely continuous in x, and thus the function $f(\cdot,t)$ belongs to the domain of H. These properties can be used to justify all the manipulations made here. We also stress that if we had not chosen the constants $A_\pm$ and $B_\pm$ in Eq. (41) so that the function is continuously differentiable, then the addition of the Gaussian cut-off would have resulted in functions which are in $L^2(\mathbb{R})$ but which do not belong to the domain of H. Thus our estimates are not valid for such initial states. For more sophisticated mathematical methods to study such problems, see, for instance, Refs. 15 and 16.

[22] M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-adjointness* (Academic Press, New York and London, 1975).

FIGURE CAPTIONS

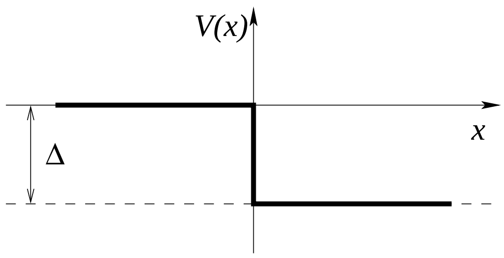

FIG. 1: A potential $V(x)$ containing a downward step.

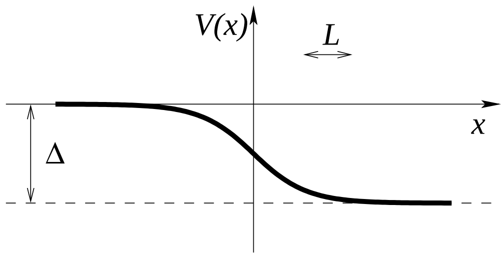

FIG. 2: A potential containing a soft step.

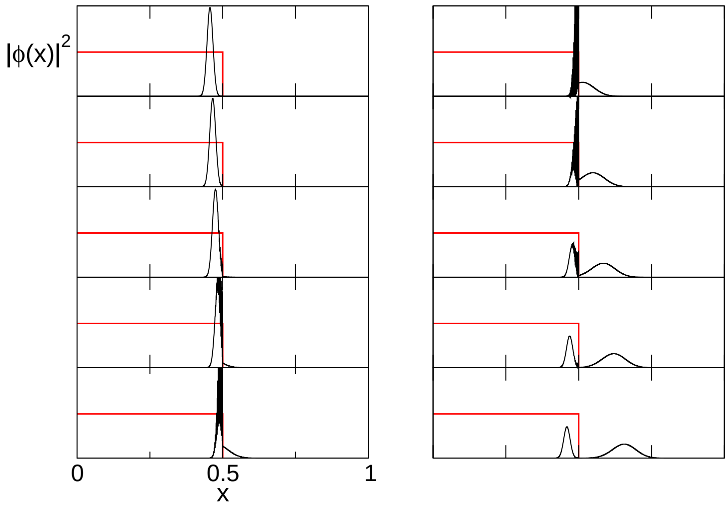

FIG. 3: Numerical simulation of the time-dependent Schrödinger equation for the hard step potential of Eq. (1). The picture shows ten snapshots of $|\psi|^2$ (black lines) at different times before, during, and after passing the potential step. (Order: left column top to bottom, then right column top to bottom.) The straight lines in the figures depict the potential in arbitrary units. It can be seen that there is a transmitted wave packet and a reflected wave packet. The initial wave function is a Gaussian wave packet centered at $x = 0.4$ with $\sigma = 0.01$ and $k_0 = 500\pi$. The simulation assumes infinite potential walls at $x = 0$ and $x = 1$. The step height is $\Delta = 15E$, and the x-interval is resolved with a linear mesh of $N = 10^4$ points. The snapshots are taken at times $6, 7, 8, \ldots, 15$ in appropriate time units.

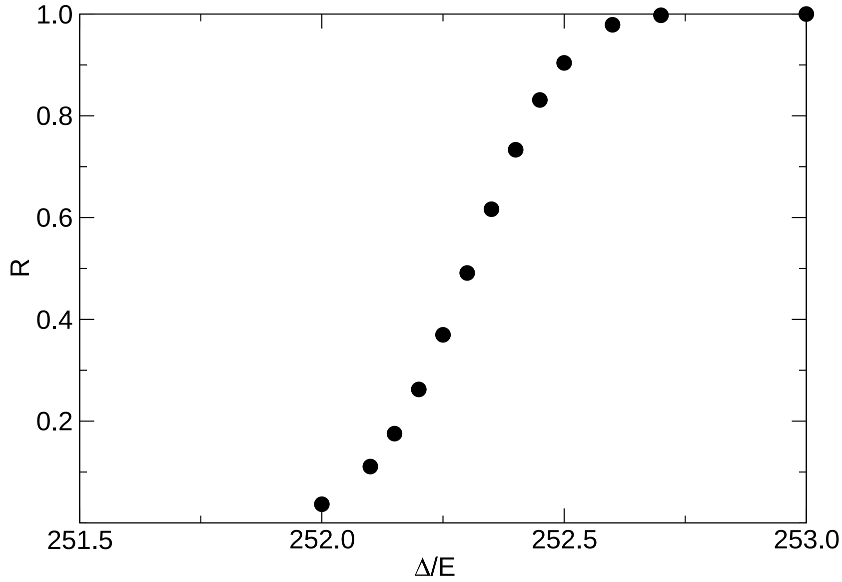

FIG. 4: An example of how numerical error may lead to wrong predictions. The simulation shown in Fig. 3 was repeated with a soft step potential as in Eq. (9) with $L = 0.005$ for different values of the step height Δ. The plot shows the values for the reflection probability $R = \|\psi_{\rm ref}\|^2$. These values cannot be correct; for the parameters used in this simulation (see the following), R cannot become close to 1 and must stay between 0 and 10^{-17} for every $\Delta > 0$. The simulation used a standard algorithm for simulating the Schrödinger equation,[6] a grid of $N = 10^4$ sites, and as the initial wave function a Gaussian packet with parameters $k_1 = 400\pi$, $x_0 = 0.4$, and $\sigma = 0.005$. The bound of 10^{-17} follows from Eq. (18) and the fact that the reflection coefficient (10) is bounded by $\exp(-2\pi\sqrt{2mE}L/\hbar) = \exp(-2\pi k_1 L)$, which here is $\exp(-4\pi^2) < 10^{-17}$.

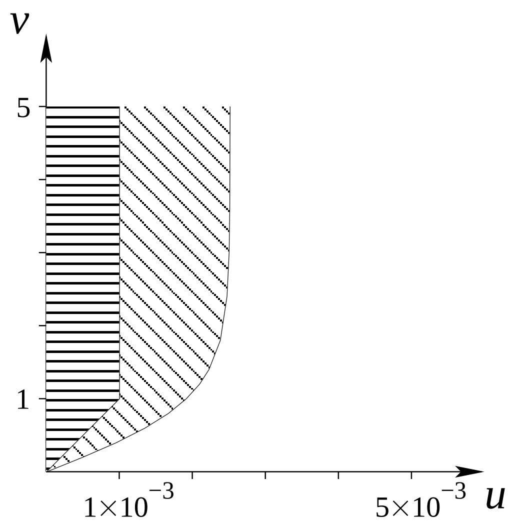

FIG. 5: The region (shaded) in the plane of the parameters u and v, defined in Eq. (24), in which the reflection probability (25) exceeds 99%. The horizontally shaded subset is the region in which Eq. (26) holds.

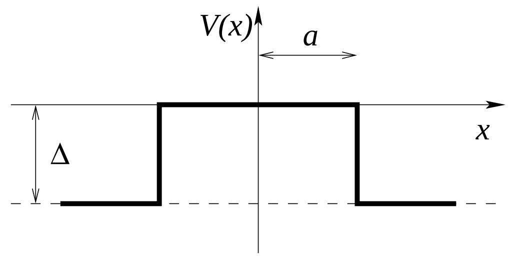

FIG. 6: Potential plateau.

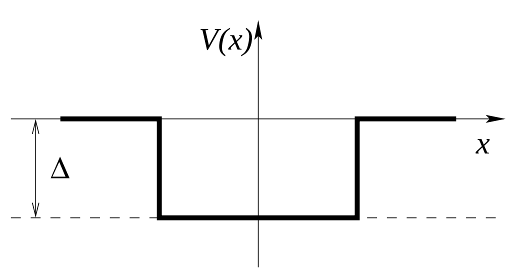

FIG. 7: Potential well.

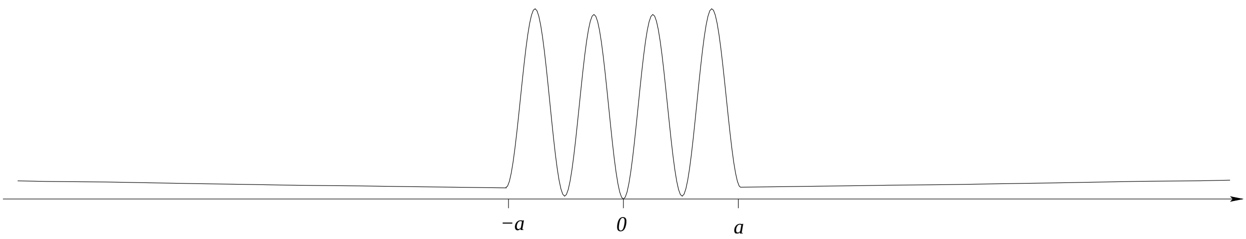

FIG. 8: Plot of $|\psi_n(x)|^2$ for an eigenfunction ψ_n with complex eigenvalue according to Eq. (36) with $V(x)$ the plateau potential as in Fig. 6. The parameters are $n = 4$ and $\Delta = 64W$, corresponding to $\Delta = 32\pi^2 = 315.8$ in units with $a = 1$, $m = 1$, and $\hbar = 1$.