

Paradoxical Reflection in Quantum Mechanics

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Abstract

This article concerns a phenomenon of elementary quantum mechanics that is quite counter-intuitive, very non-classical, and apparently not widely known: a quantum particle can get reflected at a potential step downwards. In contrast, classical particles get reflected only at upward steps. As a consequence, a quantum particle can be trapped for a long time (though not forever) in a region surrounded by downward potential steps, that is, on a plateau. Said succinctly, a quantum particle tends not to fall off a table. The conditions for this effect are that the wave length is much greater than the width of the potential step and the kinetic energy of the particle is much smaller than the depth of the potential step. We point out how the topic is accessible with elementary methods, but also with mathematical rigor and numerically.

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1 Introduction

Suppose a quantum particle moves towards a sudden drop of potential as in Figure 1, with the particle arriving from the left. As a classical analogue, we may imagine a ball rolling towards the edge of a table. Will it fall down or be reflected? Classically, the ball is certain to fall down, but a quantum particle has a chance to be reflected. That sounds paradoxical because the particle turns around and returns to the left under a

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force pointing to the right! Under suitable conditions reflection even becomes close to certain. This non-classical, counter-intuitive quantum phenomenon we call “paradoxical reflection,” or, when a region is surrounded by downward potential steps, “paradoxical confinement”—where “paradoxical” is understood in the sense of “counter-intuitive,” not “illogical.” It can be derived easily using the following simple reasoning.

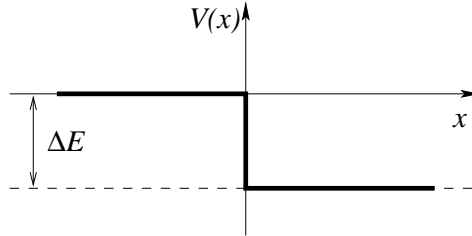


Figure 1: A potential $V(x)$ containing a step downwards

Suppose the particle moves in 1 dimension, and the potential is a rectangular step as in Figure 1,

$$V(x) = -\Delta E \Theta(x) \quad (1)$$

with Θ the Heaviside function and $\Delta E \geq 0$. A wave packet coming from the left gets partially reflected at the step and partially transmitted. The size of the reflected and the transmitted packets can be determined by a standard textbook method of calculation (e.g., [1, 2]), the *stationary analysis*, replacing the wave packet by a plane wave of energy E and solving the stationary Schrödinger equation. 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 Section 2 and observe two things: First, $R \neq 0$, implying that partial reflection occurs although the potential step is *downwards*. Second, R even converges to 1, so that reflection becomes nearly certain, as the ratio $E/\Delta E$ goes to zero. Thus, paradoxical reflection can be made arbitrarily strong by a suitable choice of parameters (e.g., for sufficiently big ΔE if E is kept fixed).

If it sounds incredible that a particle can be repelled by a potential step downwards, the following fact may add to the amazement. As derived in [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 step downwards yields the same reflection coefficient as a step upwards. (But keep in mind the difference between a step upwards and a step downwards that at a step upwards, also energies below the height of the step are possible for the incoming particle, a case in which reflection is certain, $R = 1$.)

To provide some perspective, it may be worthwhile to point to some parallels with quantum tunneling: there, the probability of a quantum particle passing through a potential barrier is positive even in cases in which this is impossible for a classical particle. In fact, paradoxical reflection is somewhat similar to what could be called

anti-tunneling, the effect that a quantum particle can have positive probability of being reflected by a barrier so small that a classical particle would be certain to cross it.

In the rest of this article, we address the following questions: Is paradoxical reflection a real physical phenomenon or an artifact of mathematical over-simplification? (We will look at numerical and rigorous mathematical results.) How does it depend on the parameters of the situation: the width L (see Figure 2) and the depth ΔE of the potential step, the wave length λ and the width σ of the incoming wave packet? Why does this phenomenon not occur in the classical regime? 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? And, could one use this phenomenon in principle for constructing a particle trap? In spring 2005, 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; these discussions inspired the present article.

2 Stationary Analysis of the Rectangular Step

We begin by providing more detail about the stationary analysis of the rectangular step (1), considering the time-independent Schrödinger equation ($m = \text{mass}$)

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

This can be solved in a standard way: for $x < 0$, let ψ be a superposition of an incoming wave e^{ik_1x} and a reflected wave Be^{-ik_1x} , while for $x > 0$, let ψ be a transmitted wave Ae^{ik_2x} , with a possibly different wave number k_2 . Indeed, from (2) we obtain that

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

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

$$A = \frac{2k_1}{k_1 + k_2}, \quad B = \frac{k_1 - k_2}{k_1 + k_2}. \quad (4)$$

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

$$R = \frac{|j_{\text{refl}}|}{j_{\text{in}}}, \quad T = \frac{j_{\text{tra}}}{j_{\text{in}}}. \quad (5)$$

Noting that $j_{\text{tra}} = \hbar k_2 |A|^2/m$, $j_{\text{refl}} = -\hbar k_1 |B|^2/m$, $j_{\text{in}} = \hbar k_1/m$, we find that

$$R = |B|^2 = 1 - \frac{k_2}{k_1} |A|^2, \quad T = \frac{k_2}{k_1} |A|^2. \quad (6)$$

Note that both R and T lie in the interval $[0, 1]$, and that $R + T = 1$. By inserting (4) into (6), we obtain

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

and make two observations: First, $R \neq 0$, implying that reflection occurs, if $k_1 \neq k_2$, which is the case as soon as $\Delta E \neq 0$. Second, R even converges to 1, so that reflection becomes nearly certain, as the ratio $r := E/\Delta E$ tends to zero; that is because

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

since both the numerator and the denominator tend to 1 as $r \rightarrow 0$. This is the simplest derivation of paradoxical reflection.

3 Soft Step

For a deeper analysis of the effect, we will gradually consider increasingly more realistic models. In this section, we consider a soft (or smooth, i.e., differentiable) potential step, as in Figure 2, for which the drop in the potential is not infinitely rapid but takes place over some distance L . The result will be that paradoxical reflection exists also for soft steps, so that the effect is not just a curious feature of rectangular steps (which could not be expected to ever occur in nature). Another result concerns how the effect depends on the width L of the step.

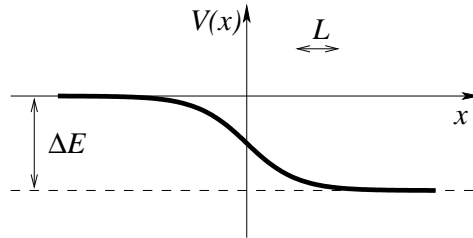


Figure 2: A potential containing a soft step

To study this case it is useful to consider the explicit function

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

depicted in Figure 2. (Recall that $\tanh = \sinh / \cosh$ converges to ± 1 as $x \rightarrow \pm\infty$.) The reflection coefficient for this potential can be calculated again by a stationary analysis, obtaining from the time-independent Schrödinger equation (2) solutions $\psi(x)$ which are asymptotic to $e^{ik_1x} + Be^{-ik_1x}$ as $x \rightarrow -\infty$ and asymptotic to Ae^{ik_2x} as $x \rightarrow \infty$, i.e.,

$\lim_{x \rightarrow \infty} (\psi(x) - Ae^{ik_2x}) = 0$. The calculation is done in [2, p. 78]: The values k_1 and k_2 are again given by (3), and the reflection coefficient turns out to be

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

From this and (3) we can read off that, again, $R \neq 0$ for $\Delta E \neq 0$, and $R \rightarrow 1$ as $E \rightarrow 0$ while ΔE and L are fixed (since then $k_1 \rightarrow 0$, $k_2 \rightarrow \sqrt{2m\Delta E}/\hbar$, so both the numerator and the denominator tend to $\sinh(\frac{\pi}{2}\sqrt{2m\Delta E}L/\hbar)$). As $\Delta E \rightarrow \infty$ while E and L are fixed, $R \rightarrow \exp(-2\pi\sqrt{2mEL}/\hbar)$ because for large arguments $\sinh \approx \frac{1}{2} \exp$.

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

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

as the numerator tends to 0 and the denominator to 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*.

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

$$\frac{df}{dL} = \frac{\alpha \cosh(\alpha L) \sinh(\beta L) - \beta \sinh(\alpha L) \cosh(\beta L)}{\sinh^2(\beta L)} < 0 \quad (12)$$

because

$$\frac{\alpha}{\tanh \alpha} < \frac{\beta}{\tanh \beta}, \quad (13)$$

as $x/\tanh x$ is increasing for $x > 0$.

How about soft steps with other shapes than that of the tanh function? Suppose that the potential $V(x)$ is a continuous, monotonically decreasing function such that $V(x) \rightarrow 0$ as $x \rightarrow -\infty$ and $V(x) \rightarrow -\Delta E$ as $x \rightarrow +\infty$. To begin with, we note that the fact, mentioned in the introduction, that the reflection coefficient is the same for particles coming from the left or from the right, still holds true for such a general potential [2, p. 76]. This suggests that paradoxical reflection occurs also for general potential steps. Unfortunately, we do not know of any general result on lower bounds for the reflection coefficient R that could be used to establish paradoxical reflection in this generality. However, an upper bound is known [3, eq. (82)], according to which R is less than or equal to the reflection coefficient (7) of the rectangular step. This agrees with our observation in the previous paragraph that reflection is the more likely the sharper the step.

4 Wave Packets

Another respect in which we can be more realistic is by admitting that the wave function with which a quantum particle reaches a potential step is not an infinitely-extended plane wave e^{ik_1x} but in fact a wave packet of finite width σ , for example a Gaussian wave packet

$$\psi_{\text{in}}(x) = G_{\mu,\sigma}(x)^{1/2} e^{ik_1x} \quad (14)$$

with $G_{\mu,\sigma}$ the Gauss function with mean μ and variance σ^2 ,

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

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

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

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

$$R = \|\psi_{\text{refl}}\|^2, \quad T = \|\psi_{\text{tra}}\|^2, \quad (17)$$

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

Because of the paradoxical feel of paradoxical reflection, one might suspect at first that the effect does not exist for wave packets but is merely an artifact of the stationary analysis. We thus address, in this section, the question as to how wave packets behave, and whether the reflection probability (17) agrees with the reflection coefficient discussed earlier. We begin with the numerical evidence confirming paradoxical reflection.

4.1 Numerical Simulation

A numerical simulation of a wave packet partly reflected from a (soft) step downwards is shown in Figure 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 of exactly Gaussian shape, one continuing to move to the right and the other, reflected one 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 step downwards (even for wave packets of finite width). That is, the numerical simulation confirms the prediction of the stationary analysis.

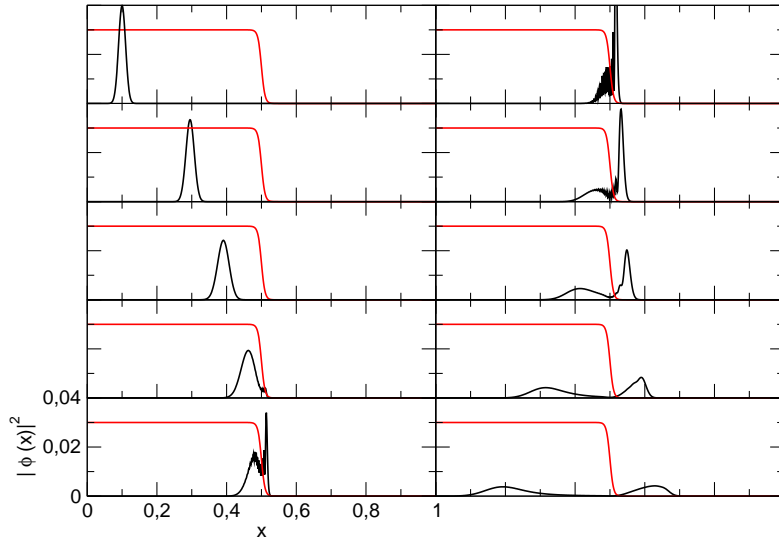


Figure 3: Numerical simulation of the time-dependent Schrödinger equation for the soft step potential (9). The picture shows ten snapshots of $|\psi|^2$ (black lines) at different times before, during, and after passing the potential step. (Order: left column top to bottom, then right column top to bottom.) It can clearly be seen that there is a transmitted wave packet and, “paradoxically,” a reflected wave packet. The initial wave function is a Gaussian wave packet centered at $x = 0.1$ with $\sigma = 0.01$ and $k_0 = 200\pi$. The simulation assumes infinite walls at $x = 0$ and $x = 1$. The parameters are $m = 1$, $L = 1/100$ and $\Delta E = 18.4 E$, and the linear mesh has $N = 1000$ points. The additional lines in the figures depict the potential in arbitrary units. The figure shows the modulus of the wave packet at times: 1, 4, 8, 11, 12, 13, 16, 18, 22, 27 Δt in arbitrary time units.

4.2 But Is It for Real?

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

Do not think the worry that numerical errors may lead to the wrong behavior of a wave packet was paranoid: There are cases in which exactly this happens. Here is an example involving the potential $V(x) = -x^2$: In some numerical simulations, a wave packet starting near the origin and moving to the right gets reflected at some point and returns to the origin, whereas in the rigorous solution of the Schrödinger equation the wave packet never returns, but accelerates more and more. As illustrated in Figure 4, the numerically predicted time of reflection depends on the mesh width (i.e., the numerical resolution): the higher the resolution, the later the predicted reflection.

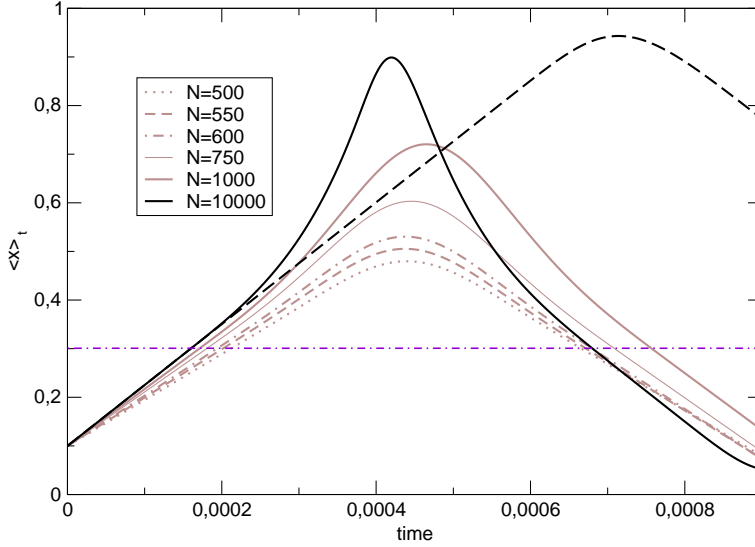


Figure 4: An example of how numerical error may lead to wrong predictions. The plot shows numerical results about the evolution of the average position of a Gaussian wave packet (initially as in Figure 3) with the parabolic potential $V(x) = -50k_0^2(x - 0.3)^2$ as a function of time for several numbers of nodes of the linear mesh, N . The black dashed line corresponds to the evolution for $V(x) = 0$. We see that there is a spurious reflection of the wave packet due to the finite size effects of the numerical simulation. Note that in the figure only in the $N = 10,000$ case the wave function collides with the $x = 1$ wall. In the other cases the reflection occurs far from the $x = 1$ wall (see for instance the $N = 500$ case).

We return to the mathematics of paradoxical reflection. The rigorous mathematical analysis of scattering problems of this type is a fairly complex and subtle topic. The main techniques and results (also for higher dimensional problems) are described in [4, 5], and the mathematical results relevant to potentials of the step type can be found in [6]. The reflection probability R of eq. (17) is given in terms of the plane wave reflection coefficients $R(k_1)$ by the following formula, expressing exactly what one would intuitively expect:

$$R = \int_0^\infty dk_1 R(k_1) |\widehat{\psi}_{\text{in}}(k_1)|^2. \quad (18)$$

The same formula holds with all R 's replaced by T 's. In (18), $R(k_1)$ is given by the stationary analysis, as in (7) or (10), with k_2 expressed in terms of k_1 and ΔE , $k_2 = \sqrt{k_1^2 + 2m\Delta E/\hbar^2}$; and $\widehat{\psi}_{\text{in}}(k_1)$ is the Fourier transform of the incoming wave packet $\psi_{\text{in}}(x)$.

(In brackets: To be precise, the incoming packet $\psi_{\text{in}}(x, t)$ is defined as the free asymptote of $\psi(x, t)$ for $t \rightarrow -\infty$, i.e., $\psi_{\text{in}}(x, t)$ evolves without the potential,

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

and

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

Similarly, $\psi_{\text{refl}} + \psi_{\text{tra}}$ is the free asymptote of ψ for $t \rightarrow +\infty$. When we write $\psi_{\text{in}}(x)$, we mean to set $t = 0$; note, however, that (18) actually does not depend on the t -value as, by the free Schrödinger equation (19), $\widehat{\psi}_{\text{in}}(k, t) = \exp(-it\hbar k^2/2m) \widehat{\psi}_{\text{in}}(k, 0)$ and thus $|\widehat{\psi}_{\text{in}}(k, t)|^2 = |\widehat{\psi}_{\text{in}}(k, 0)|^2$. Since 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 (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 also $R > 1 - \varepsilon$. 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

$$\int_0^\infty dk_1 \Theta(R(k_1) - (1 - \varepsilon)) |\widehat{\psi}_{\text{in}}(k_1)|^2 = 1 - \delta, \quad (21)$$

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

$$\begin{aligned} \int_0^\infty dk_1 R(k_1) |\widehat{\psi}_{\text{in}}(k_1)|^2 &\geq \int_0^\infty dk_1 R(k_1) \Theta(R(k_1) - (1 - \varepsilon)) |\widehat{\psi}_{\text{in}}(k_1)|^2 \geq \\ &\geq \int_0^\infty dk_1 (1 - \varepsilon) \Theta(R(k_1) - (1 - \varepsilon)) |\widehat{\psi}_{\text{in}}(k_1)|^2 = (1 - \varepsilon)(1 - \delta) > 1 - \varepsilon - \delta. \end{aligned}$$

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

5 Parameter Dependence

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

$$\frac{1}{k_1} \gg L \quad (22a)$$

$$\Delta E \gg \frac{\hbar^2 k_1^2}{2m} = E \quad (22b)$$

$$\sigma \gg \frac{1}{k_1}. \quad (22c)$$

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

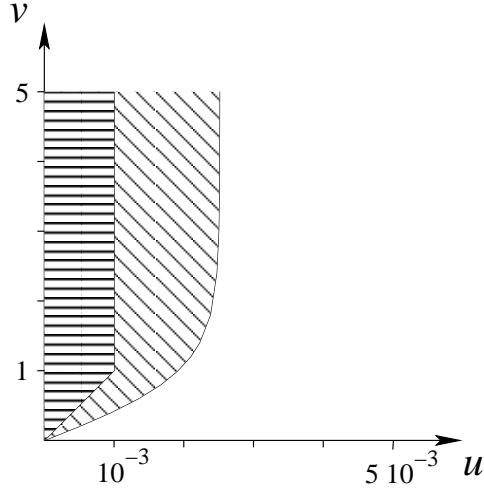


Figure 5: The region (shaded) in the plane of the parameters u and v , defined in (23), in which the reflection probability (24) exceeds 99 percent. The horizontally shaded subset is the region in which condition (25) holds.

To derive this claim from (10) and (18), consider first the case $\sigma \rightarrow \infty$ 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 (10) depends on the parameters $k_1, L, \Delta E, m$ only in the dimensionless combinations

$$u = \frac{\pi}{2} k_1 L, \quad v = \frac{\pi}{2} \sqrt{2m\Delta E} L / \hbar, \quad (23)$$

that is,

$$R = R(u, v) = \left(\frac{\sinh(\sqrt{u^2 + v^2} - u)}{\sinh(\sqrt{u^2 + v^2} + u)} \right)^2. \quad (24)$$

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

$$u < 10^{-3} \text{ and } v > 10^3 u. \quad (25)$$

More generally, for $R(u, v)$ to be very close to 1 it is sufficient that $u \ll 1$ and $v \gg u$, which means (22a) and (22b). To see this, note that

$$\begin{aligned} \sinh(\sqrt{u^2 + v^2} - u) &= \sinh(\sqrt{u^2 + v^2} + u - 2u) = \\ &= \sinh(\sqrt{u^2 + v^2} + u) \cosh(2u) - \cosh(\sqrt{u^2 + v^2} + u) \sinh(2u) \end{aligned} \quad (26)$$

so that

$$\sqrt{R(u, v)} = \frac{\sinh(\sqrt{u^2 + v^2} - u)}{\sinh(\sqrt{u^2 + v^2} + u)} = \cosh(2u) - \frac{\sinh(2u)}{\tanh(\sqrt{u^2 + v^2} + u)}. \quad (27)$$

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

$$\sqrt{R(u, v)} \approx 1 - \frac{2u}{\tanh v}. \quad (28)$$

If v is of order 1, this 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 (28) is close to 1 when $u/v \ll 1$. Thus, when (22a) and (22b) are satisfied \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 coefficient close to one. Thus, every wave number \tilde{k}_1 in the interval, say, $[k_1 - \frac{10}{\sigma}, k_1 + \frac{10}{\sigma}]$ should satisfy (22a) and (22b). This will be the case if $\frac{10}{\sigma}$ is small compared to k_1 , or $\sigma \gg 1/k_1$. Thus, (22c), which is merely what is required for (14) to be a good wave packet, i.e., an approximate plane wave, is a natural condition on σ for keeping R close to 1.

6 The Classical Limit

If paradoxical reflection exists, then why do we not see it in the classical limit? On the basis of (22) 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 wave length. For paradoxical reflection, in contrast, it is essential that the length scale of the drop in the potential be smaller than the wave length. For further discussion of the classical limit of quantum mechanics, see [7].

7 A Plateau as a Trap

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

$$V(x) = -\Delta E(\Theta(x - a) + \Theta(-x - a)), \quad (29)$$

depicted in Figure 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

$$\tau_{\text{cl}} = a\sqrt{\frac{2m}{E}}, \quad (30)$$

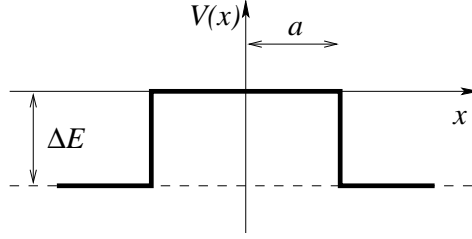


Figure 6: Potential plateau

independently of the height of the plateau. Instead, the time the quantum particle likely remains on the plateau is of the order $\sqrt{\Delta E/E} \tau_{\text{cl}}$ and is thus much larger than τ_{cl} if the height ΔE is large enough. One can say that a quantum particle on a table tends not to fall down. In this formulation, the “table” is supposed to be of an appreciable height, i.e., $\Delta E \gg E$. In fact, as we shall argue in the subsequent sections, a quantum particle starting on the plateau should leave the plateau at the rate τ_{qu}^{-1} with the decay time

$$\tau_{\text{qu}} = a \frac{\sqrt{2m\Delta E}}{4E} = \frac{1}{4} \sqrt{\frac{\Delta E}{E}} \tau_{\text{cl}}. \quad (31)$$

The lifetime (31) can be obtained in the following semi-classical way: Imagine a particle traveling along the plateau with the speed $\sqrt{2E/m}$ classically corresponding to energy E , getting reflected at the edge with probability R given by (7), traveling back with the same speed, getting reflected at the other edge with probability R , and so on. Since the transmission probability $T = 1 - R$ corresponding to (7) is

$$4\sqrt{E/\Delta E} + \text{higher powers of } E/\Delta E, \quad (32)$$

a number of reflections of order $(\sqrt{E/\Delta E})^{-1}$ should typically be required before transmission occurs, in qualitative agreement with (31). In fact, the transmission probability of $T = 4\sqrt{E/\Delta E}$, when small, corresponds to a decay rate T/τ_{cl} and hence to the decay time τ_{cl}/T given by (31).

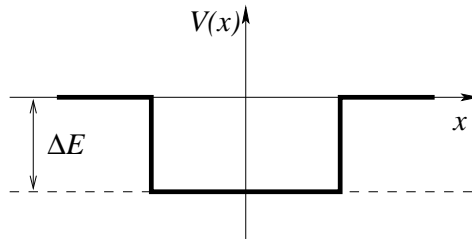


Figure 7: Potential well

One must be careful with this reasoning, since applied carelessly it would lead to the same lifetime for the potential well depicted in Figure 7 as for the potential plateau.

(That is because the reflection probability at a potential step *upwards* is, as already mentioned, the same as that at a potential step *downwards*.) 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 [2] always involves incoming waves at the same total energy $E > 0$; for a potential well it would thus say nothing about bound states, which have $E < 0$.

This is a basic difference between confinement in a potential well and paradoxical confinement on a potential plateau: In the well, the particle has positive probability to stay forever. Mathematically speaking, the potential well has bound states (i.e., eigenfunctions in the Hilbert space $L^2(\mathbb{R})$ of square-integrable functions), whereas the potential plateau does not. For the potential well, the initial wave packet will typically be a superposition $\psi = \psi_{\text{bound}} + \psi_{\text{scattering}}$ of a bound state (a superposition of one or more square-integrable eigenfunctions) and a scattering state (orthogonal to all bound states); then $\|\psi_{\text{bound}}\|^2$ is the probability that the particle remains in (a 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. Indeed, we will show that (31) is the lifetime. Our tool for the proof will be a method similar to the stationary analysis of Section 2, using special states lying outside the Hilbert space $L^2(\mathbb{R})$ (as do the stationary states of Section 2). And again like the stationary states of Section 2, the special states are similar to eigenfunctions of the Hamiltonian: they are solutions of the time-independent Schrödinger equation (2), but with complex “energy”!

8 Eigenfunctions with “Complex Energy”

We now derive the formula (31) for the lifetime $\tau = \tau_{\text{qu}}$ from the behavior of solutions to the eigenvalue equation (2), but with complex eigenvalues. To avoid confusion, let us now call the eigenvalue Z instead of E ; thus, the equation reads

$$Z\psi(x) = -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x), \quad (33)$$

where V is the plateau potential as in (29). Such “eigenfunctions of complex energy” were first considered by Gamow [8, 9] for the theoretical treatment of radioactive alpha decay.

The fact that the eigenvalue is complex may be confusing at first, since the Hamiltonian is a self-adjoint operator, and it is a known fact that the eigenvalues of a self-adjoint operator are real. However, in the standard mathematical terminology for self-adjoint operators in Hilbert spaces, the words “eigenvalue” and “eigenfunction” are reserved for such solutions of (33) that ψ is square-integrable (= normalizable), i.e., $\psi \in L^2(\mathbb{R})$. In this sense, all eigenvalues must be real indeed; for us this means that any solution ψ of (33) for $Z \in \mathbb{C} \setminus \mathbb{R}$ is not square-integrable. In fact, even the eigenfunctions with real eigenvalue E considered in (2) were not square-integrable, which means that they do not count as “eigenfunctions” in the mathematical terminology, 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. So, the eigenvalues Z we are talking about are neither eigenvalues in the standard sense, nor even elements of the spectrum. (Nevertheless we continue calling them “eigenvalues,” as they satisfy (33) 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

$$\psi(x, t) = e^{-iZt/\hbar}\psi(x, 0). \quad (34)$$

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

$$|\psi(x, t)|^2 = e^{2\text{Im} Zt/\hbar}|\psi(x, 0)|^2, \quad (35)$$

so that $2\text{Im} Z/\hbar$ is the rate of growth of the density $|\psi(x, t)|^2$. For those eigenfunctions relevant to our purposes, the imaginary part of Z is always negative, so that ψ shrinks with time. In particular, the amount of $|\psi|^2$ on top of the plateau decays with the exponential factor that occurs in (35). Assuming 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 using that the lifetime τ for which the particle remains on the plateau is reciprocal to the decay rate of the amount of probability on top of the plateau, we have that

$$\tau = -\frac{\hbar}{2\text{Im} Z}. \quad (36)$$

From (34) we can further read off that the phase of $\psi(x, t)$ at any fixed x rotates with frequency $\text{Re} Z/\hbar$, while for eigenfunctions with real eigenvalue E it does so with frequency E/\hbar , which motivates us to call $\text{Re} Z$ the energy and denote it by E . Thus,

$$Z = E - i\frac{\hbar}{2\tau}. \quad (37)$$

Below, we will determine τ by determining the relevant eigenvalues Z , i.e., those corresponding to decay eigenfunctions, see below (40).

How can it be that $|\psi|^2$ shrinks everywhere? Does that not conflict with the conservation of the total probability? Apart from the fact that $|\psi|^2$ cannot be the probability density anyway since ψ is not square-integrable, the shrinking of ψ means that there is a flow of $|\psi|^2$ to infinity (that is not compensated by an equally large flow of $|\psi|^2$ from infinity). This is indeed similar to the situation we want to consider, in which the amount of $|\psi|^2$ on top of the plateau continuously shrinks due to a flow of $|\psi|^2$ away from the plateau. It also suggests that ψ should grow exponentially in space as $x \rightarrow \pm\infty$: 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 on top of the plateau shrinks exponentially with time. As we will see now, the eigenfunctions behave exactly that way.

The general solution of (33) with $Z \in \mathbb{C}$ except $Z = 0$ or $Z = -\Delta E$ is¹

$$\psi(x) = \begin{cases} B_- e^{-i\tilde{k}x} + C_- e^{i\tilde{k}x} & \text{when } x < -a, \\ A_+ e^{ikx} + A_- e^{-ikx} & \text{when } -a < x < a, \\ B_+ e^{i\tilde{k}x} + C_+ e^{-i\tilde{k}x} & \text{when } x > a, \end{cases} \quad (38)$$

where

$$k = \sqrt{2mZ}/\hbar \quad \text{and} \quad \tilde{k} = \sqrt{2m(Z + \Delta E)}/\hbar \quad (39)$$

with the following (usual) definition of the complex square root: Given a complex number ζ other than one that is real and ≤ 0 , let $\sqrt{\zeta}$ denote the square root with positive real part, $\text{Re} \sqrt{\zeta} > 0$. For $\zeta \leq 0$, we let $\sqrt{\zeta} = i\sqrt{|\zeta|}$. (Since (38) remains invariant under changes in the signs of k and \tilde{k} , choosing the positive branch for the square roots is not a restriction for the solutions.) We are interested only in those solutions for Z with $\text{Re} Z = E > 0$; these are the ones that should be relevant to the behavior of states starting out on the plateau (with positive energy). Nevertheless, for mathematical simplicity, we will also allow $\text{Re} Z \leq 0$ but exclude any Z that is real and negative or zero. For any $Z \in \mathbb{C} \setminus (-\infty, 0]$ we have that $\text{Re} \tilde{k} > 0$, so that the probability current j associated with $\exp(i\tilde{k}x)$ is positive (i.e., a vector pointing to the right). Since we do not want to consider any contribution with a current from infinity to the plateau, we assume that

$$C_+ = C_- = 0. \quad (40)$$

We thus define a *decay eigenfunction* or *Gamow eigenfunction* to be a nonzero function ψ of the form (38) with (39) and $C_{\pm} = 0$, satisfying the eigenvalue equation (33) 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 that possess a decay eigenfunction we call *decay eigenvalues* or *Gamow eigenvalues*.²

The remaining coefficients A_{\pm}, B_{\pm} are determined up to an overall factor by the requirement that both ψ and its derivative ψ' be continuous at $\pm a$, the ends of the plateau. We will see that $\text{Im} \tilde{k} < 0$, so that, indeed, $|\psi(x)| \rightarrow \infty$ exponentially as $x \rightarrow \pm\infty$. Continuity of ψ and ψ' determines the possible values of (not only A_{\pm}, B_{\pm} but also) Z and thus k, \tilde{k} . We have collected the details of the computations into Appendix A, and report here the results. To describe the solutions, let

$$\lambda_0 = \frac{2\pi\hbar}{\sqrt{2m\Delta E}}, \quad \alpha = \frac{a}{\pi\hbar} \sqrt{2m\Delta E} = \frac{2a}{\lambda_0}. \quad (41)$$

λ_0 is the de Broglie wavelength corresponding to the height ΔE of the potential plateau, and α is the width of the plateau in units of λ_0 .

¹For $Z = 0$, the line for $-a < x < a$ has to be replaced by $A_0 + A_1 x$; for $Z = -\Delta E$, $\psi(x) = D_- + E_- x$ for $x < -a$ and $\psi(x) = D_+ + E_+ x$ for $x > a$.

²Here is a look at the negative Z 's that we excluded in this definition: In fact, for $Z \in (-\infty, 0] \setminus \{-\Delta E\}$ there exist no nonzero functions with $C_{\pm} = 0$ satisfying the eigenvalue equation (33) for all $x \neq \pm a$ such that ψ and ψ' are continuous. (But we have not included the proof in this paper.) For $Z = -\Delta E$, the coefficients C_{\pm} are not defined, so the condition (40) makes no sense.

Proposition 1 *If $\alpha \geq 10$, then the number N of decay eigenvalues Z of (33) with $|Z| \leq \Delta E/4$ lies in the range $\alpha - 2 < N \leq \alpha + 2$. There is a natural way of numbering these eigenvalues as Z_1, \dots, Z_N . (There is no formula for the eigenvalue 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 $x \rightarrow \pm\infty$. Furthermore, for $n \ll \alpha$,*

$$Z_n \approx \frac{n^2 \Delta E}{4\alpha^2} \left(1 - i \frac{2}{\pi\alpha}\right). \quad (42)$$

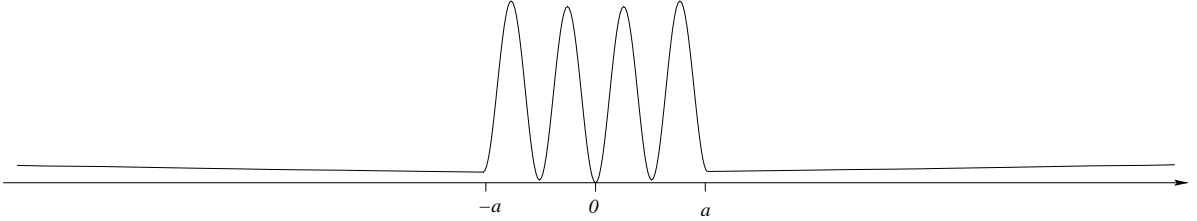


Figure 8: Plot of $|\psi_n(x)|^2$ for an eigenfunction ψ_n with complex eigenvalue according to (33) with $V(x)$ the plateau potential as in Figure 6; the parameters are $n = 4$ and $\alpha = 8$; in units with $a = 1$, $m = 1$, and $\hbar = 1$, this corresponds to $\lambda_0 = 1/4$ and $\Delta E = 32\pi^2 = 315.8$.

The proof is given in Appendix A; the values (42) are not (to our knowledge) in the literature so far. What can we read off about the lifetime τ ? In the regime $a\sqrt{2m\Delta E} \gg \hbar$ of large ΔE , which corresponds to $\alpha \gg 1$, the n -th complex eigenvalue Z_n with $n \ll \alpha$ is such that

$$\text{Re } Z_n \approx \frac{\hbar^2 \pi^2 n^2}{8ma^2}, \quad \text{Im } Z_n \approx -\frac{2\hbar}{a\sqrt{2m\Delta E}} \text{Re } Z_n. \quad (43)$$

(Readers familiar with the infinite well potential, $V(x) = 0$ when $-a \leq x \leq a$ and $V(x) = \infty$ when $|x| > a$, which corresponds to the limit $\Delta E \rightarrow \infty$ of very deep wells of the type shown in Figure 7, will notice that $\text{Re } Z_n$ given above actually coincides with the eigenvalues of the infinite well potential of length $2a$.) Using (36) and $E = \text{Re } Z$, one finds that

$$\tau = a \frac{\sqrt{2m\Delta E}}{4E} = \frac{1}{4} \sqrt{\frac{\Delta E}{E}} \tau_{\text{cl}} = \tau_{\text{qu}}, \quad (44)$$

the same value as specified in (31). This completes our derivation of the lifetime (31) from complex eigenvalues. As we did for the potential step, we now also look at the question whether wave packets behave in the same way as the eigenfunctions, that is, whether a wave packet can remain on top of the plateau for the time span (31).

9 Wave Packets on the Plateau

Now consider the long-time asymptotics for a normalized (square-integrable) wave function of more or less definite energy such that the reflection coefficient is near 1, confined

initially in the plateau interval. As time proceeds, with the wave function slowly leaking out exponentially, a quasi-steady-state situation should be approached—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 state corresponds to a fixed point of the dynamics on projective space.) This situation should be described by a wave function of the sort discussed in the previous section, one that corresponds to a complex eigenvalue Z with negative imaginary part and that grows exponentially as $|x| \rightarrow \infty$.

On the rigorous mathematical level, we can use the eigenfunctions with complex eigenvalue to establish that initial wave functions originating in the plateau region and involving only sufficiently low energy components have decay times given by τ_{qu} as in (31) for the lowest relevant energy. As mentioned earlier, the complex Z_n are not eigenvalues of the quantum Hamiltonian in the standard mathematical terminology, and the corresponding eigenfunctions are not at all localized, but rather grow exponentially with increasing distance from the plateau. They nevertheless can be used for the mathematical analysis. As a first step, we construct special states approximately localized in the plateau region which have the slow decay just described. This is the essence of Proposition 2 below. We then conclude in Corollary 1 that the slow decay applies to much more general initial states.

Proposition 2 *Let n be a fixed positive integer; keep a and m fixed and consider the regime $\hbar^2/2ma^2 \ll \Delta E \rightarrow \infty$, so that $\alpha \gg n$. There exists a normalized wave function $\phi_n(x)$ such that (i) on the plateau ϕ_n agrees (up to a factor) with the eigenfunction ψ_n with complex eigenvalue $Z = Z_n = E - i\hbar/2\tau$; (ii) the initial probability of the particle being on the plateau is close to 1; (iii) for every $0 < t < \tau$, the time-evolved wave function $\phi_{n,t} = e^{-iHt/\hbar}\phi_n$ is close, on the plateau $[-a, a]$, to (a factor times) the time-evolved eigenfunction $\psi_{n,t} = e^{-iZ_n t/\hbar}\psi_n$. Put differently,*

$$(i) \phi_n(x) = A_n \psi_n(x) \text{ for } -a \leq x \leq a \text{ with some constant } A_n \in \mathbb{C};$$

$$(ii) 1 - \int_{-a}^a |\phi_n(x)|^2 dx \ll 1;$$

$$(iii) \int_{-a}^a |\phi_{n,t}(x) - A_n \psi_{n,t}(x)|^2 dx \ll 1.$$

The proof is included in Appendix B. As a consequence of Proposition 2, the amount of probability on the plateau indeed shrinks at rate $1/\tau$, at least up to time τ . In particular, the particle has probability $\approx 1/e = 0.3679$ to stay on the plateau until τ .

Let us describe how ϕ_n is chosen. We make the n -th decay eigenfunction ψ_n normalizable by multiplying it outside the plateau by a Gaussian function with width $\sigma > 0$. We assume that $\sigma = O(a)$, i.e., it does not grow with α . Finally, we multiply the resulting function by a constant A_n which is so chosen that ϕ_n has norm 1. Explicitly, then

$$\phi_n(x) = A_n \times \begin{cases} B_- e^{-ikx - \frac{1}{4\sigma^2}(x+a)^2} & \text{when } x < -a, \\ B_+ e^{ikx - \frac{1}{4\sigma^2}(x-a)^2} & \text{when } x > a, \\ A_+ e^{ikx} + A_- e^{-ikx} & \text{when } -a \leq x \leq a. \end{cases} \quad (45)$$

That is, ϕ_n is obtained from the eigenfunction ψ_n by “cutting off” the function around $x = \pm(a + \sigma)$. Among the statements in Proposition 2, property (i) is immediate, and property (ii) is quite straightforward: Using the explicit form of A_{\pm} and B_{\pm} given in Appendix A, one can compute that, in the regime $n \ll \alpha$,

$$\int_{-a}^a |\psi_n(x)|^2 dx \approx a, \quad (46)$$

while the integrals

$$\int_a^{\infty} \left| \frac{\phi_n(x)}{A_n} \right|^2 dx \quad \text{and} \quad \int_{-\infty}^{-a} \left| \frac{\phi_n(x)}{A_n} \right|^2 dx \quad (47)$$

can be neglected in comparison, as they become small when α is large: They are of order $1/\alpha^2$. This can be understood by noticing that $|\psi_n(a)|^2$, the value at the left end of the interval $[a, \infty)$, is of order $1/\alpha^2$, and the width σ of the Gaussian is independent of α , so that the integral is of order $1/\alpha^2$, since $|\psi_n|^2$ grows with rate of order $1/\alpha^2$, so slowly that the increase is negligible over an interval of length σ . Property (iii) will be established in Appendix B.

Corollary 1 *For any initial wave function ψ on the plateau with contributions only from eigenfunctions ψ_n with low n , i.e.,*

$$\psi(x) = \begin{cases} \sum_{n=1}^{n_{\max}} c_n \psi_n(x) & \text{when } -a \leq x \leq a, \\ 0 & \text{otherwise,} \end{cases} \quad (48)$$

with α -independent n_{\max} and coefficients c_n , the time-evolved wave function $\psi_t = e^{-iHt/\hbar}\psi$ is close, on the plateau, to $\sum_n c_n \psi_{n,t}$, at least up to time $\min(\tau_1, \dots, \tau_{n_{\max}})$, where $\tau_n = -\hbar/2\text{Im} Z_n$. That is,

$$\int_{-a}^a \left| \psi_t(x) - \sum_n c_n \psi_{n,t}(x) \right|^2 dx \ll 1. \quad (49)$$

This means that any such wave packet ψ will have a long decay time on the plateau, namely at least $\min(\tau_1, \dots, \tau_{n_{\max}})$ (with each τ_n given by the quantum formula (31) and not by the classical formula (30)!); indeed, (49) 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 $|c_n|^2$. The proof of Corollary 1 is simple; it is included in Appendix C.

As another remark, the proof in Appendix B actually shows more than just Proposition 2, namely the following. Considering the eigenfunction ψ_n , we introduce the abbreviation

$$v = \frac{\hbar}{m} \text{Re } \tilde{k}, \quad (50)$$

which equals the speed at which an escaping particle moves away from the plateau. The maximal region in which we can expect a wave packet originally on the plateau to agree with an eigenfunction is the neighborhood of the plateau growing at speed v ; that is, the region at time t is the interval $[-a - vt, a + vt]$. And indeed, the wave function initially as in (45) stays close to (a factor times) the eigenfunction in this growing region:

$$\int_{-a-vt}^{a+vt} |\phi_{n,t}(x) - A_n \psi_{n,t}(x)|^2 dx \ll 1 \quad (51)$$

for $0 \leq t \leq \tau$. Moreover, in the same way in which Corollary 1 is obtained from Proposition 2, one obtains the following from (51): For ψ as in Corollary 1, $v = \min(v_1, \dots, v_{n_{\max}})$, v_n given by (50) for ψ_n , and $0 < t < \min(\tau_1, \dots, \tau_{n_{\max}})$,

$$\int_{-a-vt}^{a+vt} |\psi_t(x) - \sum_n c_n \psi_{n,t}(x)|^2 dx \ll 1. \quad (52)$$

This justifies the qualitative description in the beginning of this section.

As a final remark we note that the decay results described here, both qualitative and quantitative, presumably apply as well to the standard tunnelling 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 [10] by other methods based on analytic continuation.

10 Conclusions

We have argued that paradoxical reflection and paradoxical confinement, the phenomenon that a quantum particle tends not to fall off a table, are real phenomena and not artifacts of the stationary analysis. We have pointed out that the effect is a robust prediction of the Schrödinger equation, as it 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 counter-argument to note that paradoxical reflection is classically impossible. We conclude that paradoxical reflection is a fact, not an artifact. Finally, we have computed that a state (of sufficiently low energy) on a potential plateau as in Figure 6 has a long decay time, no less than τ_{qu} given by (31). We conclude from this that a plateau potential can, for suitable parameters, effectively be confining. Thus, the effect could indeed be used for constructing a (metastable) particle trap.

A Solving the Plateau Eigenvalue Equation

We now prove Proposition 1; that is, we determine all decay eigenfunctions of (33), as defined after (40). The continuity of ψ requires that

$$A_+ e^{ika} + A_- e^{-ika} = B_+ e^{i\tilde{k}a}, \quad (53)$$

$$A_+ e^{-ika} + A_- e^{ika} = B_- e^{i\tilde{k}a}, \quad (54)$$

and continuity of ψ' that also

$$k (A_+ e^{ika} - A_- e^{-ika}) = \tilde{k} B_+ e^{i\tilde{k}a}, \quad (55)$$

$$k (A_+ e^{-ika} - A_- e^{ika}) = -\tilde{k} B_- e^{i\tilde{k}a}. \quad (56)$$

Recall that both k and \tilde{k} can be complex. Since we assume $\Delta E > 0$, and since, by (33), $\tilde{k}^2 = k^2 + 2m\Delta E/\hbar^2$, we have that $k \pm \tilde{k} \neq 0$, and these equations are readily solved. First, we find the relations

$$A_- = e^{i2ak} \frac{k - \tilde{k}}{k + \tilde{k}} A_+, \quad (57)$$

$$B_+ = e^{ia(k-\tilde{k})} \frac{2k}{k + \tilde{k}} A_+, \quad (58)$$

$$B_- = e^{-ia(k+\tilde{k})} \frac{2k}{k - \tilde{k}} A_+, \quad (59)$$

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

$$\left(\frac{k + \tilde{k}}{k - \tilde{k}} \right)^2 = e^{i4ak}. \quad (60)$$

Let λ_0 and α be defined by (41), and, in order to express k in natural units, let

$$\kappa := \frac{\lambda_0 k}{2\pi}. \quad (61)$$

Then

$$k = \frac{2\pi}{\lambda_0} \kappa, \quad \tilde{k} = \frac{2\pi}{\lambda_0} \sqrt{1 + \kappa^2}, \quad (62)$$

and we have that

$$\frac{k + \tilde{k}}{k - \tilde{k}} = \frac{\kappa + \sqrt{1 + \kappa^2}}{\kappa - \sqrt{1 + \kappa^2}} = - \left(\kappa + \sqrt{1 + \kappa^2} \right)^2. \quad (63)$$

Thus (60) is equivalent to

$$\left(\kappa + \sqrt{1 + \kappa^2} \right)^4 = e^{i4\pi\kappa\alpha}. \quad (64)$$

The solutions of this equation coincide with those of the equation

$$\ln\left(\kappa + \sqrt{1 + \kappa^2}\right) = i\pi\kappa\alpha - i\frac{\pi n}{2} \quad (65)$$

where $n \in \mathbb{Z}$ is arbitrary and \ln denotes the principal branch of the complex logarithm.³

Thus, with every decay eigenfunction ψ is associated a solution κ of (65) (with $\operatorname{Re} \kappa > 0$, since $\operatorname{Re} k > 0$ by definition of k) and an integer n . Furthermore, $n \geq -1$, because $\operatorname{Re} \kappa > 0$ and the imaginary part of the left hand side of (65) must lie between $-\pi$ and π . Conversely, with every solution κ of (65) with $\operatorname{Re} \kappa > 0$ there is associated a decay eigenvalue

$$Z = \kappa^2 \Delta E \quad (66)$$

and an eigenfunction ψ that is unique up to a factor: Indeed, (61) and (62) provide the values of k and \tilde{k} and imply (66) and (60); $\operatorname{Re} \kappa > 0$ implies $Z \notin (-\infty, 0]$, as well as $\operatorname{Re} k > 0$, so that indeed $k = \sqrt{2mZ}/\hbar$; $k \pm \tilde{k} \neq 0$; A_+ can be chosen arbitrarily in $\mathbb{C} \setminus \{0\}$, and if A_- and B_\pm are chosen according to (57)–(59) then ψ is nonzero (as, e.g., $B_+ \neq 0$ when $k \neq 0$ and $A_+ \neq 0$) and a decay eigenfunction. We note that the condition $\operatorname{Re} \kappa > 0$ is automatically satisfied when $n \geq 2$, as we can read off from the imaginary part of (65) using that \ln has imaginary part in $(-\pi, \pi]$.

To determine ψ explicitly, note that $e^{i2ak\frac{k-\tilde{k}}{k+\tilde{k}}} = (-1)^{n+1}$, and thus $A_- = (-1)^{n+1}A_+$, $B_- = (-1)^{n+1}B_+$; setting $A_+ = \frac{1}{2}$ and introducing the notation

$$B := B_+ e^{ia\tilde{k}} = e^{iak} \frac{k}{k + \tilde{k}} = e^{i\pi\kappa\alpha} \frac{\kappa}{\sqrt{1 + \kappa^2} + \kappa} = i^n \kappa, \quad (67)$$

we obtain that for odd n

$$\psi(x) = B \left[\chi(x > a) e^{i\tilde{k}(x-a)} + \chi(x < -a) e^{-i\tilde{k}(x+a)} \right] + \chi(-a \leq x \leq a) \cos(kx), \quad (68)$$

and for even n

$$\psi(x) = B \left[\chi(x > a) e^{i\tilde{k}(x-a)} - \chi(x < -a) e^{-i\tilde{k}(x+a)} \right] + \chi(-a \leq x \leq a) \sin(kx). \quad (69)$$

We have used here the notation $\chi(Q)$ to denote the characteristic function of a condition Q :

$$\chi(Q) = \begin{cases} 1 & \text{when } Q \text{ is true,} \\ 0 & \text{otherwise.} \end{cases} \quad (70)$$

To sum up what we have so far, the decay eigenvalues are characterized, via (66), through the solutions κ of (65) with $\operatorname{Re} \kappa > 0$. In order to study existence, uniqueness, and the asymptotics for $\alpha \rightarrow \infty$ of these solutions, let us now assume, as in Proposition 1,

³For $\zeta \in \mathbb{C} \setminus \{0\}$, the equation $e^z = \zeta$ has infinitely many solutions z , all of which have real part $\ln|\zeta|$, and the imaginary parts of which differ by integer multiples of 2π ; by $\ln \zeta$ we denote that z which has $-\pi < \operatorname{Im} z \leq \pi$.

that $\alpha \geq 10$ and $|Z| \leq \Delta E/4$. By virtue of (66), the latter assumption is equivalent to $|\kappa| \leq 1/2$. We first show that solutions with $|\kappa| \leq 1/2$ must have $|n| \leq \alpha + 2$: Since \ln has imaginary part in $(-\pi, \pi]$, (65) implies that $\operatorname{Re} \kappa \in (\frac{n-2}{2\alpha}, \frac{n+2}{2\alpha}]$, and hence

$$\frac{1}{2} \geq |\kappa| \geq |\operatorname{Re} \kappa| \geq \frac{|n| - 2}{2\alpha}, \quad (71)$$

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

We now show that there exists a unique solution κ of (65) for every n with $|n| \leq \alpha + 2$. Let

$$F(\kappa) = \frac{n}{2\alpha} - \frac{i}{\pi\alpha} \ln \left(\kappa + \sqrt{1 + \kappa^2} \right), \quad (72)$$

so that (65) can equivalently be rewritten as the fixed point equation

$$F(\kappa) = \kappa. \quad (73)$$

We use the Banach fixed point theorem [11] to conclude the existence and uniqueness of κ . Since

$$F'(\kappa) = -\frac{i}{\pi\alpha} \frac{1}{\sqrt{1 + \kappa^2}}, \quad (74)$$

we have, by the triangle inequality, that

$$|F'(\kappa)| = \frac{1}{\pi\alpha|1 + \kappa^2|^{1/2}} \leq \frac{1}{\pi\alpha|1 - |\kappa|^2|^{1/2}}. \quad (75)$$

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

$$|F(\kappa)| \leq |F(\kappa) - F(0)| + |F(0)| \leq rK + \frac{|n|}{2\alpha} \leq r, \quad (76)$$

provided that

$$|n| \leq 2\alpha r(1 - K). \quad (77)$$

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 then a unique solution to the equation $F(\kappa) = \kappa$ in the ball $|\kappa| \leq r$. Even though we are ultimately interested in the radius $1/2$, let us set $r = 1/\sqrt{2}$, which satisfies $r < \sqrt{1 - 1/\pi^2\alpha^2}$ as $\alpha \geq 10$; also (77) is satisfied because $|n| \leq \alpha + 2$ and $\alpha \geq 10 > 2(1 + 1/\pi)/(\sqrt{2} - 1) = 6.37$. Hence, for every n with $|n| \leq \alpha + 2$, there is a unique solution κ_n with $|\kappa_n| \leq 1/\sqrt{2}$.

Getting back to the ball of radius $1/2$, while some of the κ_n may have modulus greater than $1/2$, we can at least conclude that there is at most one solution with modulus $\leq 1/2$

for every n with $|n| \leq \alpha + 2$. In addition, by setting $r = 1/2$, we obtain from (77) that $|\kappa_n| \leq 1/2$ for every n with $|n| \leq \alpha - 1$. If $n = 0$, then $F(0) = 0$ and $\kappa_0 = 0$ is the unique solution, which would lead to $\psi = 0$. This excludes $n = 0$. Which of the solutions have $\text{Re } \kappa_n > 0$, as required for decay eigenvalues? For any n with $|n| \leq \alpha + 2$, 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 $r = 1/\sqrt{2}$, $\kappa_n^{(j)} \rightarrow \kappa_n$ as $j \rightarrow \infty$, and

$$|\kappa_n - \kappa_n^{(j)}| \leq \frac{K^j}{1-K} |\kappa_n^{(1)} - \kappa_n^{(0)}| \leq |n| \alpha^{-(j+1)}. \quad (78)$$

For $n = -1$ and $j = 1$, this gives us that $|\kappa_{-1} - \kappa_{-1}^{(1)}| \leq \alpha^{-2}$, and with $\kappa_{-1}^{(1)} = -1/2\alpha$ and $\alpha \geq 10$, we can conclude that $\text{Re } \kappa_{-1} < 0$. This excludes $n = -1$. 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 $\text{Re } \kappa_n > 0$. Hence, the decay eigenvalues with $|Z| \leq \Delta E/4$ 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, as we have shown, be greater than $\alpha - 2$ and less than or equal to $\alpha + 2$.

Furthermore, for these κ_n , $\text{Im } \kappa_n < 0$: Computing $\kappa_n^{(2)}$ explicitly yields

$$\kappa_n^{(2)} = \nu - i \frac{1}{\pi\alpha} \ln(\nu + \sqrt{1 + \nu^2}) \quad \text{with } \nu = \frac{n}{2\alpha}. \quad (79)$$

Using (78) as before, the claim follows if we can show that $\text{Im } \kappa_n^{(2)} < -n\alpha^{-3}$, which is equivalent to

$$\frac{2\pi}{\alpha} \nu < \ln(\nu + \sqrt{1 + \nu^2}). \quad (80)$$

Note that $0 < \nu \leq (\alpha + 2)/2\alpha \leq 0.6$ since $\alpha \geq 10$. In fact, (80) holds for all $0 < \nu < 1$ and $\alpha \geq 10$ because $\sqrt{1 + \nu^2} > 1$ and $\ln(\nu + 1)/\nu$ for $\nu > 0$ is a decreasing function⁴ whose value at $\nu = 1$ is $\ln 2 = 0.693 > 0.628 = 2\pi/10 \geq 2\pi/\alpha$. As a consequence of $\text{Im } \kappa_n < 0$ (and $\text{Re } \kappa_n > 0$), also $\text{Im } \tilde{k} < 0$, so that $|\psi(x)|$ grows exponentially as $x \rightarrow \pm\infty$.

Now let us consider the asymptotics for $n \ll \alpha$. From (78) we have that κ_n is given by the right hand side of (79) up to an error of order $O(n\alpha^{-3})$. Therefore, for integers n with $0 < n \ll \alpha$ we have that

$$k \approx \frac{\pi n}{2a} - i \frac{n}{2a\alpha}, \quad \tilde{k} \approx \frac{\pi\alpha}{a} - i \frac{n^2}{4a\alpha^2}, \quad Z_n = \kappa_n^2 \Delta E \approx \frac{n^2 \Delta E}{4\alpha^2} \left(1 - i \frac{2}{\pi\alpha} \right). \quad (81)$$

B Derivation of the Lifetime Estimates for the Metastable States on the Plateau

We now prove Proposition 2. What remains to be shown is property (iii); we will establish the stronger statement (51). We will do this by constructing a function $f(x, t)$

⁴To see this, note that its derivative is of the form $f(\nu)/g(\nu)$ with $f(\nu) = \nu - (1 + \nu) \ln(1 + \nu)$ and $g(\nu) = \nu^2(1 + \nu)$. Since $g(\nu) > 0$ for $\nu > 0$, it suffices to show that $f(\nu) < 0$ for $\nu > 0$. This follows from $f(0) = 0$ and $f'(\nu) = -\ln(1 + \nu) < 0$ for $\nu > 0$.

which remains close to the time-evolved eigenfunction in a growing region around the plateau. We then prove that this function forms an excellent approximation of $\phi_{n,t}(x)$. $f(x, t)$ will be defined by multiplying the time-evolved eigenfunction $e^{-itZ_n/\hbar}\psi_n$ again by Gaussians, but now with time-dependent parameters.

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

$$\beta = -\text{Im } \tilde{k} \approx \frac{n^2}{4a\alpha^2} \quad (82)$$

and recall

$$v = \frac{\hbar}{m}\text{Re } \tilde{k} \approx \frac{\hbar\pi\alpha}{ma}, \quad (83)$$

whence $\tilde{k} = \frac{m}{\hbar}v - i\beta$ with $v, \beta > 0$. We define further

$$R(t) = a + vt, \quad b(t) = \sigma^2 + i\frac{\hbar}{2m}t. \quad (84)$$

The Gaussians will be attached symmetrically to $x = \pm R(t)$ with a ‘‘variance’’ $b(t)$, which yields explicitly

$$f(x, t) = A_n e^{-itZ_n/\hbar} \times \begin{cases} \pm B e^{i\tilde{k}(-x-a) - \frac{1}{4b(t)}(-x-R(t))^2}, & \text{when } x < -R(t), \\ B e^{i\tilde{k}(x-a) - \frac{1}{4b(t)}(x-R(t))^2}, & \text{when } x > R(t), \\ \psi_n(x), & \text{when } |x| \leq R(t). \end{cases} \quad (85)$$

Clearly, $f(x, 0) = \phi_n(x)$. Also $f(x, t)$ is continuously differentiable in x for all $t > 0$ 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 computation⁵ to check that for all $t > 0$

$$\begin{aligned} (H - Z)f(x, t) &= -\frac{\hbar^2}{2m}\partial_x^2 f(x, t) + (V(x) - Z)f(x, t) \\ &= -\frac{\hbar^2}{2m}[g_1(x - R(t), t) \pm g_1(-x - R(t), t)]f(x, t), \end{aligned} \quad (86)$$

with

$$g_1(y, t) = \chi(y > 0) \left(\frac{y^2}{4b(t)^2} - \frac{1}{2b(t)} - i\tilde{k}\frac{y}{b(t)} \right). \quad (87)$$

In addition, we have

$$i\hbar\partial_t f(x, t) = Zf(x, t) - \frac{\hbar^2}{2m}[g_2(x - R(t), t) \pm g_2(-x - R(t), t)]f(x, t), \quad (88)$$

⁵The computation can be given the following mathematical justification: Since the potential V is bounded, by an application of the Kato–Rellich theorem [12, Theorem X.15], the Hamiltonian $H = -\frac{\hbar^2}{2m}\partial_x^2 + V$ 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 . This can be used to justify all the manipulations made here. Let us also use the opportunity to stress that, if we had not chosen the constants A_{\pm} and B_{\pm} in (38) 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 [13].

with $g_2 = g_1 + g_3$ where

$$g_3(y, t) = \chi(y > 0) \frac{1 + 2\beta y}{2b(t)}. \quad (89)$$

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

$$t \mapsto F(t) = e^{itH/\hbar} f(\cdot, t) - \phi_n. \quad (90)$$

with $F(t) \in L^2$ for all $t \geq 0$ and $F(0) = 0$. F is differentiable and by the above estimates for all $t > 0$,

$$\partial_t F(t) = e^{itH/\hbar} \left[\frac{i}{\hbar} H f(\cdot, t) + \partial_t f(\cdot, t) \right] = e^{itH/\hbar} g(\cdot, t) \quad (91)$$

where

$$g(x, t) = i \frac{\hbar}{2m} [g_3(x - R(t), t) \pm g_3(-x - R(t), t)] f(x, t). \quad (92)$$

As the derivative is continuous (in the L^2 -norm) in t , it can be integrated to yield $F(t) = \int_0^t ds \partial_s F(s)$. Then, by the unitarity of the time evolution, we find

$$\|f(\cdot, t) - \phi_{n,t}\| = \|F(t)\| \leq \int_0^t ds \|\partial_s F(s)\| = \int_0^t ds \|g(\cdot, s)\|. \quad (93)$$

Thus we only need to estimate the magnitude of $\int_0^t ds \|g(\cdot, s)\|$. Let us first point out that for all $|x| > R(t)$, with $y = |x| - R(t)$,

$$|f(x, t)|^2 = |A_n|^2 |B|^2 \exp\left(2 \operatorname{Re} \left[-i \frac{t}{\hbar} Z + i \tilde{k}(y + vt) - \frac{1}{4b(t)^2} y^2 \right]\right). \quad (94)$$

Here the argument of the exponential can be simplified using $Z = \frac{\hbar^2}{2m} \tilde{k}^2 - \Delta E$ to

$$2\beta y - \frac{\sigma^2}{4|b_t|^2} y^2 = \frac{1}{2} c_t^2 - \frac{1}{2} \left[\frac{2\beta}{c_t} y - c_t \right]^2, \quad \text{with } c_t = 2\beta |b(t)| \sigma^{-1}. \quad (95)$$

Therefore,

$$\begin{aligned} \|g(\cdot, t)\|^2 &= \left(\frac{\hbar}{2m} \right)^2 2 \int_0^\infty dy |f(y + R(t), t)|^2 |g_3(y, t)|^2 \\ &= \left(\frac{\hbar |A_n| |B|}{2m |b_t|} \right)^2 \frac{1}{2} \int_0^\infty dy (1 + 2\beta y)^2 \exp\left(2\beta y - \frac{\sigma^2}{4|b_t|^2} y^2\right) \\ &= \left(\frac{\hbar \beta |A_n| |B|}{m \sigma c_t} \right)^2 \frac{c_t}{4\beta} e^{\frac{1}{2} c_t^2} \int_{-c_t}^\infty dx (1 + c_t^2 + c_t x)^2 e^{-\frac{1}{2} x^2} \\ &\leq \left(\frac{\hbar \beta |A_n| |B|}{m \sigma c_t} \right)^2 \frac{c_t}{4\beta} e^{\frac{1}{2} c_t^2} \int_{-\infty}^\infty dx ((1 + c_t^2)^2 + c_t^2 x^2) e^{-\frac{1}{2} x^2} \\ &= \left(\frac{\hbar \sqrt{\beta} |A_n| |B|}{2m \sigma} \right)^2 \frac{1}{c_t} e^{\frac{1}{2} c_t^2} \sqrt{2\pi} ((1 + c_t^2)^2 + c_t^2). \end{aligned} \quad (96)$$

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

$$\begin{aligned} c_t \leq c_\tau &= 2\beta|b(\tau)|\sigma^{-1} = \frac{2}{\sigma}\beta\sqrt{\sigma^4 + \left(\frac{\hbar}{2m}\right)^2\tau^2} \\ &\approx \frac{2}{\sigma}\frac{n^2}{4a\alpha^2}\sqrt{\sigma^4 + \left(\frac{a^2}{\pi n^2}\right)^2\alpha^2} \leq \frac{a}{\pi\sigma}\frac{1}{\alpha}, \end{aligned} \quad (97)$$

and therefore

$$\|g(\cdot, t)\| \leq \frac{\hbar\sqrt{\beta}|A_n||B|}{2m\sigma}\frac{2}{\sqrt{c_t}}. \quad (98)$$

Since

$$c_s = \sqrt{(2\beta\sigma)^2 + (s\beta\hbar/(m\sigma))^2} \geq s\frac{\beta\hbar}{m\sigma}, \quad (99)$$

we can estimate the integral over s by

$$\int_0^t ds \frac{1}{\sqrt{c_s}} \leq \int_0^t ds \sqrt{\frac{m\sigma}{\beta\hbar s}} = 2\sqrt{\frac{m\sigma t}{\beta\hbar}}. \quad (100)$$

This proves that for all $0 \leq t \leq \tau$,

$$\|f(\cdot, t) - \phi_{n,t}\|^2 \leq 4|A_n|^2|B|^2\frac{\hbar}{m\sigma}t \approx \frac{2a}{\pi\sigma}\frac{t}{\tau}\frac{1}{\alpha} \ll 1. \quad (101)$$

Since on the interval $[-a - vt, a + vt]$, $f(x, t) = A_n\psi_{n,t}(x)$, we have that

$$\int_{-a-vt}^{a+vt} |\phi_{n,t}(x) - A_n\psi_{n,t}(x)|^2 dx \leq \int_{-\infty}^{\infty} |\phi_{n,t}(x) - f(x, t)|^2 dx = \|f(\cdot, t) - \phi_{n,t}\|^2 \ll 1, \quad (102)$$

which is what we wanted to show.

C Longevity of Wave Packets on the Plateau

We now prove Corollary 1. Define

$$\phi(x) := \sum_{n=1}^{n_{\max}} \frac{c_n}{A_n} \phi_n(x)$$

and note that, since $\phi(x) = \psi(x)$ for $-a \leq x \leq a$, and by virtue of property (ii) in Proposition 2,

$$\|\psi - \phi\| = \|\phi \chi(x < -a \text{ or } x > a)\| \leq \sum_n \left| \frac{c_n}{A_n} \right| \|\phi_n \chi(x < -a \text{ or } x > a)\| \ll 1.$$

As a consequence, also ψ_t will be close to

$$\phi_t = e^{-iHt/\hbar}\phi = \sum_n \frac{c_n}{A_n} \phi_{n,t},$$

so that, provided $0 < t < \tau_n$ for each n ,

$$\left\| \left(\psi_t - \sum_n c_n \psi_{n,t} \right) \chi(-a \leq x \leq a) \right\| \quad (103)$$

$$\leq \left\| (\psi_t - \phi_t) \chi(-a \leq x \leq a) \right\| + \left\| \left(\phi_t - \sum_n c_n \psi_{n,t} \right) \chi(-a \leq x \leq a) \right\| \quad (104)$$

$$\leq \left\| \psi_t - \phi_t \right\| + \sum_n \left| \frac{c_n}{A_n} \right| \left\| \left(\phi_{n,t} - A_n \psi_{n,t} \right) \chi(-a \leq x \leq a) \right\| \ll 1 \quad (105)$$

by virtue of property (iii) of Proposition 2.

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