2.3: Particle Reflection and Tunneling

Now, let us proceed to the cases when a 1D particle moves in various potential profiles $U(x)$ that are constant in time. Conceptually, the simplest of such profiles is a potential step - see Fig. 3.

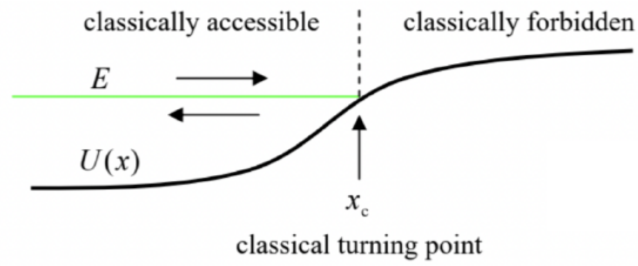

Fig. 2.3. Classical 1D motion in a potential profile $U(x)$.

As I am sure the reader knows, in classical mechanics the particle's kinetic energy $p^2/2m$ cannot be negative, so if the particle is incident on such a step (in Fig. 3, from the left), it can only travel through the classically accessible region, where its (conserved) full energy,

$$E = \frac{p^2}{2m} + U(x), \tag{2.3.1}$$

is larger than the local value $U(x)$. Let the initial velocity $v = p/m$ be positive, i.e. directed toward the step. Before it has reached the classical turning point x_c, defined by equality

$$U(x_c) = E \tag{2.3.2}$$

the particle's kinetic energy $p^2/2m$ is positive, so that it continues to move in the initial direction. On the other hand, a classical particle cannot penetrate that classically forbidden region $x > x_c$, because there its kinetic energy would be negative. Hence when the particle reaches the point $x = x_c$, its velocity has to change its sign, i.e. the particle is reflected back from the classical turning point.

In order to see what does the wave mechanics say about this situation, let us start from the simplest, sharp potential step shown with the bold black line in Fig. 4:

$$U(x) = U_0\theta(x) \equiv \begin{cases} 0, & \text{at } x < 0, \\ U_0, & \text{at } 0 < x. \end{cases} \tag{2.3.3}$$

For this choice, and any energy within the interval $0 < E < U_0$, the classical turning point is $x_c = 0$.

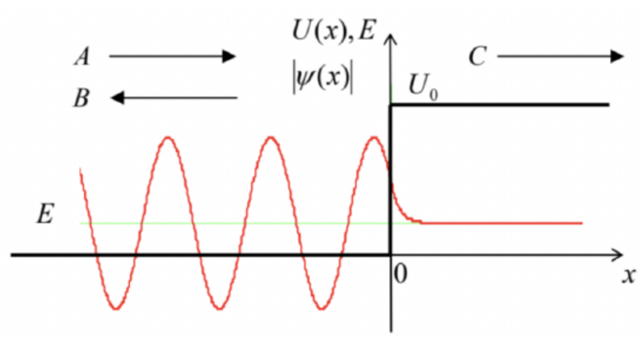

Fig. 2.4. The reflection of a monochromatic wave from a potential step $U_0 > E$. (This particular wavefunction's shape is for $U_0 = 5E$.) The wavefunction is plotted with the same schematic vertical offset by E as those in Fig. 1.8.

Let us represent an incident particle with a wave packet so long that the spread $\delta k \sim 1/\delta x$ of its wave-number spectrum is sufficiently small to make the energy uncertainty $\delta E = \hbar\delta\omega = \hbar(d\omega/dk)\delta k$ negligible in comparison with its average value $E < U_0$, as well as with $(U_0 - E)$. In this case, E may be considered as a given constant, the time dependence of the wavefunction is given by Eq. (1.62), and we can calculate its spatial factor $\psi(x)$ from the 1D version of the stationary Schrödinger equation (1.65) : 11

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi. \tag{2.3.4}$$

At $x<0$, i.e. at $U=0$, the equation is reduced to the Helmholtz equation (1.78), and may be satisfied with either of two traveling waves, proportional to $\exp\{+ikx\}$ and $\exp\{-ikx\}$ correspondingly, with k satisfying the dispersion equation (1.30):

$$k^2 \equiv \frac{2mE}{\hbar^2}. \tag{2.3.5}$$

Thus the general solution of Eq. (53) in this region may be represented as

$$\psi_-(x) = Ae^{+ikx} + Be^{-ikx} \tag{2.3.6}$$

The second term on the right-hand side of Eq. (55) evidently describes a (formally, infinitely long) wave packet traveling to the left, arising because of the particle's reflection from the potential step. If $B=-A$, this solution is reduced to Eq. (1.84) for the potential well with infinitely high walls, but for our current case of a finite step height U_0, the relation between the coefficients B and A may be different.

To show this, let us solve Eq. (53) for $x>0$, where $U=U_0>E$. In this region the equation may be rewritten as

$$\frac{d^2\psi_+}{dx^2} = \kappa^2\psi_+, \tag{2.3.7}$$

where κ is a real and positive constant defined by a formula similar in structure to Eq. (54):

$$\kappa^2 \equiv \frac{2m(U_0-E)}{\hbar^2} > 0. \tag{2.3.8}$$

The general solution of Eq. (56) is the sum of $\exp\{+\kappa x\}$ and $\exp\{-\kappa x\}$, with arbitrary coefficients. However, in our particular case the wave function should be finite at $x\rightarrow+\infty$, so only the latter exponent forbidden is acceptable:

$$\psi_+(x) = Ce^{-\kappa x}. \tag{2.3.9}$$

Such penetration of the wavefunction to the classically forbidden region, and hence a non-zero probability to find the particle there, is one of the most fascinating predictions of quantum mechanics, and has been repeatedly observed in experiment - e.g., via tunneling experiments - see the next section. [12] From Eq. (58), it is evident that the constant κ, defined by Eqs. (57), may be interpreted as the reciprocal penetration depth. Even for the lightest particles, this depth is usually very small. Indeed, for $E<<U_0$ that relation yields

$$\delta \equiv \left.\frac{1}{\kappa}\right|_{E\rightarrow 0} = \frac{\hbar}{(2mU_0)^{1/2}}. \tag{2.3.10}$$

For example, let us consider a conduction electron in a typical metal, which runs, at the metal's surface, into a sharp potential step whose height is equal to metal's workfunction $U_0 \approx 5\text{eV}$ - see the discussion of the photoelectric effect in Sec. 1.1. In this case, according to Eq. (59), δ is close to 0.1 nm, i.e. is close to a typical size of an atom. For heavier elementary particles (e.g., protons) the penetration depth is correspondingly lower, and for macroscopic bodies, it is hardly measurable.

Returning to Eqs. (55) and (58), we still should relate the coefficients B and C to the amplitude A of the incident wave, using the boundary conditions at $x=0$. Since E is a finite constant, and $U(x)$ is a finite function, Eq. (53) says that $d^2\psi/dx^2$ should be finite as well. This means that the first derivative should be continuous:

$$\lim_{\varepsilon\rightarrow 0}\left(\left.\frac{d\psi}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{x=-\varepsilon}\right) = \lim_{\varepsilon\rightarrow 0}\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\psi}{dx^2}dx = \frac{2m}{\hbar^2}\lim_{\varepsilon\rightarrow 0}\int_{-\varepsilon}^{+\varepsilon}[U(x)-E]\psi dx = 0 \tag{2.3.11}$$

Repeating such calculation for the wavefunction $\psi(x)$ itself, we see that it also should be continuous at all points, including the border point $x=0$, so that the boundary conditions in our problem are

$$\psi_-(0) = \psi_+(0), \quad \frac{d\psi_-}{dx}(0) = \frac{d\psi_+}{dx}(0) \tag{2.3.12}$$

Plugging Eqs. (55) and (58) into Eqs. (61), we get a system of two linear equations

$$A+B=C, \quad ikA-ikB=-\kappa C, \tag{2.3.13}$$

whose (easy :-) solution allows us to express B and C via A:

$$B = A\frac{k-i\kappa}{k+i\kappa}, \quad C = A\frac{2k}{k+i\kappa}. \tag{2.3.14}$$

We immediately see that the numerator and denominator in the first of these fractions have equal moduli, so that $|B| = |A|$. This means that, as we could expect, a particle with energy $E < U_0$ is totally reflected from the step – just as in classical mechanics. As a result, at $x < 0$ our solution (55) may be represented as a standing wave

$$\psi_- = 2iAe^{i\theta}\sin(kx-\theta), \quad \text{with } \theta \equiv \tan^{-1}\frac{k}{\kappa}. \tag{2.3.15}$$

Note that the shift $\Delta x \equiv \theta/k = \left(\tan^{-1} k/\kappa\right)/k$ of the standing wave to the right, due to the partial penetration of the wavefunction under the potential step, is commensurate with, but generally not equal to the penetration depth $\delta \equiv 1/\kappa$. The red line in Fig. 4 shows the exact behavior of the wavefunction, for a particular case $E = U_0/5$, at which $k/\kappa \equiv [E/(U_0-E)]^{1/2} = 1/2$.

According to Eq. (59), as the particle's energy E is increased to approach U_0, the penetration depth $1/\kappa$ diverges. This raises an important issue: what happens at $E > U_0$, i.e. if there is no classically forbidden region in the problem? In classical mechanics, the incident particle would continue to move to the right, though with a reduced velocity, corresponding to the new kinetic energy $E - U_0$, so there would be no reflection. In quantum mechanics, however, the situation is different. To analyze it, it is not necessary to re-solve the whole problem; it is sufficient to note that all our calculations, and hence Eqs. (63) are still valid if we take [13]

$$\kappa = -ik', \quad \text{with} \quad k'^2 \equiv \frac{2m(E-U_0)}{\hbar^2} > 0. \tag{2.3.16}$$

With this replacement, Eq. (63) becomes [14]

$$B = A\frac{k-k'}{k+k'}, \quad C = A\frac{2k}{k+k'}. \tag{2.3.17}$$

The most important result of this change is that now the particle's reflection is not total: $|B| < |A|$. To evaluate this effect quantitatively, it is fairer to use not the B/A or C/A ratios, but rather that of the probability currents (5) carried by the de Broglie waves traveling to the right, with amplitudes C and A, in the corresponding regions (respectively, for $x > 0$ and $x < 0$):

$$\mathscr{T} \equiv \frac{I_C}{I_A} = \frac{k'|C|^2}{k|A|^2} = \frac{4kk'}{(k+k')^2} \equiv \frac{4[E(E-U_0)]^{1/2}}{\left[E^{1/2}+(E-U_0)^{1/2}\right]^2} \tag{2.3.18}$$

(The parameter $\mathscr{T}$ so defined is called the transparency of the system, in our current case of the potential step of height U_0, at particle's energy E.) The result given by Eq. (67) is plotted in Fig. 5a as a function of the U_0/E ratio. Note its most important features:

(i) At $U_0 = 0$, the transparency is full, $\mathscr{T} = 1$ - naturally, because there is no step at all.

(ii) At $U_0 \to E$, the transparency drops to zero, giving a proper connection to the case $E < U_0$.

(iii) Nothing in our solution's procedure prevents us from using Eq. (67) even for $U_0 < 0$, i.e. for the step-down (or "cliff") potential profile - see Fig. 5b. Very counter-intuitively, the particle is (partly) reflected even from such a cliff, and the transmission diminishes (though rather slowly) at $U_0 \to -\infty$.

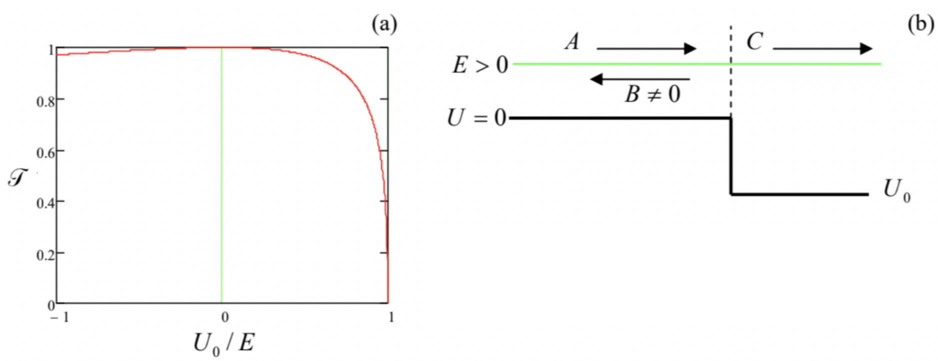

Fig. 2.5. (a) The transparency of a potential step with $U_0 < E$ as a function of its height, according to Eq. (75), and (b) the "cliff" potential profile, with $U_0 < 0$.

The most important conceptual conclusion of this analysis is that the quantum particle is partly reflected from a potential step with $U_0 < E$, in the sense that there is a non-zero probability $\mathscr{T} < 1$ to find it passed over the step, while there is also some probability, $(1 - \mathscr{A} > 0$, to have it reflected.

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The last property is exhibited, but for any relation between E and U_0, by another simple potential profile $U(x)$, the famous potential (or "tunnel") barrier. Fig. 6 shows its simple, "rectangular" version:

$$U(x)=\begin{cases}0, \text{ for } x<-d/2, \\ U_0, \text{ for } -d/2<x<+d/2, \\ 0, \text{ for } +d/2<x.\end{cases}$$

To analyze this problem, it is sufficient to look for the solution to the Schrödinger equation in the form (55) at $x \leq -d/2$. At $x>+d/2$, i.e., behind the barrier, we may use the arguments presented above (no wave source on the right!) to keep just one traveling wave, now with the same wave number:

$$\psi_{+}(x)=F e^{i k x}. \tag{2.3.19}$$

However, under the barrier, i.e. at $-d/2 \leq x \leq +d/2$, we should generally keep both exponential terms,

$$\psi_b(x)=C e^{-\kappa x}+D e^{+\kappa x}, \tag{2.3.20}$$

because our previous argument, used in the potential step problem's solution, is no longer valid. (Here k and κ are still defined, respectively, by Eqs. (54) and (57).) In order to express the coefficients B, C, D, and F via the amplitude A of the incident wave, we need to plug these solutions into the boundary conditions similar to Eqs. (61), but now at two boundary points, $x=\pm d/2$.

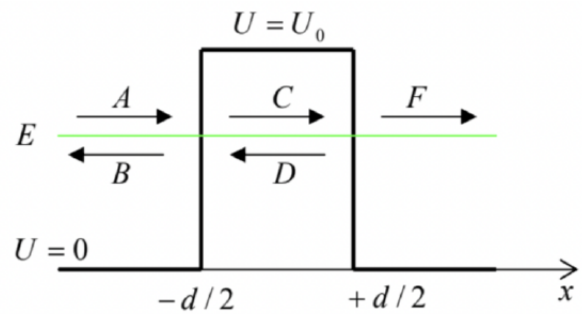

Fig. 2.6. A rectangular potential barrier, and the de Broglie waves taken into account in its analysis.

Solving the resulting system of 4 linear equations, we get four ratios $B/A, C/A$, etc.; in particular,

$$\frac{F}{A}=\left[\cosh \kappa d+\frac{i}{2}\left(\frac{\kappa}{k}-\frac{k}{\kappa}\right) \sinh \kappa d\right]^{-1} e^{-i k d}, \tag{2.3.21}$$

and hence the barrier's transparency

$$\text{Rectangular tunnel barrier's transparency} \qquad \mathscr{T} \equiv\left|\frac{F}{A}\right|^2=\left[\cosh ^2 \kappa d+\left(\frac{\kappa^2-k^2}{2 \kappa k}\right)^2 \sinh ^2 \kappa d\right]^{-1}. \tag{2.3.22}$$

So, quantum mechanics indeed allows particles with energies $E<U_0$ to pass "through" the potential barrier – see Fig. 6 again. This is the famous effect of quantum mechanical tunneling. Fig. 7a shows the barrier transparency as a function of the particle energy E, for several characteristic values of its thickness d, or rather of the ratio d/δ, with δ defined by Eq. (59).

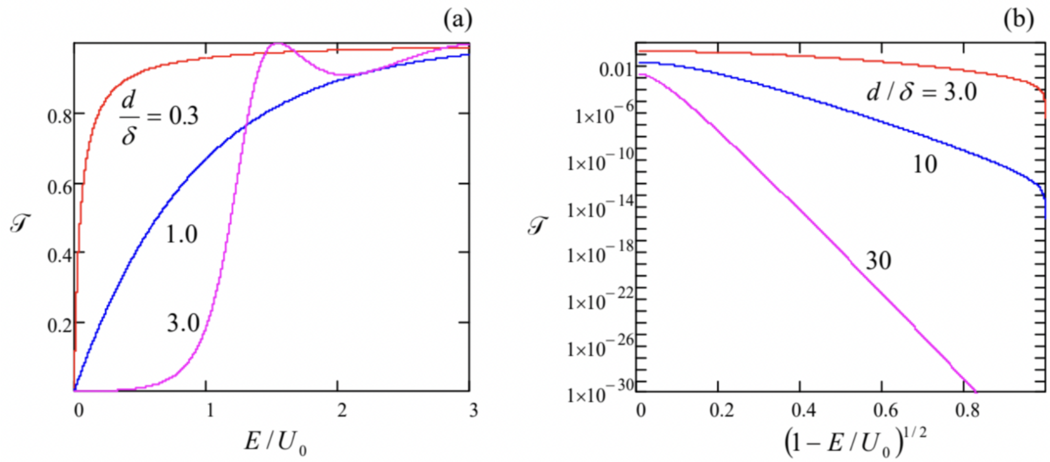

Fig. 2.7. The transparency of a rectangular potential barrier as a function of the particle's energy E.

The plots show that generally, the transparency grows gradually with the particle's energy. This growth is natural because the penetration constant κ decreases with the growth of E, i.e., the wavefunction penetrates more and more into the barrier, so that more and more of it is "picked up" at the second interface $(x = +d/2)$ and transferred into the wave $F\exp\{ikx\}$ propagating behind the barrier.

Now let us consider the important limit of a very thin and high rectangular barrier, $d << \delta, E << U_0$, giving $k << \kappa << 1/d$. In this limit, Eq. (71) yields

$$\mathscr{T} \equiv \left|\frac{F}{A}\right|^2 \rightarrow \frac{1}{|1+i\alpha|^2} = \frac{1}{1+\alpha^2}, \quad \text{where } \alpha \equiv \frac{1}{2}\left(\frac{\kappa^2 - k^2}{\kappa k}\right)\kappa d \approx \frac{1}{2}\frac{\kappa^2 d}{k} \approx \frac{m}{\hbar^2 k} U_0 d, \tag{2.3.23}$$

The last product, $U_0 d$, is just the "energy area" (or the "weight")

$$w \equiv \int_{U(x)>E} U(x) dx \tag{2.3.24}$$

of the barrier. This fact implies that the very simple result (72) may be correct for a barrier of any shape, provided that it is sufficiently thin and high.

To confirm this guess, let us consider the tunneling problem for a very thin barrier with $\kappa d, kd << 1$, approximating it with the Dirac's δ-function (Fig. 8):

$$U(x) = w\delta(x), \tag{2.3.25}$$

so that the parameter w satisfies Eq. (73).

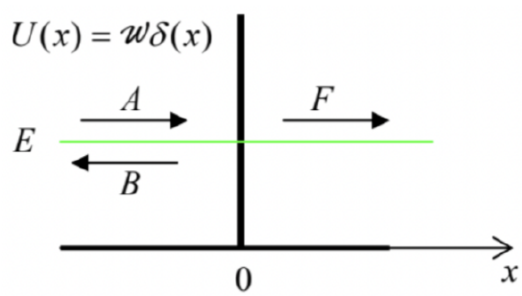

Fig. 2.8. A delta-functional potential barrier.

The solutions of the tunneling problem at all points but $x = 0$ still may be taken in the form of Eqs. (55) and (69), so we only need to analyze the boundary conditions at that point. However, due to the special character of the δ-function, we should be careful here. Indeed, instead of Eq. (60) we now get

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\psi}{dx}\right|_{x=+\varepsilon}-\left.\frac{d\psi}{dx}\right|_{x=-\varepsilon}\right)=\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\psi}{dx^2}dx=\lim_{\varepsilon\to 0}\frac{2m}{\hbar^2}\int_{-\varepsilon}^{+\varepsilon}[U(x)-E]\psi dx$$
$$=\frac{2m}{\hbar^2}w_\psi(0).$$

According to this relation, at a finite w, the derivatives $d\psi/dx$ are also finite, so that the wavefunction itself is still continuous:

$$\lim_{\varepsilon\to 0}\left(\psi|_{x=+\varepsilon}-\psi|_{x=+\varepsilon}\right)=\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon}\frac{d\psi}{dx}dx=0 \tag{2.3.26}$$

Using these two boundary conditions, we readily get the following system of two linear equations,

$$A+B=F,\quad ikF-(ikA-ikB)=\frac{2mw}{\hbar^2}F, \tag{2.3.27}$$

whose solution yields

$$\frac{B}{A}=\frac{-i\alpha}{1+i\alpha},\quad \frac{F}{A}=\frac{1}{1+i\alpha},\quad \text{where } \alpha\equiv\frac{mw}{\hbar^2 k}. \tag{2.3.28}$$

(Taking Eq. (73) into account, this definition of α coincides with that in Eq. (72).) For the barrier transparency $\mathscr{T}\equiv|F/A|^2$, this result again gives the first of Eqs. (72), which is therefore general for such thin barriers. That formula may be recast to give the following simple expression (valid only for $E<<U_{\max}$:

$$\mathcal{T}=\frac{1}{1+\alpha^2}\equiv\frac{E}{E+E_0},\quad \text{where } E_0\equiv\frac{mW^2}{2\hbar^2}, \tag{2.3.29}$$

which shows that as energy becomes larger than the constant E_0, the transparency approaches 1 .

Now proceeding to another important limit of thick barriers $(d>>\delta)$, Eq. (71) shows that in this case, the transparency is dominated by what is called the tunnel exponent:

$$\mathscr{T}=\left(\frac{4k\kappa}{k^2+\kappa^2}\right)^2 e^{-2\kappa d} \tag{2.3.30}$$

- the behavior which may be clearly seen as the straight-line segments in semi-log plots (Fig. 7b) of $\mathscr{T}$ as a function of the combination $(1-E/U_0)^{1/2}$, which is proportional to $\kappa-$ see Eq. (57). This exponential dependence on the barrier thickness is the most important factor for various applications of quantum-mechanical tunneling - from the field emission of electrons to vacuum [15] to the scanning tunneling microscopy. [16] Note also very substantial negative implications of the effect for the electronic technology progress, most importantly imposing limits on the so-called Dennard scaling of field-effect transistors in semiconductor integrated circuits (which is the technological basis of the well-known Moore's law), due to the increase of tunneling both through the gate oxide and along the channel of the transistors, from source to drain. [17]

Finally, one more feature visible in Fig. 7a (for case $d=3\delta$) are the oscillations of the transparency as a function of energy, at $E>U_0$, with $\mathcal{T}=1$, i.e. the reflection completely vanishing, at some points. [18] This is our first glimpse at one more interesting quantum effect: resonant tunneling. This effect will be discussed in more detail in Sec. 5 below, using another potential profile where it is more clearly pronounced.

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[11] Note that this is not the eigenproblem like the one we have solved in Sec. 1.4 for a potential well. Indeed, now the energy E is considered given - e.g., by the initial conditions that launch a long wave packet upon the potential step - in Fig. 4, from the left.

[12] Note that this effect is pertinent to waves of any type, including mechanical waves (see, e.g., CM Secs. 6.4 and 7.7) and electromagnetic waves (see, e.g., EM Secs. 7.3-7.7).

[13] Our earlier discarding of the particular solution $\exp\{x\}$, now becoming $\exp\{-ik'x\}$, is still valid, but now on different grounds: this term would describe a wave packet incident on the potential step from the right, and this is not the problem under our current consideration.

[14] These formulas are completely similar to those describing the partial reflection of classical waves from a sharp interface between two uniform media, at normal incidence (see, e.g., CM Sec. 6.4 and EM Sec. 7.4), with the effective impedance Z of de Broglie waves being proportional to their wave number k.

[15] See, e.g., G. Fursey, Field Emission in Vacuum Microelectronics, Kluwer, New York, 2005.

[16] See, e.g., G. Binning and H. Rohrer, Helv. Phys. Acta $\mathbf{55}$, $\mathbf{726}$ (1982).

[17] See, e.g., V. Sverdlov et al., IEEE Trans. on Electron Devices 50, 1926 (2003), and references therein. (A brief discussion of the field-effect transistors, and literature for further reading, may be found in SM Sec. 6.4.)

[18] Let me mention in passing the curious case of the potential well $U(x) = -\left(\hbar^2/2m\right)\varkappa(v+1)/\cosh^2(x/a)$, with any positive integer v and any real a, which is reflection-free $(\mathscr{T} = 1)$ for the incident de Broigle wave of any energy E, and hence for any incident wave packet. Unfortunately, a proof of this fact would require more time/space than I can afford. (Note that it was first described in a 1930 paper by Paul Sophus Epstein, before the 1933 publication by G. Pöschl and E. Teller, which is responsible for the common name of this Pöschl-Teller potential.)

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