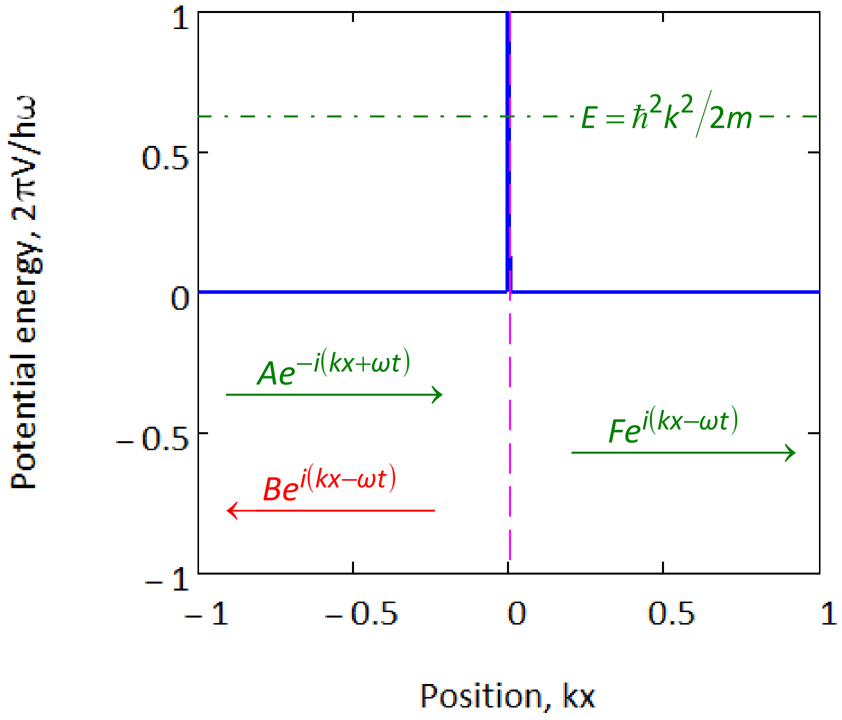
Today in Physics 237: scattering

- The Dirac delta function
- The delta function potential well:
  - bound state
  - transmission and reflection of free quanta
  - tunneling
- The finite square well: outline



The Dirac delta function

- The **delta function** is an infinite-amplitude, infinitesimally narrow object with unit integral. In 1-D, it's

$$\int_{\mathcal{C}} \delta(x)\,dx = \begin{cases} 1 & \text{if } \mathcal{C} \text{ contains the origin,} \\ 0 & \text{otherwise} \end{cases}$$

- Defined in this way by its integral, it has no official functional form; mathematicians therefore refer to it as a distribution rather than a function.

- It usually arises in one's proofs as the limiting case of sharply-peaked functional forms, as demonstrated in the green pages of Lecture 7:

$$\lim_{\varepsilon \to 0} \frac{e^{-x^2/2\varepsilon^2}}{\sqrt{2\pi}\,\varepsilon} = \delta(x) \quad ,$$

  but it is not necessarily a Gaussian underneath the integral; any sharply-peaked function will do, as long as it satisfies the definition at the top.

The Dirac delta function (continued)

- Its basic properties, taking $x = a$ to lie on $\mathcal{C}$, and introducing the Heaviside step function $\vartheta(x-a)=\begin{cases}0 & x\le a\\ 1 & x>a\end{cases}$:

$$\int_{\mathcal{C}} \delta(x-a)\,dx = 1$$

$$\int_{\mathcal{C}} f(x)\,\delta(x-a)\,dx = f(a)$$

$$\left.\begin{aligned} &\int_{\mathcal{C}} \delta(cx-a)\,dx = \frac{1}{|c|} \\[2em] &\delta(x-a) = \frac{d}{dx}\vartheta(x-a) \end{aligned}\right\}\qquad \text{Problem set \#4}$$

$$\frac{d}{dx}\delta(x-a) = -\frac{1}{x-a}\delta(x-a) \qquad \text{Try integrating by parts}$$

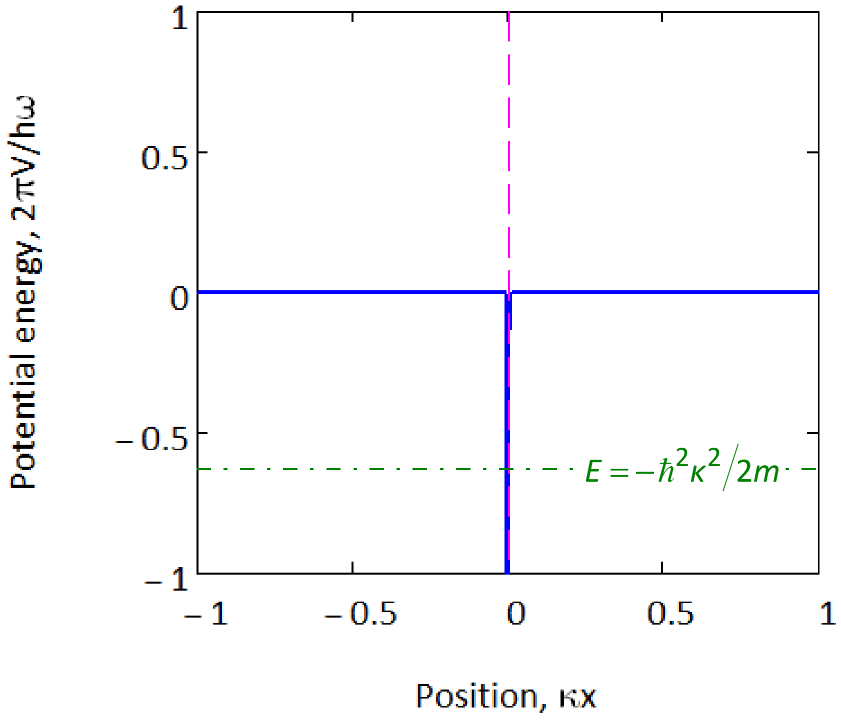
The Dirac delta function (continued)

- Its uses:
  - $\int f(x)\delta(x-a)dx = f(a)$: it picks out its argument's value in the rest of the integrand.
  - Thus it's the world's easiest object to integrate. May all your integrands contain $\delta(x)$.
- Its origins:
  - Independently developed and used by many mathematicians and physicists as far back as Fourier himself, in precisely the manner used in Lecture 7. Like the Maxwell equations, $\delta(x)$ was eventually codified by Heaviside.
  - Dirac gave it its current, distribution-like, definition and its prominent role in quantum mechanics, so in this form it is named after him. Its foundation in the theory of distributions was made rigorous about a decade later, by Schwartz.

The delta-function potential well

Suppose $V(x) = -\alpha\delta(x), \alpha > 0$: solve the Schrödinger equation.

- $V(x)$ reaches $-\infty$ at $x = 0$; any value of energy is eligible, according to our results in G&S problems 2.2-2.3, problem set 2.
- So there are free-quantum (**scattering**) solutions, and may be spatially-confined, quantized (**bound**) solutions.
- For the bound – spatially-confined – case, we look to the separation solution. Use the time-independent Schrödinger equation and $E < 0$, so the particular solutions are **real-exponent** exponentials. Abbreviating $\kappa = \sqrt{-2mE}/\hbar$ and avoiding $x = 0$,



$$x \neq 0: \quad \frac{d^2\psi}{dx^2} = \kappa^2\psi \quad \begin{cases} x < 0: & \psi(x) = \cancelto{0}{A}e^{-\kappa x} + Be^{\kappa x} \\ x > 0: & \psi(x) = Fe^{-\kappa x} + \cancelto{0}{G}e^{\kappa x} \end{cases}$$

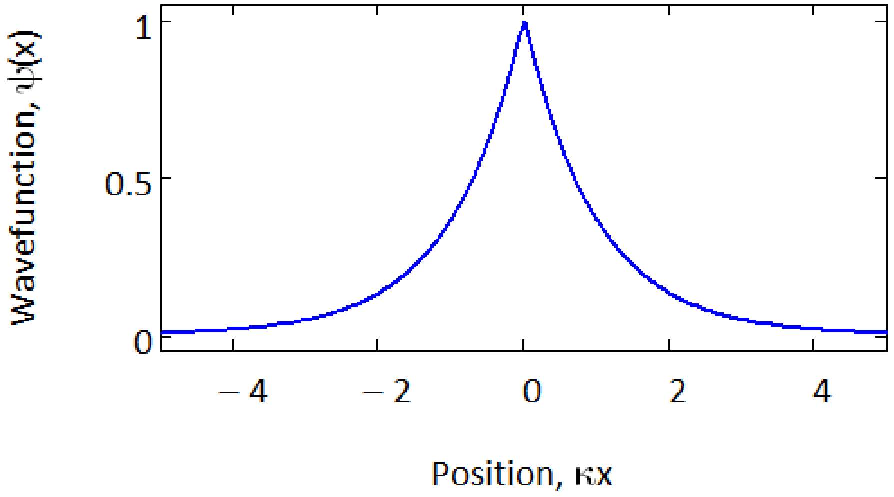
otherwise ψ blows up

The delta-function potential well (continued)

- To evaluate the remaining constants *B*, *F*, and *κ*, and to stitch the solution through $x = 0$, our first constraint is the **continuity of *ψ*.** Apply this at $x = 0$ and we find that $B = F$, so that

$$\psi(x)=Be^{\pm\kappa x}\quad,\quad x\underset{>}{\leq}0\quad;\quad\text{or, better yet,}\ \boxed{\psi(x)=Be^{-\kappa|x|}}\quad,$$

as plotted at right, which is just like the $t = 0$ wavefunction we encountered in G&S problem 2.20 (Lecture 7).

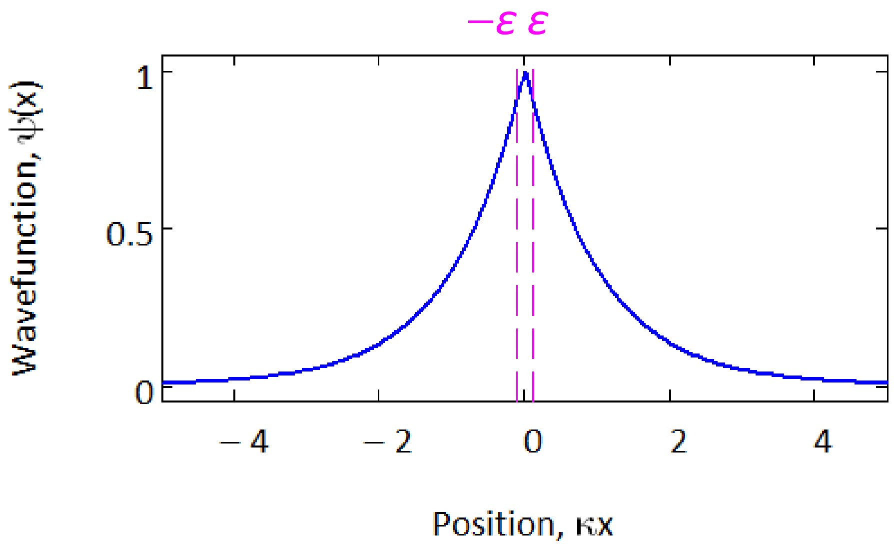


- Next we would use continuity of $d\psi/dx$ at $x = 0$ to determine *κ*. But we can tell by a glance to our right that the slope is *not* continuous there: $x = 0$ is a sharp corner in *ψ*.

- So instead we seek to exploit the properties of delta functions, as follows:

The delta function well (continued)

- Restore the potential energy term $V(x) = -\alpha\delta(x)$.
- Integrate the time-independent Schrödinger equation directly between $x = \pm\varepsilon$, $\varepsilon \ll 1$, aiming to let $\varepsilon \rightarrow 0$:



$$\int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi}{dx^2}dx + \frac{2m\alpha}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = \kappa^2\int_{-\varepsilon}^{\varepsilon}\psi(x)dx$$

$$\lim_{\varepsilon\rightarrow 0}\left(\left.\frac{d\psi}{dx}\right|_{\varepsilon} - \left.\frac{d\psi}{dx}\right|_{-\varepsilon}\right) + \frac{2m\alpha}{\hbar^2}\psi(0) = \kappa^2 \lim_{\varepsilon\rightarrow 0}\cancelto{0}{\int_{-\varepsilon}^{\varepsilon}\psi(x)dx}$$

- The last term approaches zero as $\varepsilon \rightarrow 0$, since $\psi(x) \approx 1$ in the neighborhood of x = 0 and is continuous there.

The delta function well (continued)

- Insert $\psi(x) = Be^{-\kappa|x|}$:

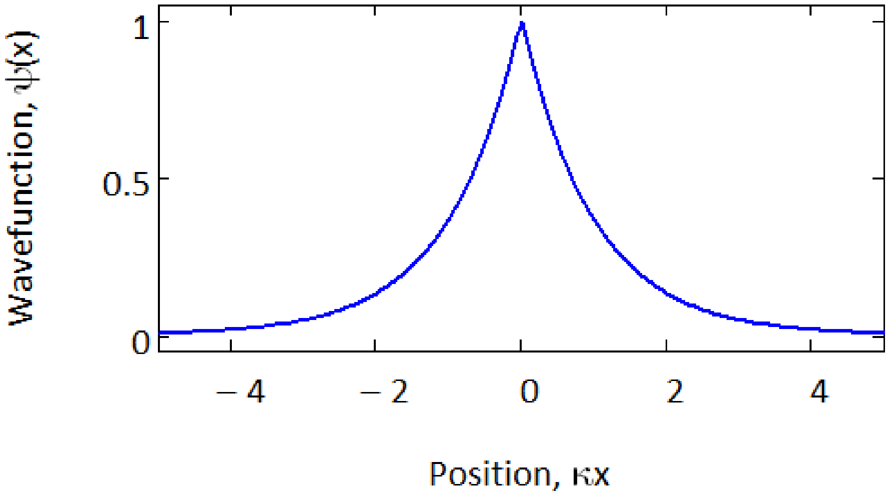
$$\Delta\left(\frac{d\psi}{dx}\right)\Big|_0 \equiv \lim_{\varepsilon\to 0}\left(-B\kappa e^{-\kappa\varepsilon} - B\kappa e^{\kappa\varepsilon}\right) = -\frac{2m\alpha}{\hbar^2}B$$

$$\Rightarrow \quad \kappa = \frac{m\alpha}{\hbar^2} \quad \Rightarrow \quad E = -\frac{\hbar^2\kappa^2}{2m} = \boxed{-\frac{m\alpha^2}{2\hbar^2}}\ .$$

- And normalize:

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 2|B|^2 \int_{-\infty}^{\infty} e^{-2\kappa x} dx = \frac{|B|^2}{\kappa}\left[-e^{-u}\right]_{-\infty}^{\infty}$$

$$= \frac{|B|^2}{\kappa} \quad \Rightarrow \quad B = \sqrt{\kappa} = \boxed{\frac{\sqrt{m\alpha}}{\hbar}}\ .$$



The delta function well (continued)

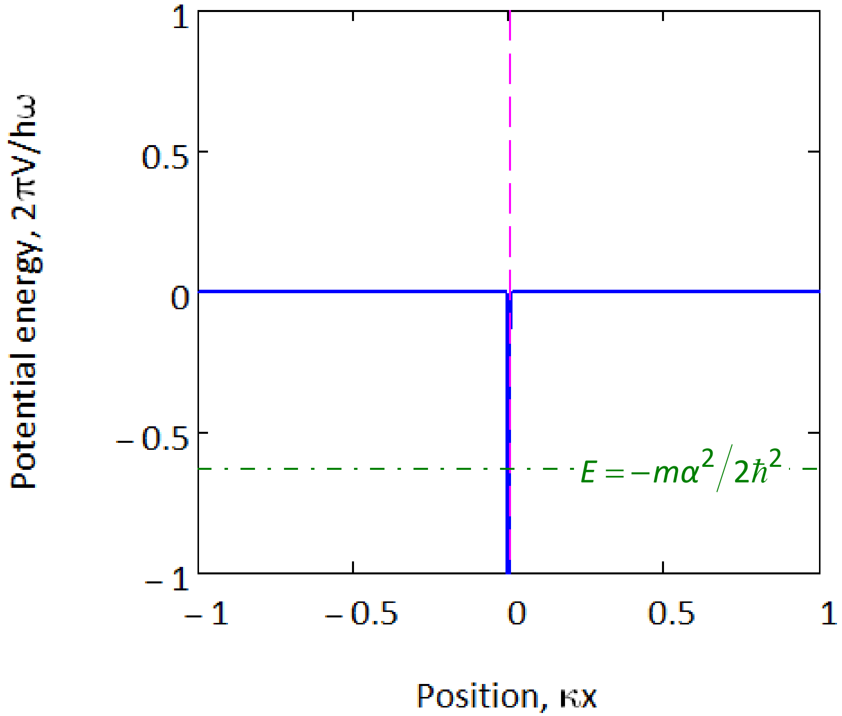
- So there is exactly one bound state in the delta-function well:

$$\boxed{\psi(x)=\frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2} \quad , \quad E=-\frac{m\alpha^2}{2\hbar^2} \quad .}$$

  Changing the value of α moves the state up or down in energy, but does not change the number of states.

  - Unless the **sign** of α is changed too; see page 18 below.

- And we have found that, although $d\psi/dx$ is not continuous at x = 0, the **magnitude of the discontinuity** is well defined – both thanks to the properties of the delta function – and that's just as good.

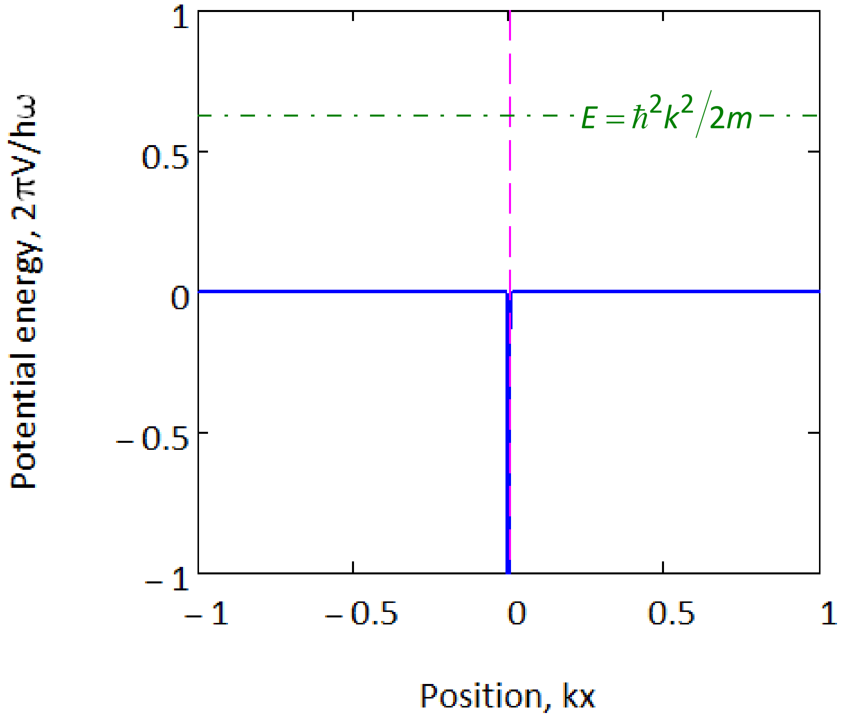


Scattering from the delta-function well

By scattering we mean free quanta – travelling waves – **bouncing off** or **skipping over** the delta-function well.

  - We cannot consider capture by the well until we learn about quantum-mechanical transitions.

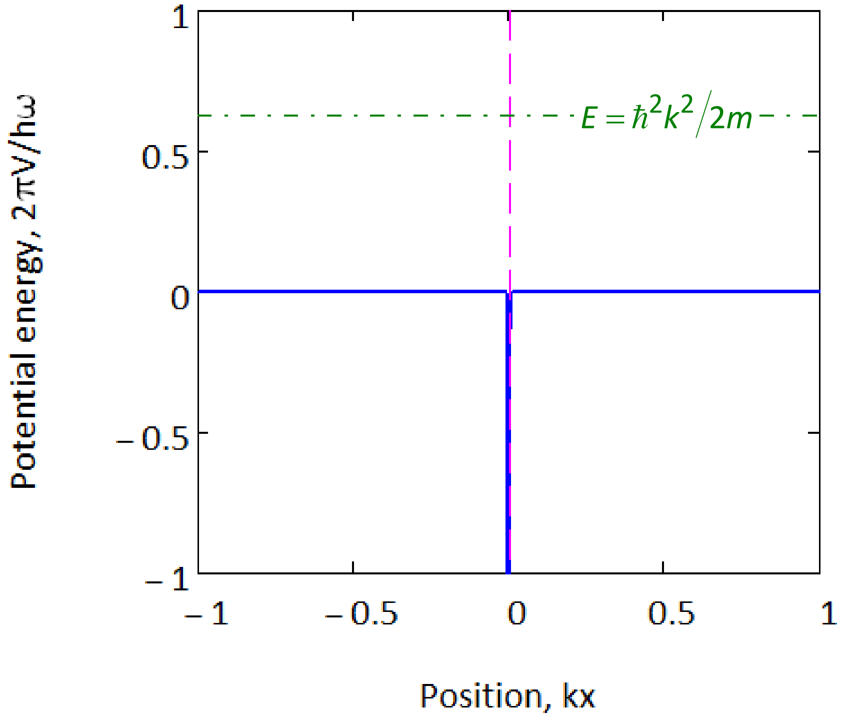
- First, what we're looking for:
  - There turn out to be too few constraints to solve for all the unknowns. This is expected, as the separation solutions cannot be normalized.
  - It turns out we can, however, calculate the fractions of **incident** wavepackets that bounce and skip.
  - As usual, we use the separation solutions $\psi(x)$ as the basis set for wavepackets. It will suffice, and be simpler to calculate the fractions for those solutions, rather than using Fourier-integral versions of wavepackets.



Scattering from the delta-function well (continued)

- As with the bound state we consider left or right of the delta function separately.
- Note that $E > 0$ this time, so we get complex-exponential particular solutions.
- Abbreviate $k = \sqrt{2mE}\big/\hbar$:

$$x \neq 0: \quad \frac{d^2\psi}{dx^2} = k^2\psi \quad \begin{cases} x < 0: & \psi(x) = Ae^{-ikx} + Be^{ikx} \\ x > 0: & \psi(x) = Fe^{-ikx} + Ge^{ikx} \end{cases} \quad .$$



- All four complex exponentials oscillate. There are none which approach ∞ at large ±*x*, as was the case for the bound state. Thus we have four unknown constants, not counting *E*.
  - We won’t find them all, but it will be OK.

Scattering from the delta-function well (continued)

- As with the bound state, we can invoke continuity of ψ to sew the solutions together at x = 0:

$$A+B=F+G \quad \Rightarrow \quad \boxed{\psi(0)=A+B \text{ or } F+G} \quad .$$

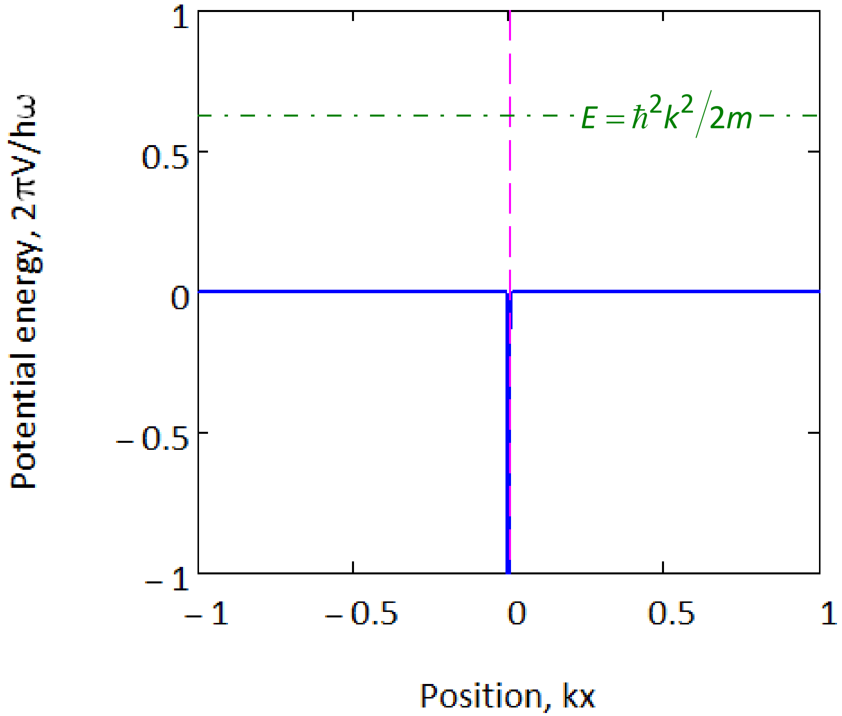
- Again we calculate the derivatives so that their discontinuity can be matched with $\int \delta(x)\psi(x)dx$:

$$\frac{d\psi}{dx}=ik\left(Fe^{ikx}-Ge^{-ikx}\right), x>0 \qquad \left.\frac{d\psi}{dx}\right|_{+\varepsilon}=ik(F-G)$$

$$\Rightarrow$$

$$=ik\left(Ae^{ikx}-Be^{-ikx}\right), x<0 \qquad \left.\frac{d\psi}{dx}\right|_{-\varepsilon}=ik(A-B)$$

$$\Rightarrow \quad \Delta\left(\frac{d\psi}{dx}\right)_0=ik(F-G-A+B) \quad .$$



Scattering from the delta-function well (continued)

- Again, back into the integral over $-\varepsilon \le x \le \varepsilon$ of the time-independent Schrödinger equation, and $\varepsilon \to 0$:

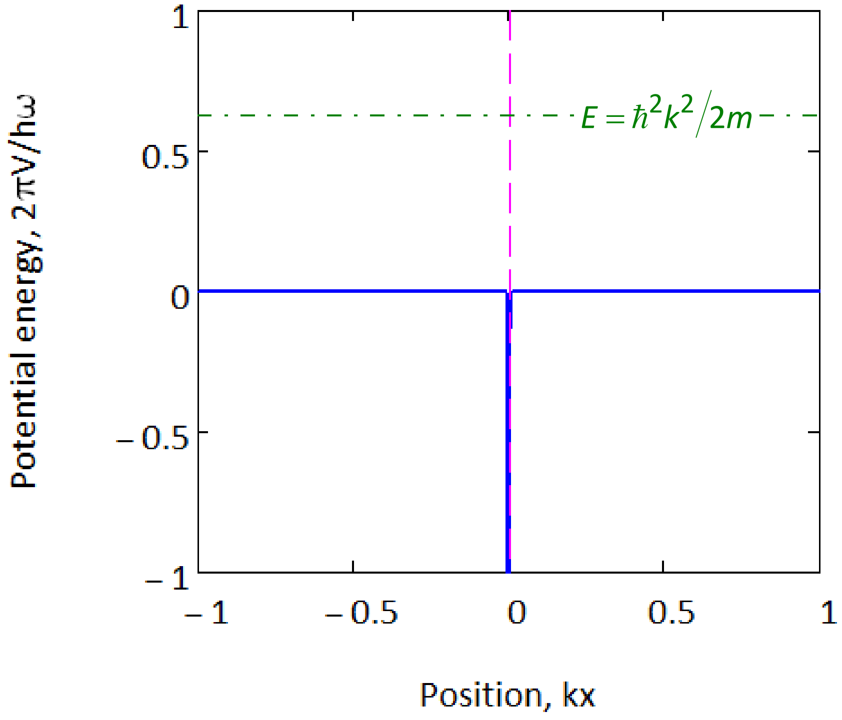
$$\int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi}{dx^2} dx + \frac{2m\alpha}{\hbar^2} \int_{-\varepsilon}^{\varepsilon} \delta(x)\psi(x) dx = \kappa^2 \int_{-\varepsilon}^{\varepsilon} \psi(x) dx$$

$$\xrightarrow[\varepsilon \to 0]{} \quad \Delta\left(\frac{d\psi}{dx}\right)\bigg|_0 + \frac{2m\alpha}{\hbar^2}\psi(0) = 0$$

$$\Rightarrow \quad ik(F - G - A + B) + \frac{2m\alpha}{\hbar^2}(A + B) = 0$$

- Abbreviate $\beta = m\alpha / \hbar^2 k$ and collect terms:

$$\boxed{F - G = A(1 + 2i\beta) - B(1 - 2i\beta)} \; .$$



Scattering from the delta-function well (continued)

- Then include the time-dependent, $e^{-i\omega t}$ part of the separation solution.

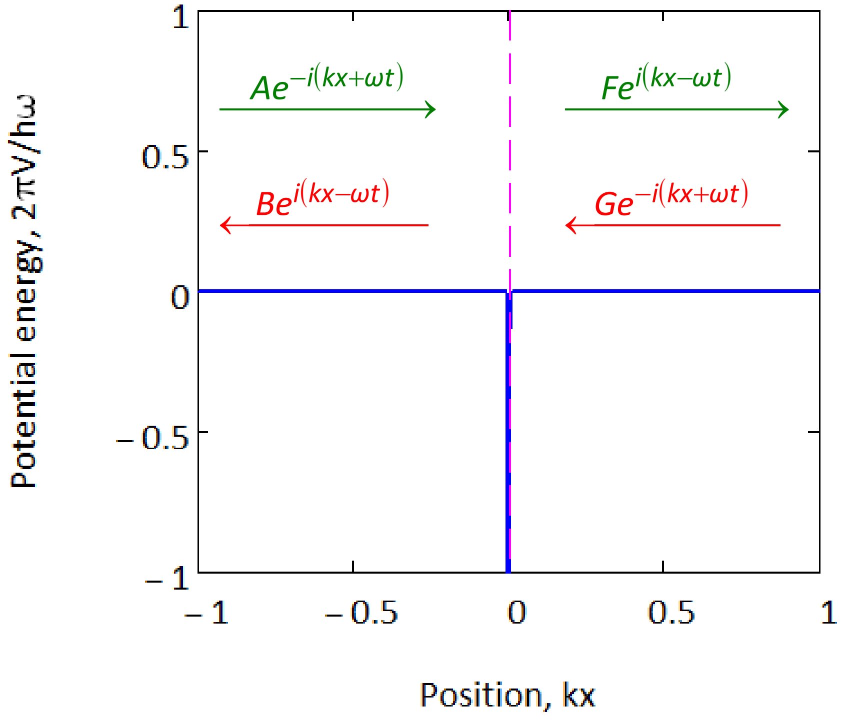
- A given peak or trough of each sinusoidal wave travels in the direction that keeps the complex exponent (phase) constant.

- Suppose the exponent is zero for a given peak. The propagation direction, + or -, is the sign of the phase velocity $v_p = \omega/k$:

$$x<0: \quad \Psi_k(x,t) = Ae^{-ikx-i\omega t} + Be^{ikx-i\omega t}$$

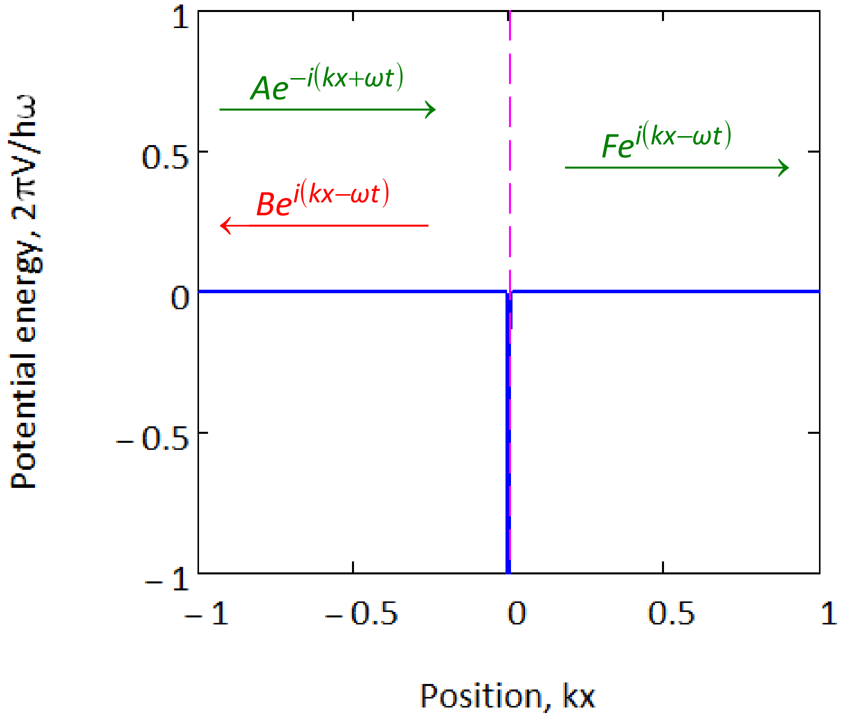
$$x>0: \quad \Psi_k(x,t) = Fe^{ikx-i\omega t} + Ge^{-ikx-i\omega t}$$

$$\Rightarrow \begin{array}{ll} A: \dfrac{\omega}{k} = -\dfrac{x}{t} > 0 & B: \dfrac{\omega}{k} = \dfrac{x}{t} < 0 \\ F: \dfrac{\omega}{k} = \dfrac{x}{t} > 0 & G: \dfrac{\omega}{k} = -\dfrac{x}{t} < 0 \end{array} .$$



Scattering from the delta-function well (continued)

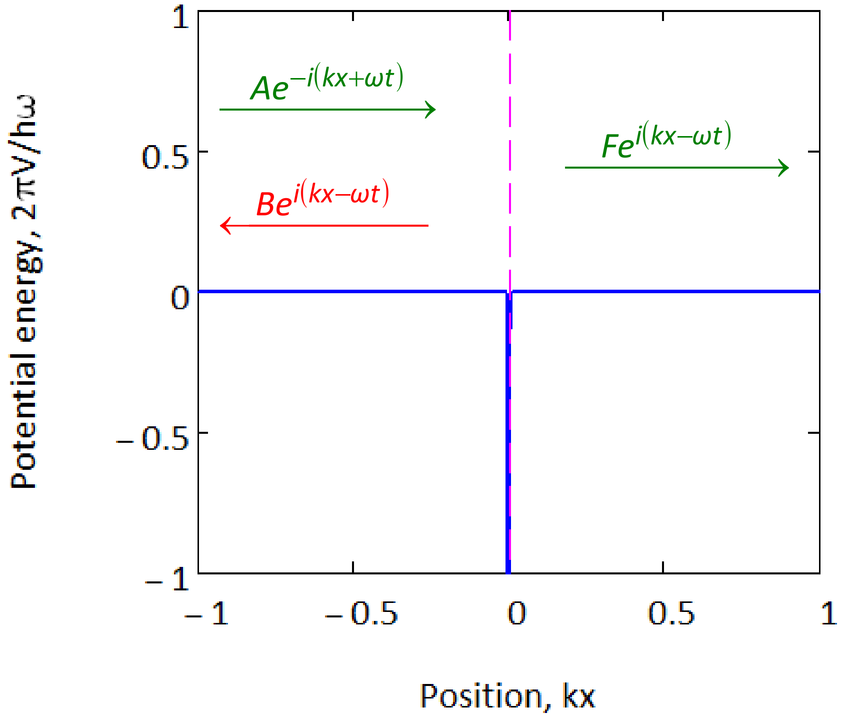
- Now we return to what we mean by scattering.
  - Suppose that we have agency: we send a wavepacket from far left ($x < 0$) toward $+x$, the same direction as component *A.*
  - It encounters the well. Its components are all subject to the same continuity conditions as above. So
    - some of it scatters toward $+x$, like component *F.*
    - some of it scatters toward $-x$, like component *B.*
    - We didn't send anything from the right, so we can take the amplitudes of all the *G*-like components to be zero.
  - What fraction *T* of the packet is transmitted, and what fraction *R* reflects?



Scattering from the delta-function well (continued)

- We would have to construct a wavefunction for the packet to find out for sure.
- But let's see what we would get if it acted like the separation solution. Let $\Psi_I(x,t)$, $\Psi_T(x,t)$, and $\Psi_R(x,t)$ be the incident, transmitted and reflected packets, and assume they behave like components A, F, and B respectively.
- Then $T = \left|\Psi_T\right|^2 / \left|\Psi_I\right|^2 = \left|F\right|^2 / \left|A\right|^2 \equiv \left|f\right|^2$ and $R = \left|\Psi_R\right|^2 / \left|\Psi_I\right|^2 = \left|B\right|^2 / \left|A\right|^2 \equiv \left|b\right|^2$. And we have just enough constraints to solve for these ratios:

$$\left.\begin{array}{l} A + B = F \quad , \quad F = A(1+2i\beta) - B(1-2i\beta) \\ \\ 1 + b = f \quad , \quad f = 1 + 2i\beta - b(1-2i\beta) \\ \\ \Rightarrow \quad b = \dfrac{i\beta}{1-i\beta} \quad , \quad f = 1 + b = \dfrac{1}{1-i\beta} \end{array}\right\} \left\{ \boxed{\begin{array}{l} T = \left|f\right|^2 = \dfrac{1}{1+\beta^2} \\ \\ R = \left|b\right|^2 = \dfrac{\beta^2}{1+\beta^2} \end{array}} \right. \begin{array}{l} , \\ \\ . \end{array}$$



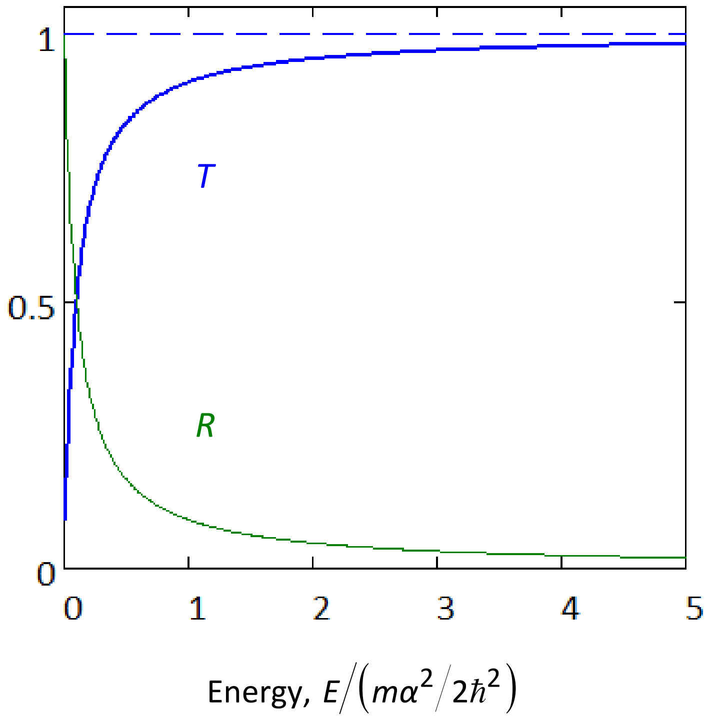
Scattering from the delta-function well (continued)

- Undo the abbreviations in favor of *m*, *α*, and *E*:

$$\boxed{T=\frac{1}{1+m\alpha^2/2\hbar^2E}}\ ,\ \boxed{R=\frac{m\alpha^2/2\hbar^2E}{1+m\alpha^2/2\hbar^2E}}=\frac{1}{1+2\hbar^2E/m\alpha^2}\quad .$$

- Note that *T* + *R* = 1: the "packet" is certain either to scatter forward or to scatter backward.

- Note also that $\lim_{E\to\infty} T=1$ and $\lim_{E\to\infty} R=0$; also that $\lim_{\alpha\to\infty} T=0$ and $\lim_{\alpha\to\infty} R=1.$

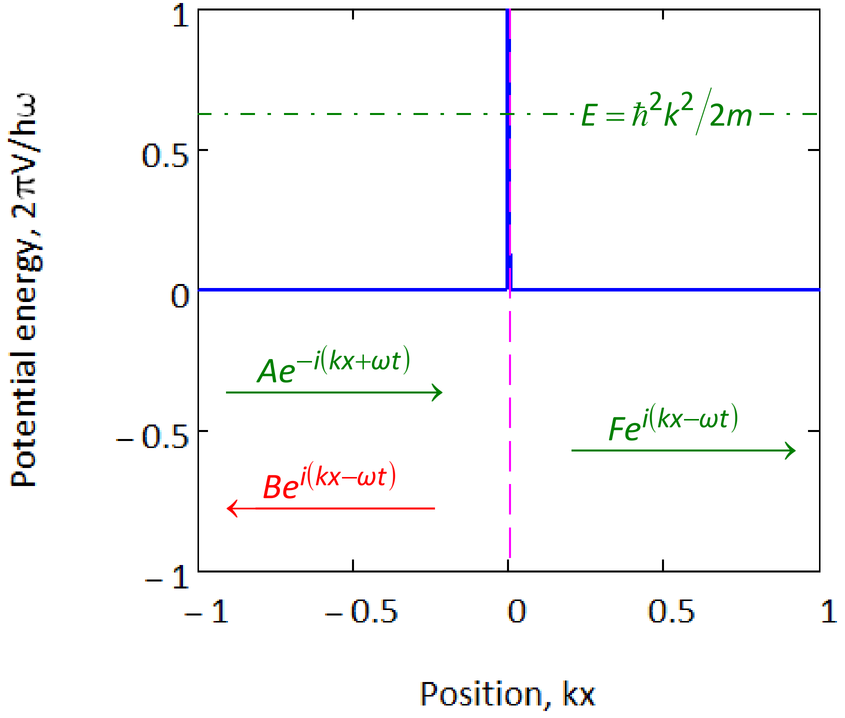


Scattering from the delta-function barrier: tunnelling

Now change the sign of the potential: $V(x)=-\alpha\delta(x), \quad \alpha\boxed{\overset{!}{<}}0 \quad .$

- This does away with the bound state: such states have $E < 0$, but no such state can have E less than the minimum of V (G&S problems 2.2 and 2.3, on problem set 2).
- But because the results we just got depend on α^2, not α, T and R are the same for the barrier as they are for the well.
- So, as unlikely as it sounds from our classical-physics experience, a wavepacket can **tunnel** through an infinite potential-energy barrier.
  - Maybe even more unlikely-sounding, the packet can overcome an infinite force, too (see page 3):

$$F=-\left.\frac{dV}{dx}\right|_{-\varepsilon}=+\left.\frac{-\alpha\delta(x)}{x}\right|_{-\varepsilon}\xrightarrow[\varepsilon\to 0]{}-\infty \quad .$$

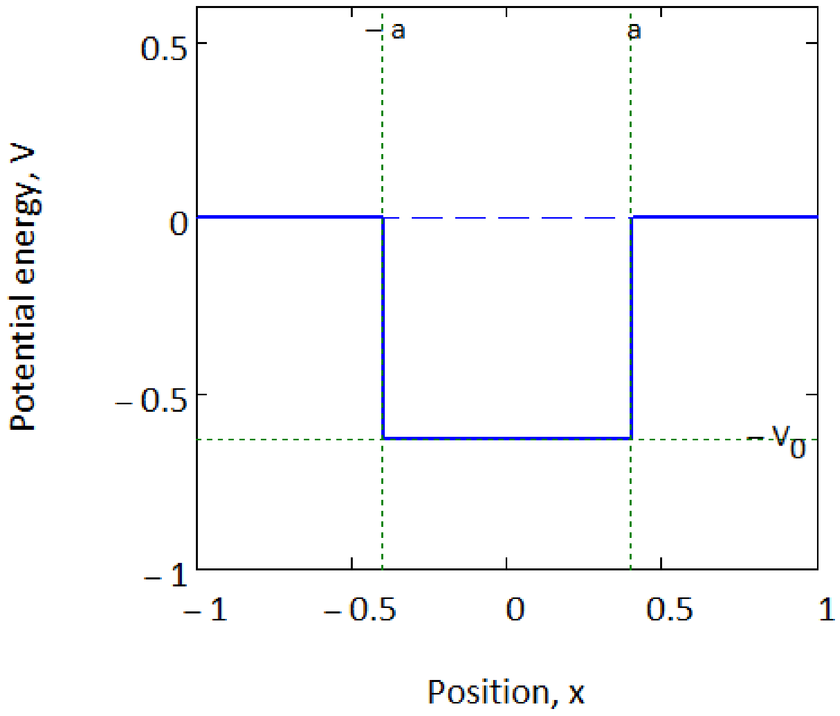


The finite square well

Our last 1-D Schrödinger-equation solution for a while:

$$V(x) = -V_0 \quad , \quad -a \le x \le a \quad , \quad = 0 \quad \text{otherwise.}$$

- This also has bound states with E = < 0 and scattering states with E > 0.
- The scattering states are constrained by continuity of ψ and $d\psi/dx$ at two boundaries instead of one.
- The bound states are constrained by boundary conditions in a way similar to the infinite square well. But not similar enough to give that sort of simplicity: one can't take ψ to be zero outside the well's edge, and this makes the problem analytical intractable.
- Since a solution takes so much writing and algebra, without any new principles introduced, we will only outline the solution. You'll get enough practice in how the solution works (G&S problem 2.32).



The finite square well: bound states

- Energies of the bound states must lie between $E = 0$ and $-V_0$. The time-independent Schrödinger equation for these is

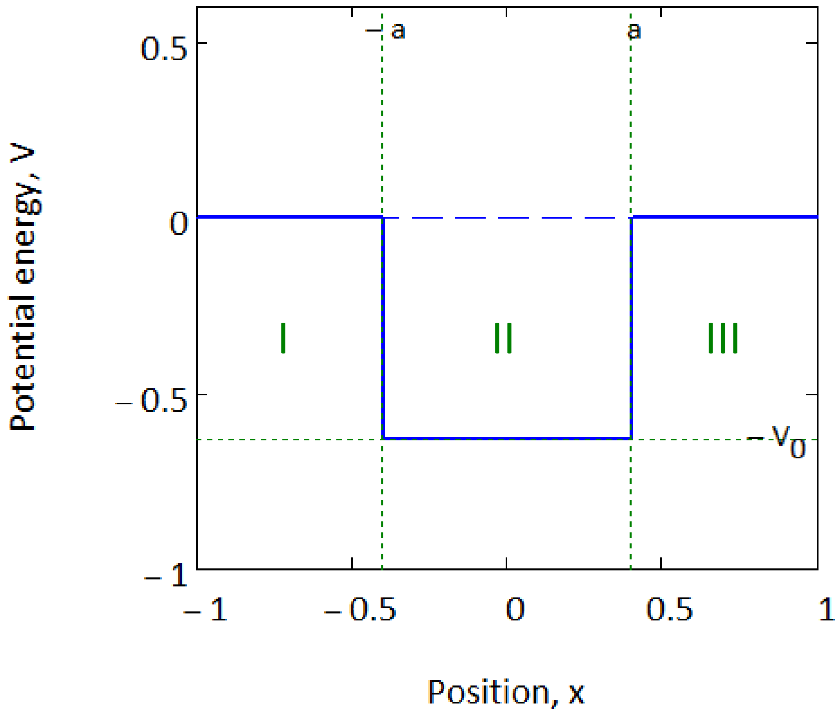
$$\frac{d^2\psi}{dx^2} - \kappa^2\psi = 0 \quad , \quad \kappa = \frac{\sqrt{-2mE}}{\hbar} \quad (\mathrm{I}, \mathrm{III});$$

$$\frac{d^2\psi}{dx^2} + \ell^2\psi = 0 \quad , \quad \ell = \frac{\sqrt{2m(E+V_0)}}{\hbar} \quad (\mathrm{II}).$$

- Set to zero the amplitudes of terms that would blow up as $x \to \pm\infty$ (page 5). The bound-state problem is symmetric about $x = 0$, so $\psi(x) = \psi(-x)$; only one boundary needs to be considered:

$$\psi(x) = D\cos\ell x \quad (\mathrm{II}), \quad Fe^{-\kappa x} \quad (\mathrm{III}) \quad .$$

Imposing continuity of ψ and $d\psi/dx$ leads to a **transcendental** equation for the quantized energy: $\kappa^2 = \ell^2 \tan^2 \ell a$, which as usual can only be solved numerically or graphically (G&S page 72).

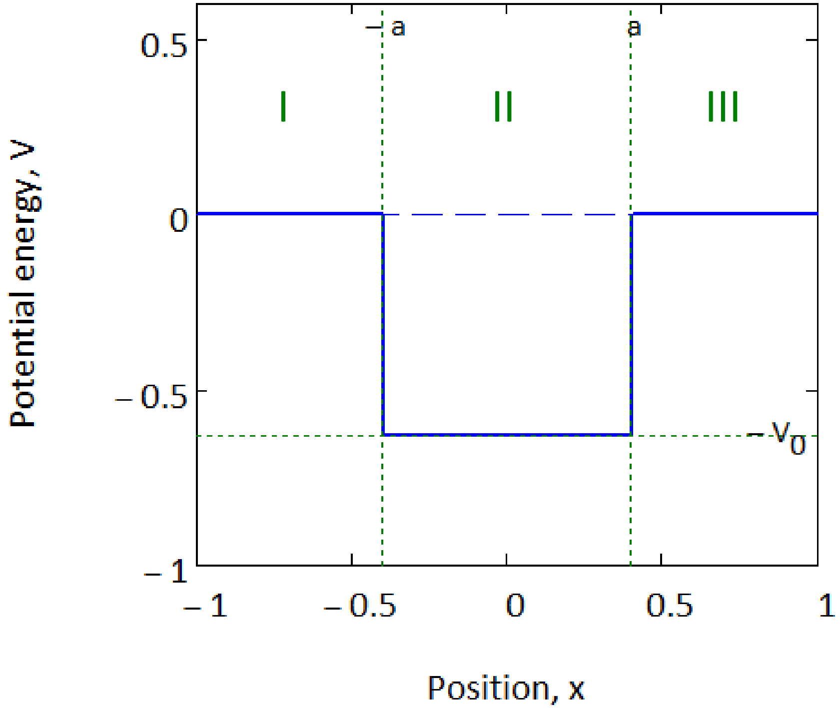


The finite square well: scattering states

- And for the scattering states ($E > 0$),

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad , \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (\mathrm{I, III});$$

$$\frac{d^2\psi}{dx^2} + \ell^2\psi = 0 \quad , \quad \ell = \frac{\sqrt{2m\left(E + V_0\right)}}{\hbar} \quad (\mathrm{II}).$$



- No solutions blow up as $x \to \pm\infty$ (page 5); let's at least suppose that there's no incident wavepacket from region III:

$$\psi(x) = Ae^{-ikx} + Be^{ikx} \quad (\mathrm{I}), \quad C\sin\ell x + D\cos\ell x \quad (\mathrm{II}), \quad Fe^{ikx} \quad (\mathrm{III}) \quad .$$

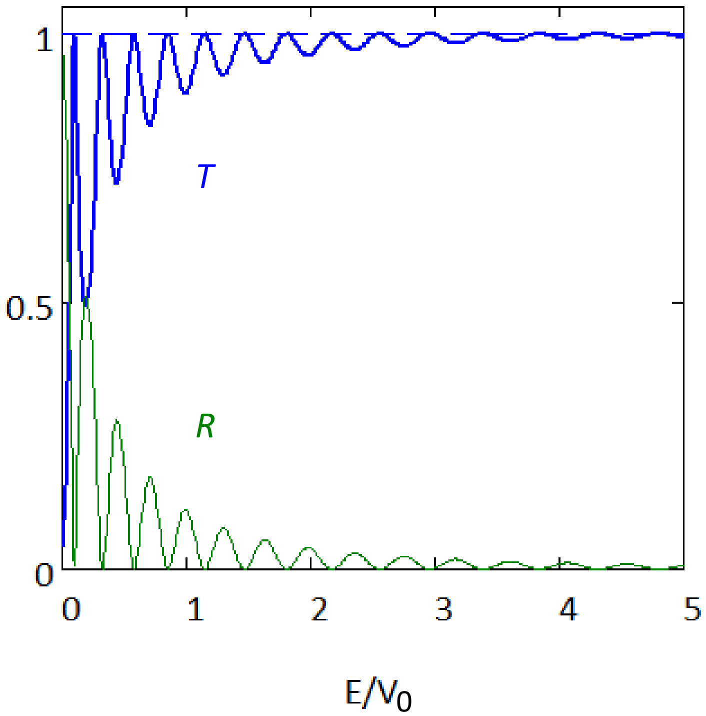
Trig functions are used in region II because it is finite in length, so the boundary conditions are anticipated to produce quantization.

The finite square well: scattering states (continued)

- Applying continuity of ψ and $d\psi/dx$ give four equations, in five unknowns not counting *E.*
- But, as for the δ-function well, this is enough to solve for the transmission and reflection coefficients:

$$\boxed{\begin{aligned} T &= \frac{1}{1+\dfrac{V_0^2}{4E(E+V_0)}\sin^2\left(\dfrac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)} \\ R &= \frac{\dfrac{V_0^2}{4E(E+V_0)}\sin^2\left(\dfrac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}{1+\dfrac{V_0^2}{4E(E+V_0)}\sin^2\left(\dfrac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)} \end{aligned}}$$

- $T = 1$ when $\boxed{E_n + V_0 = n^2\pi^2\hbar^2/8ma^2}$: comfortingly, the same as in the infinite square well (Lecture 4; note that 2*a* here is *a* there).



Quantum interference!
Compare page 17.