Quantum Mechanics I

Quantum Mechanics

The Schrödinger Equation:

Piecewise Constant Potentials

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Pink Floyd: "Another Brick in the Wall (Pt. II)"

Piecewise Constant Potentials

Reminder

- Consider the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = H\Psi(\vec{r},t) \qquad H = -\tfrac{\hbar^2}{2M}\vec{\nabla}^2 + W(\vec{r})$$

- Use stationary states

$$\Psi(\vec{r},t) = e^{-iEt/\hbar}\,\psi_E(\vec{r}) \qquad \big[-\tfrac{\hbar^2}{2M}\vec{\nabla}^2 + W(\vec{r})\big]\psi_E(\vec{r}) = E\,\psi_E(\vec{r})$$

- Reduce to 1-dimensional space

$$k(x) := \frac{\sqrt{2M[E-W(x)]}}{\hbar} \qquad \psi_E''(x) + \underbrace{\tfrac{2M}{\hbar^2}[E-W(x)]}_{:=[k(x)]^2}\psi_E(x) = 0$$

- With the $W(x)$ constant in some region, so is $k(x)$:

$$\begin{aligned}\psi(x) &= A\sin(kx) + B\cos(kx) &&= A'\sinh(\kappa x) + B'\cosh(\kappa x)\\ &= C_+e^{+ikx} + C_-e^{-ikx} &&= C_+e^{+\kappa x} + C_-e^{-\kappa x}\\ &= N\sin(kx+\delta) && \kappa := ik\end{aligned}$$

oscillatory

non-oscillatory

Piecewise Constant Potentials

Reminder & a 2nd Look

$$\psi''_E(x) + \frac{2M}{\hbar^2}[E - W(x)]\,\psi_E(x) = 0$$

- Orthogonality and normalizability:

$$\int_{\text{all space}} \mathrm{d}x\, \psi^*_{E'}(x)\,\psi_E(x) = 0 \quad \text{if } E' \neq E$$

if $E' = E$, normalize

  - ...depending on the energy spectrum:

$$\int_{\text{all space}} \mathrm{d}x\, \psi^*_{E'}(x)\,\psi_E(x) = \begin{cases} \delta_{E',E} & \text{if } E \text{ is discrete,} \\ \delta(E'-E) & \text{if } E \text{ is continuous.} \end{cases}$$

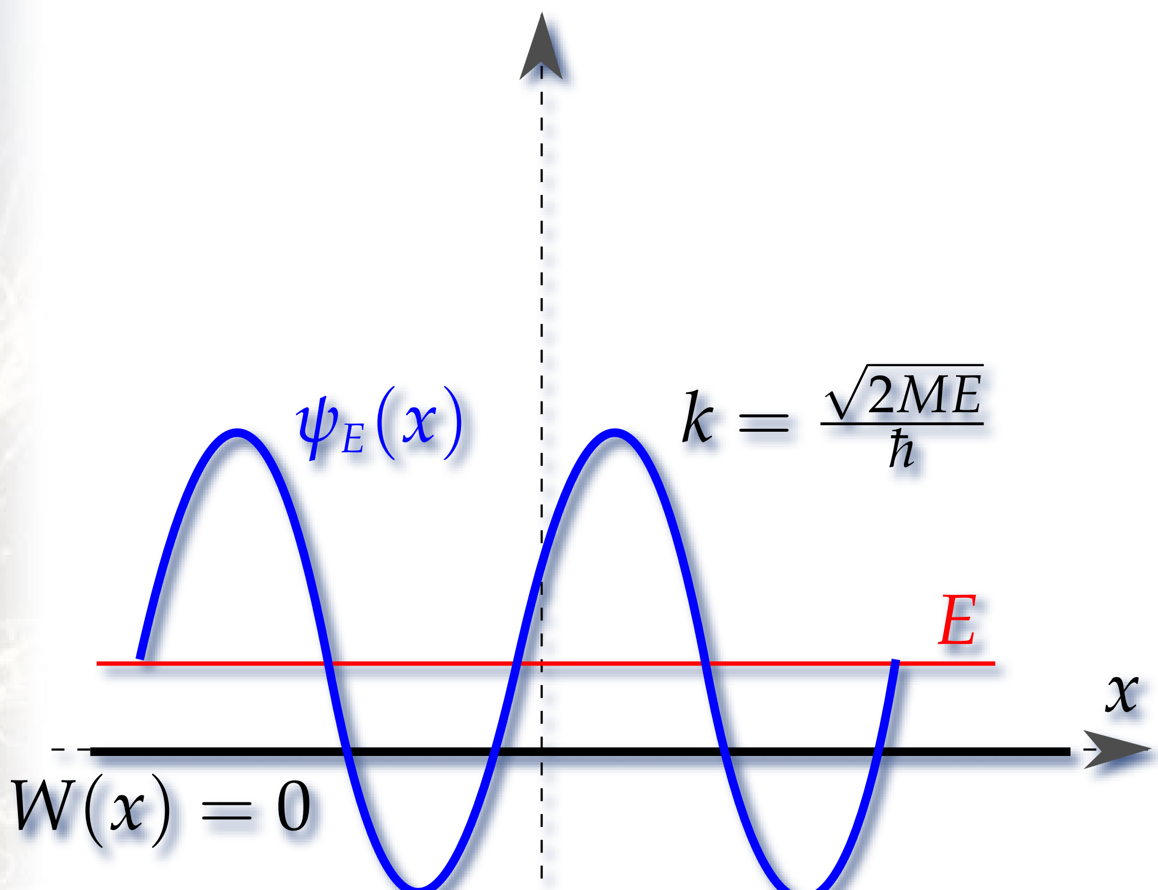
- Matching conditions
  - Everywhere continuous: $\Delta\psi_E(x) := \lim_{\epsilon\to 0}[\psi_E(x+\epsilon) - \psi_E(x-\epsilon)] = 0$
  - Unless $W(x)$ crosses E continuously*,
  - Wherever $\Delta W(x) < \infty$, $\quad \Delta\psi'_E(x) = 0$
  - Where $W(x) = w(x) + \lambda\,\delta(x-a)$, $\quad \Delta\psi'_E(x) = \frac{2M\lambda}{\hbar^2}\psi_E(a)$
  - Where $W(x) = \infty$, for $x \in [a,b]$, $\quad \psi_E(x) = 0,\ \ \psi'_E(x)$ free

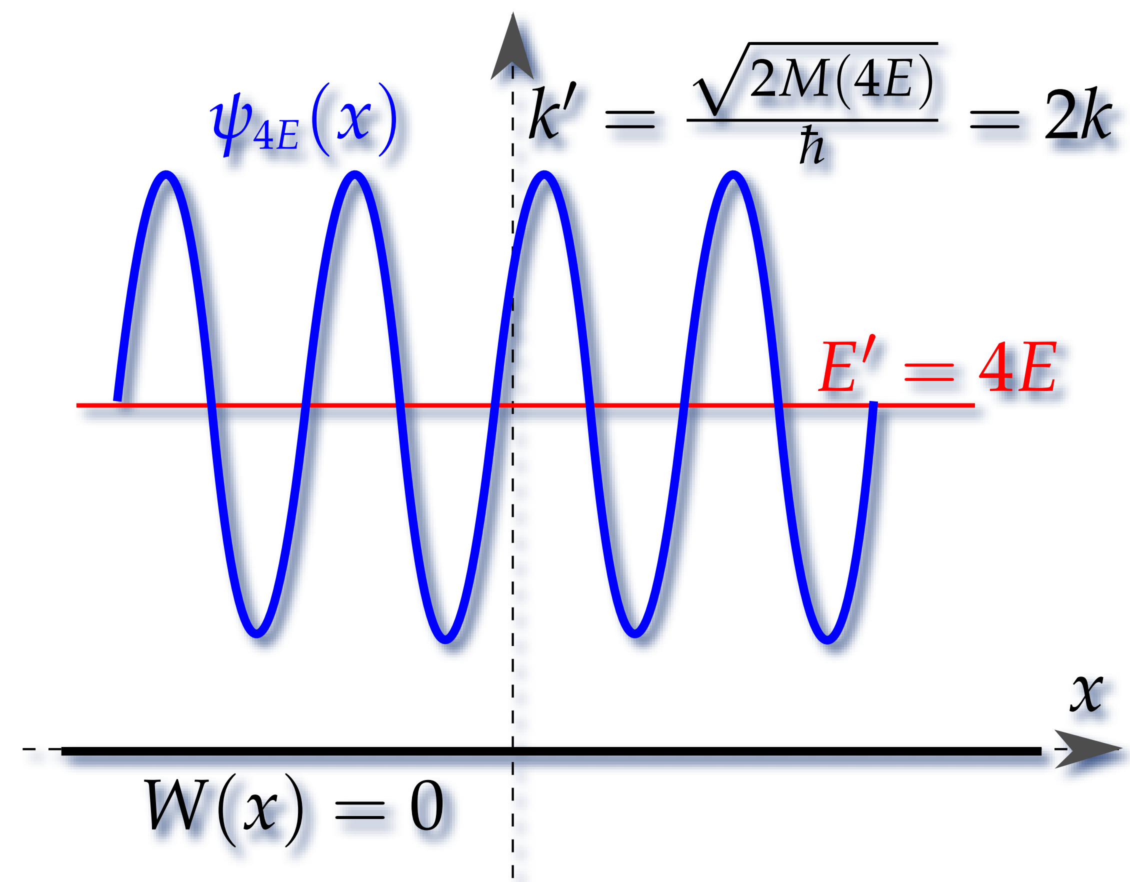
* I'll be back

Piecewise Constant Potentials

A Few Pointers...

- Sketch: x horizontally, $W(x)$ vertically w/E as a reference



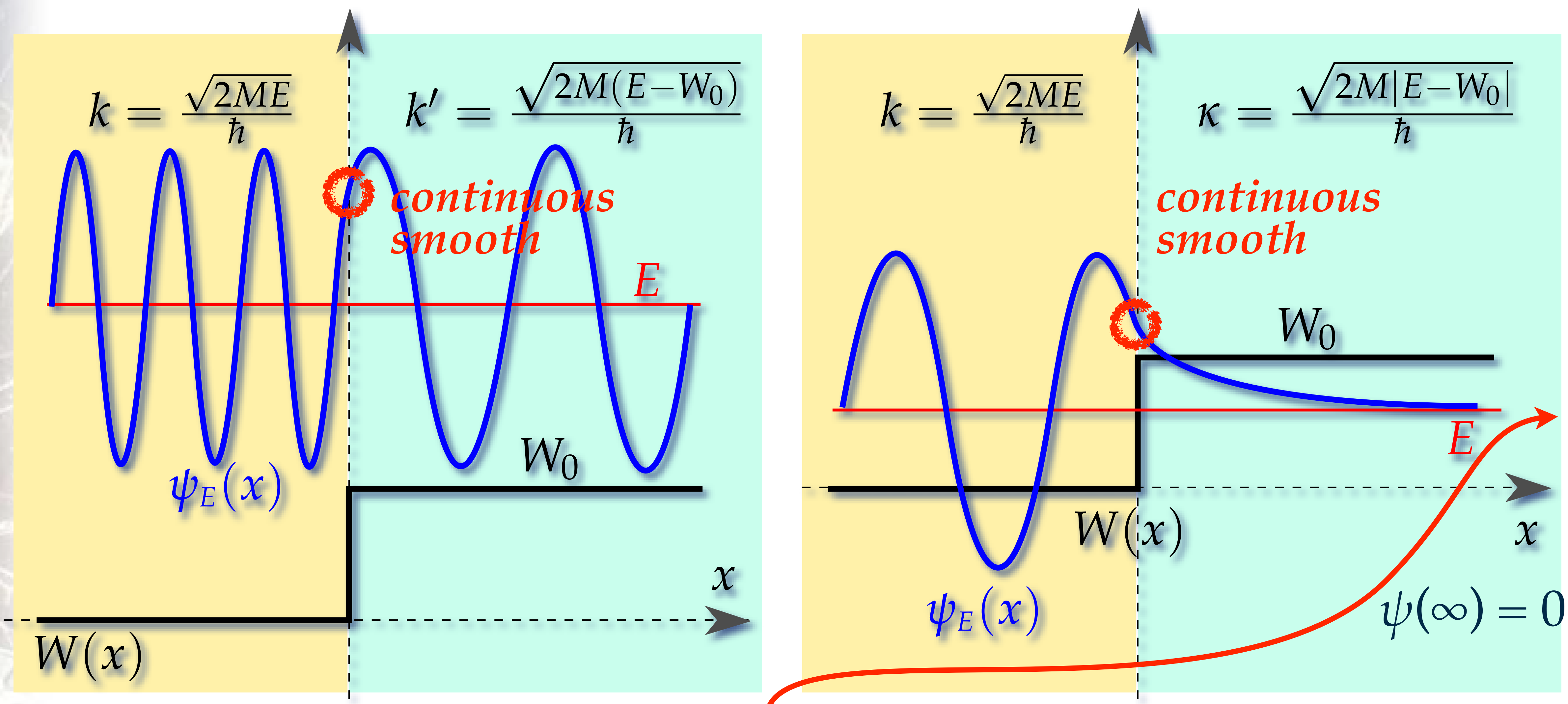


- Use the E-level as the horizontal axis for $\psi_E(x)$
- Solutions are oscillatory since $E - W(x) > 0$, and k is real
- The wave-number grows with the square-root of $E - W(x)$

Piecewise Constant Potentials

A Potential Step: Sketch

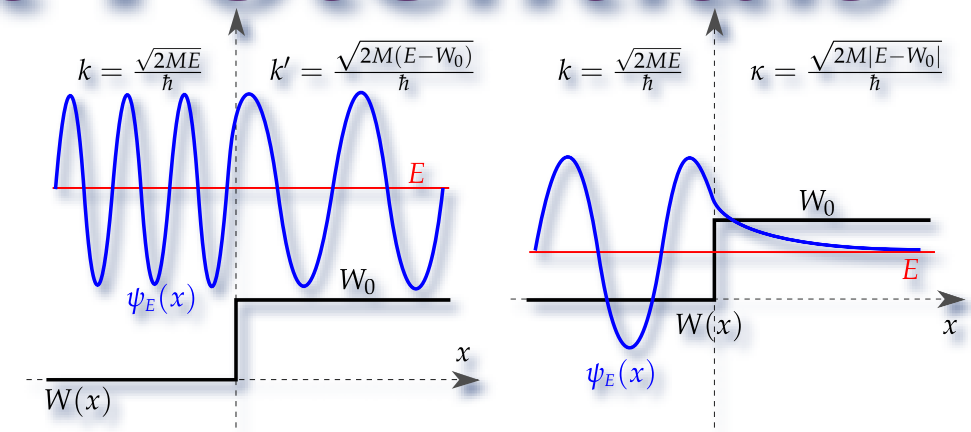
- The step function: $W(x)=0$ for $x<0$, $W(x)=W_0>0$ for $x>0$
  - Region I: $x\in(-\infty,0)$, and region II: $x\in(0,+\infty)$



- Matching: @ $x=0$, and @ $x\to\infty$ only if $E<W_0$.

Piecewise Constant Potentials

A Potential Step



- Now, do the math; $E > W_0$, using standard solutions:

$$\psi_I(x) = N\sin(kx+\delta) \qquad \psi_{II}(x) = N'\sin(k'x+\delta')$$

$$N\sin(\delta) = \psi_I(0) \stackrel{!}{=} \psi_{II}(0) = N'\sin(\delta') \qquad \text{continuity}$$

$$kN\cos(\delta) = \psi_I'(0) \stackrel{!}{=} \psi_{II}'(0) = k'N'\cos(\delta') \qquad \text{smoothness}$$

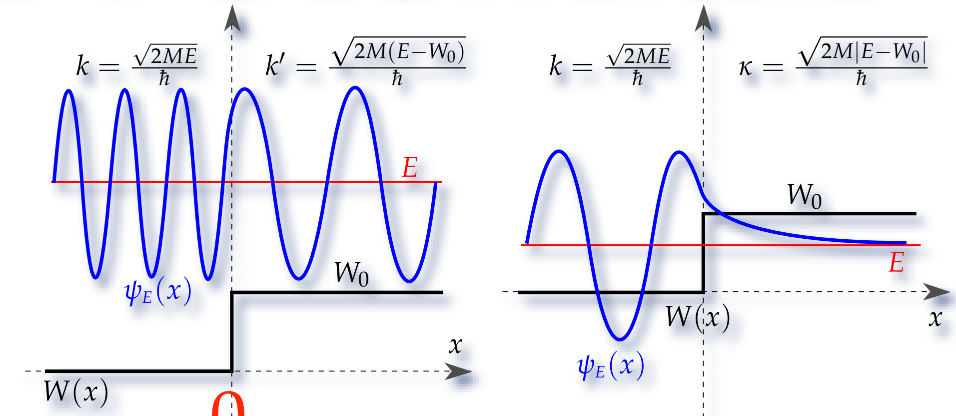
- Solve:

$$N' = N\frac{\sqrt{k^2\cos^2(\delta)+k'^2\sin^2(\delta)}}{k'} \qquad \delta' = \tan^{-1}\left(\tfrac{k'}{k}\tan(\delta)\right) + 2n\pi$$

  - Two conditions leave two integration constants, N and δ
  - N is fixed by normalization; δ and E are free & continuous
  - Continuous (unquantized!) energy is a hallmark of quantum scattering states (freely oscillate in all allowed directions)
  - The dependence on E is convoluted, through k and k'

Piecewise Constant Potentials

A Potential Step



- Now, do the math; $0 < E < W_0$, using standard solutions:

$$\psi_I(x) = N\sin(kx+\delta) \qquad \psi_{II}(x) = \underbrace{C_+}_{\text{diverges};\ \to 0} e^{+\kappa x} + \underbrace{C_-}_{\text{keep}} e^{-\kappa x}$$

$$N\sin(\delta) = \psi_I(0) \stackrel{!}{=} \psi_{II}(0) = C_-\cdot 1 \qquad C_- = \frac{kN}{\sqrt{k^2+\kappa^2}}$$

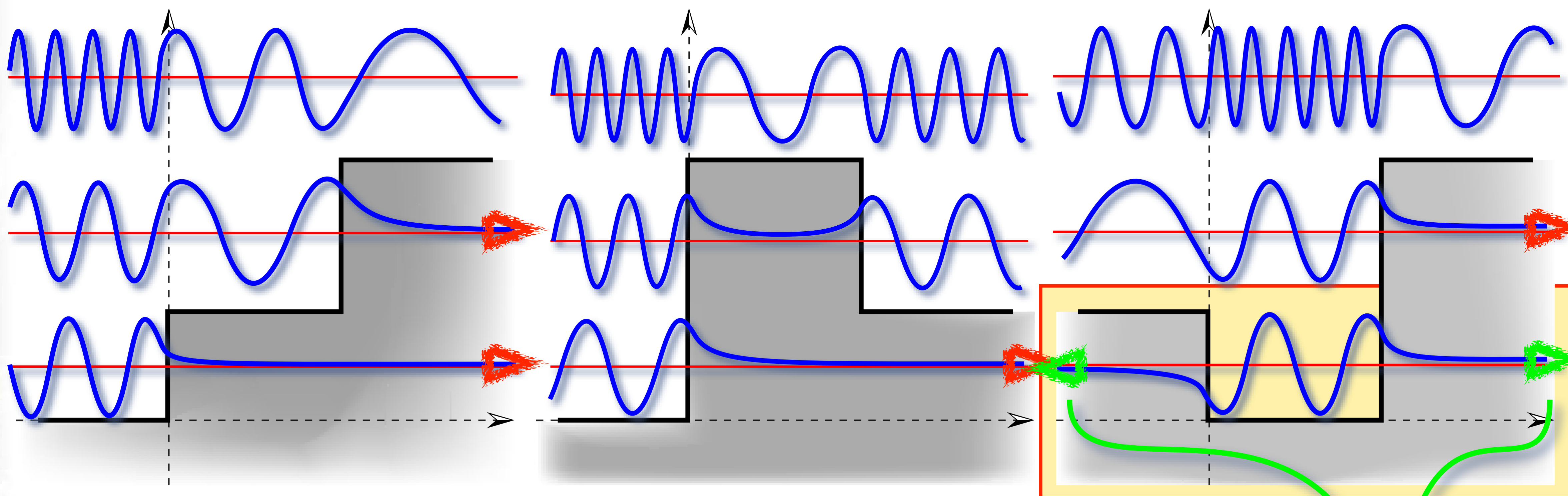
$$kN\cos(\delta) = \psi_I'(0) \stackrel{!}{=} \psi_{II}'(0) = -\kappa C_-\cdot 1 \qquad \delta = \tan\left(\frac{k}{\kappa}\right) + 2n\pi$$

- Three conditions leave only one integration constant, N,
- which is fixed by normalization; E is free & continuous
- though now the phase δ did become fixed
- Continuous (unquantized!) energy is a hallmark of quantum scattering states (freely oscillate in all allowed directions)
- The dependence on E is convoluted, through k and k'
- $1/\kappa$ is called the "skin depth": the system penetrates the step

Piecewise Constant Potentials

Two Potential Steps: Sketch

- Repeat the previous analysis in two steps
  - Three radically different situations

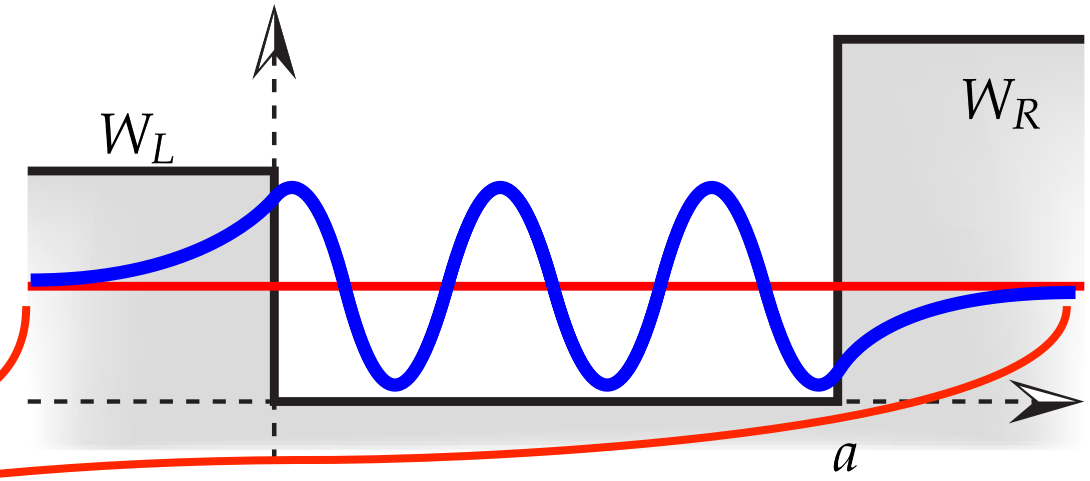


  - Inter-region matching (cont's+smooth) leaves two constants
  - Normalization fixes one constant (amplitude)
  - Each B.C. @ ∞ (normalizability) fixes a constant } free E
  - The lower-right case has "one too many conditions" fixes E

Piecewise Constant Potentials

Potential Well

- Do the math; $0 < E < \min(W_L, W_R)$ using standard solutions:



$$\psi_I(x) = C_+ e^{+\kappa x} + C_- e^{-\kappa x} \qquad \kappa = \sqrt{2M|E-W_L|}/\hbar$$

($C_- = 0$)

$$\psi_{II}(x) = A\cos(kx) + B\sin(kx) \qquad k = \sqrt{2ME}/\hbar$$

$$\psi_{III}(x) = D_+ e^{+\varkappa x} + D_- e^{-\varkappa x} \qquad \varkappa = \sqrt{2M|E-W_R|}/\hbar$$

($D_+ = 0$)

- Matching:

$$c := \cos(ka) \qquad s := \sin(ka)$$

$$0 \stackrel{!}{=} [A\cos(0)+B\sin(0)] - [C_+ e^0]$$

$$0 \stackrel{!}{=} [-kA\sin(0)+kB\cos(0)] - [\kappa C_+ e^0]$$

$$0 \stackrel{!}{=} [D_- e^{-\varkappa a}] - [A\cos(ka)+B\sin(ka)]$$

$$0 \stackrel{!}{=} [-\varkappa D_- e^{-\varkappa a}] - [-kA\sin(ka)+kB\cos(ka)]$$

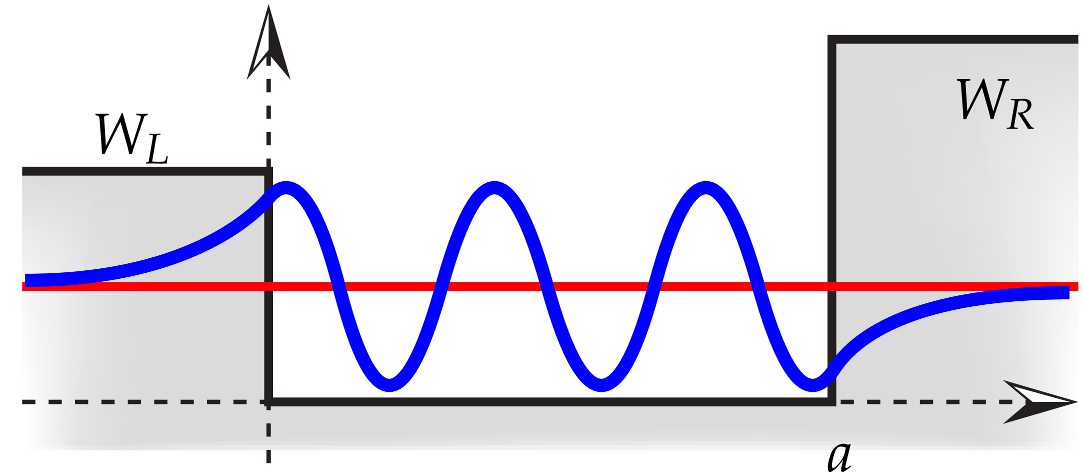
$$0 = \underbrace{\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\kappa & 0 & k & 0 \\ 0 & -c & -s & e^{-\varkappa a} \\ 0 & ks & -kc & -\varkappa e^{-\varkappa a} \end{bmatrix}}_{\det=0} \begin{bmatrix} C_+ \\ A \\ B \\ D_- \end{bmatrix}$$

A condition on E only

Piecewise Constant Potentials

Potential Well

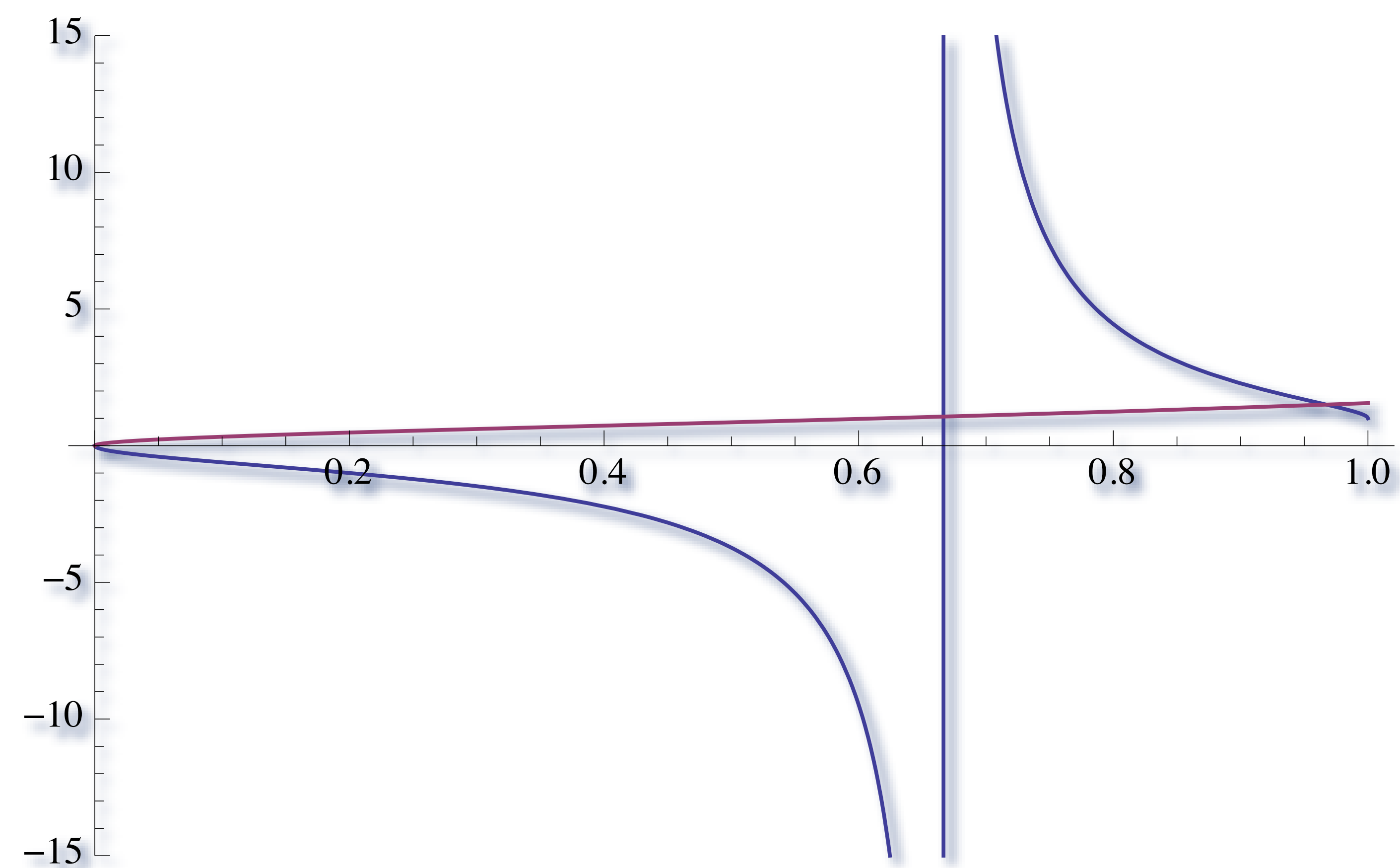
- The det=0 condition gives



$$\tan(k\,a) = \frac{k(\kappa + \varkappa)}{k^2 - \kappa\varkappa}$$

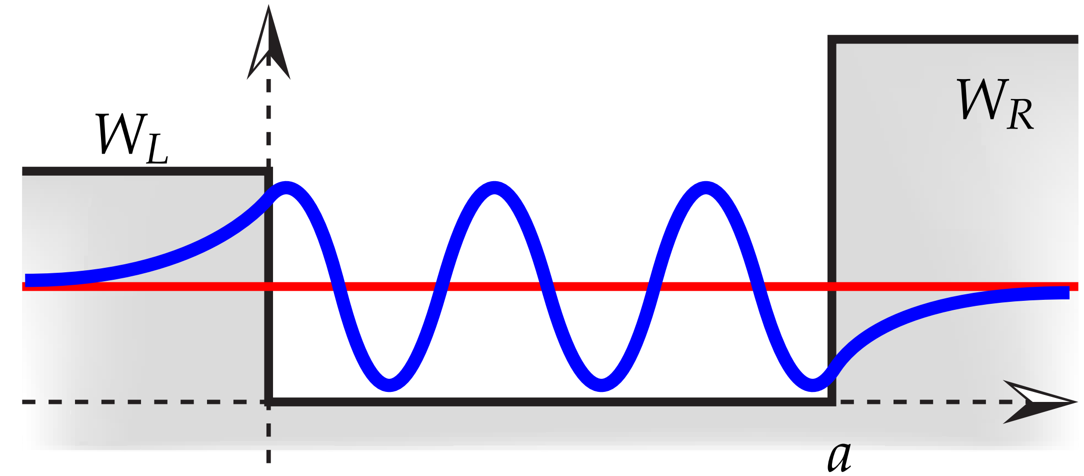
$$\tan\left(\frac{\sqrt{2ME}\,a}{\hbar}\right) = \frac{\sqrt{ME}\left[\sqrt{M(W_L-E)}+\sqrt{M(W_R-E)}\,\right]}{ME-\sqrt{M(W_L-E)}\sqrt{M(W_R-E)}}$$

- This cannot be solved analytically
- ...but graphically + numerically



Piecewise Constant Potentials

Potential Well



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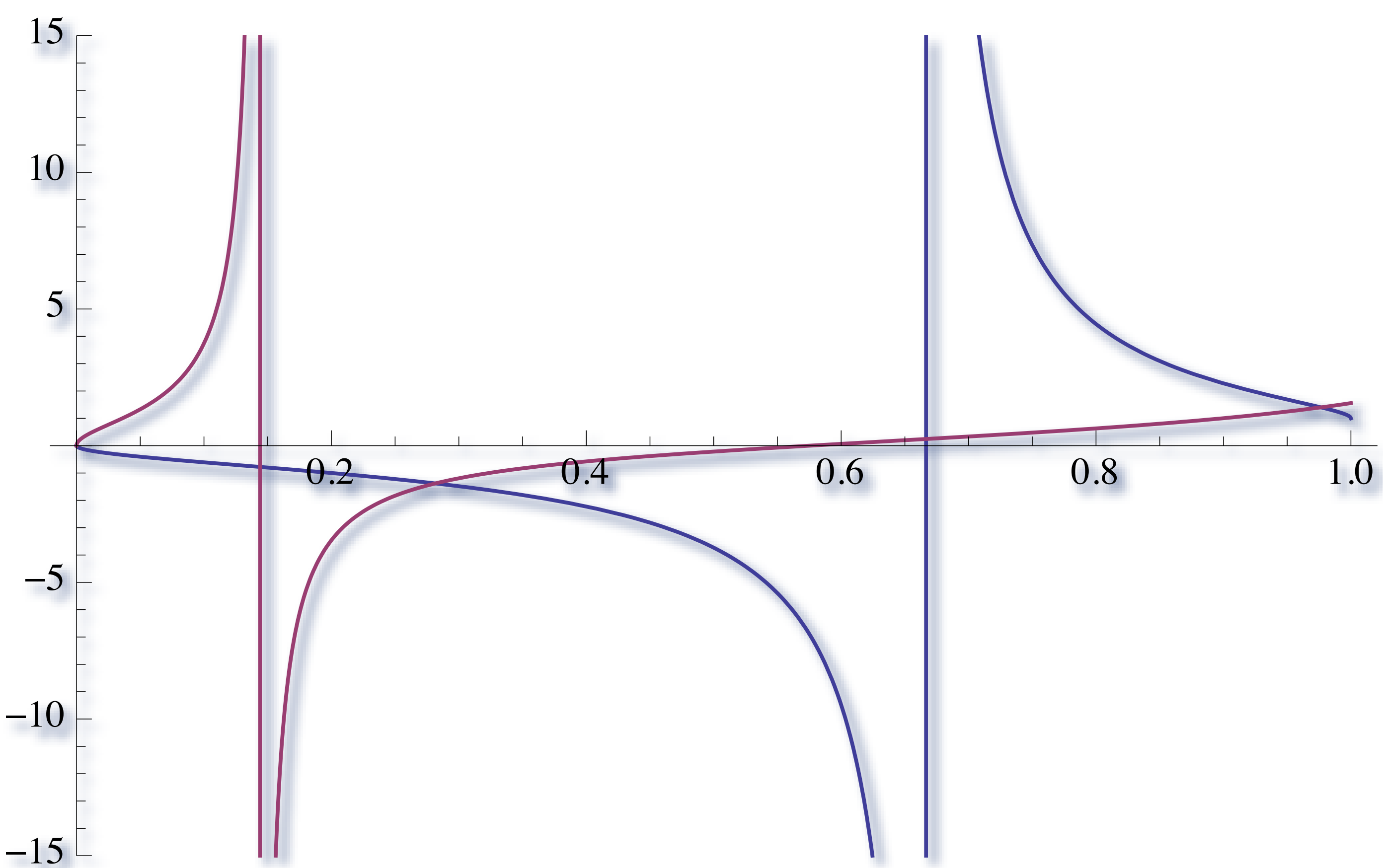
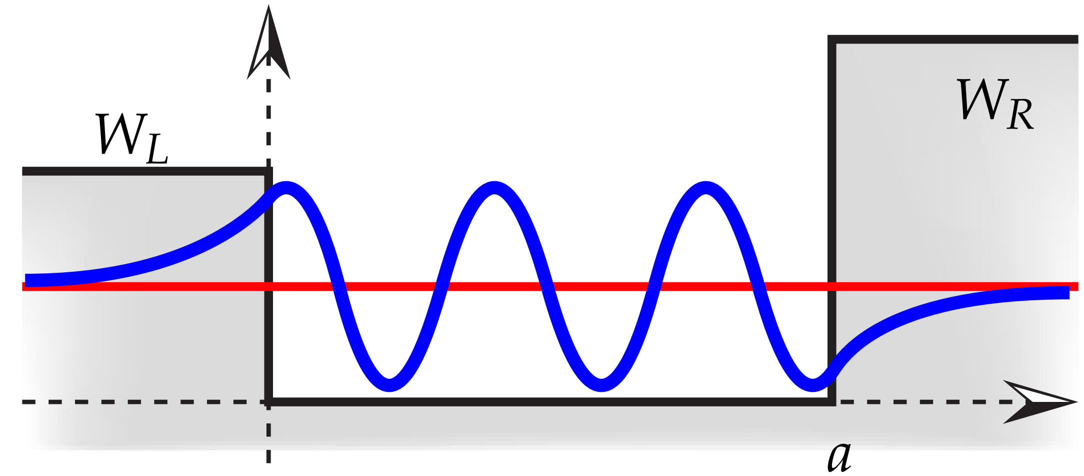


Piecewise Constant Potentials

Potential Well



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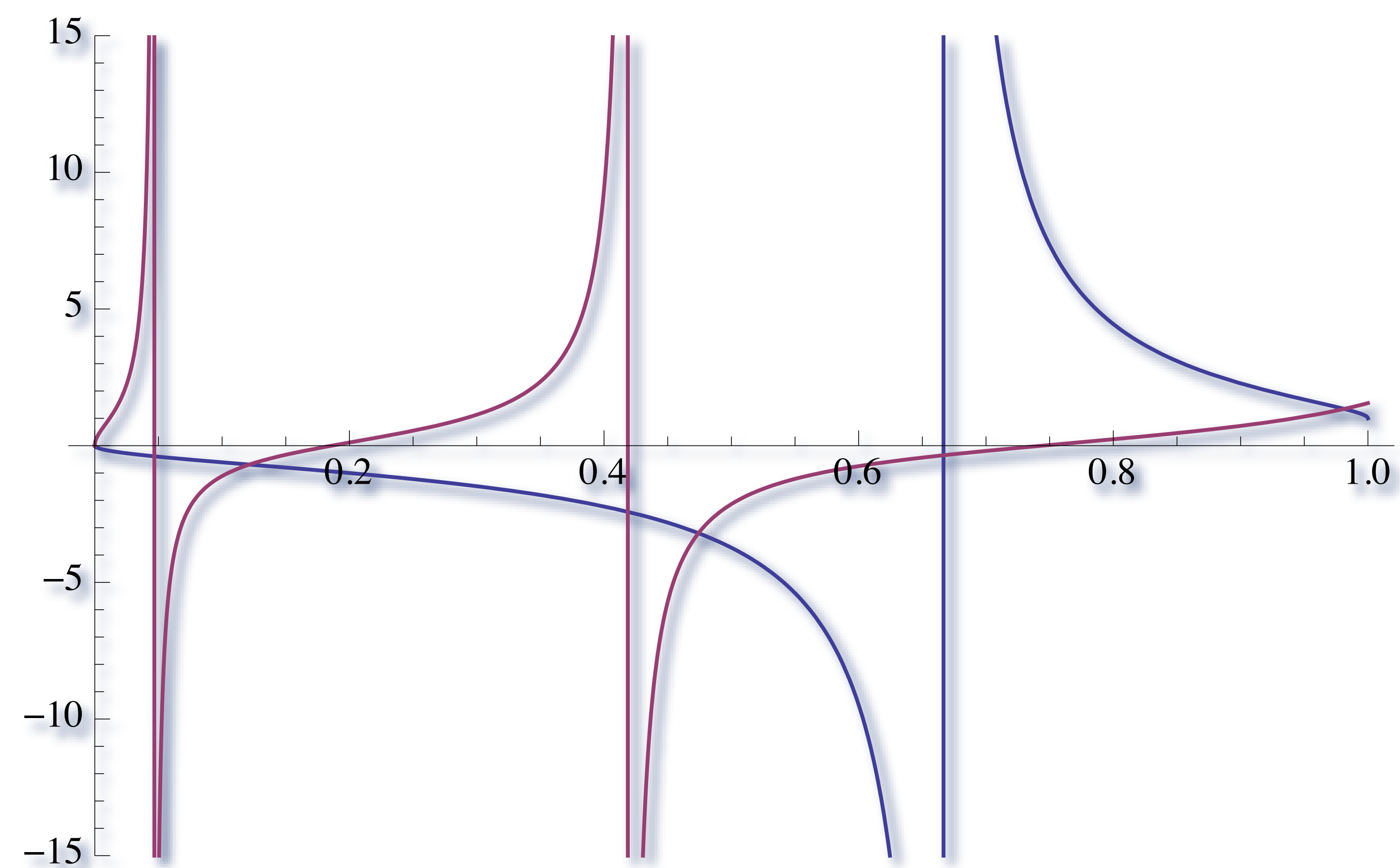
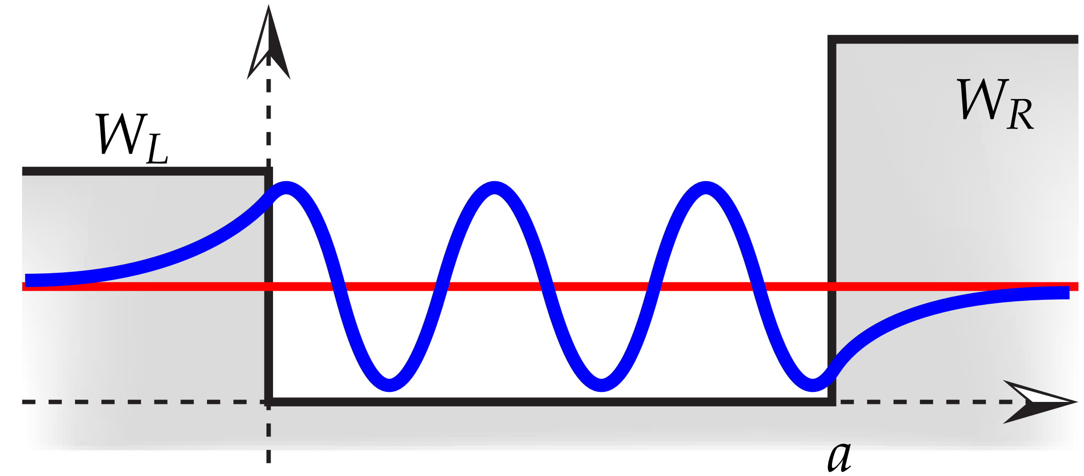


Piecewise Constant Potentials

Potential Well



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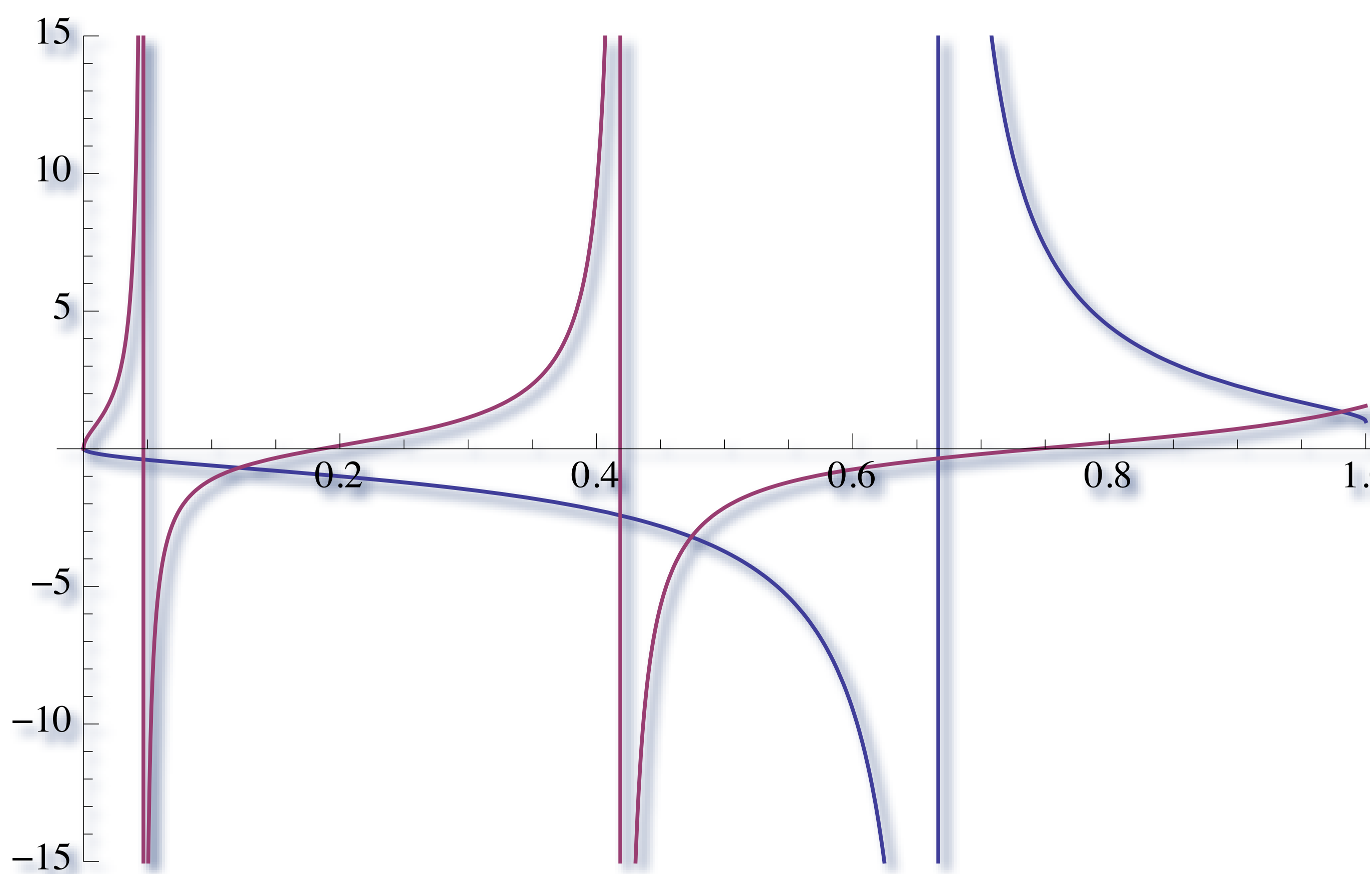
- This cannot be solved analytically
- ...but graphically + numerically
- Lift $W_R \to \infty$:

$$\tan\left(\frac{\sqrt{2ME}\,a}{\hbar}\right) = -\sqrt{\frac{E}{W_L - E}}$$

- Lift also $W_L \to \infty$:

$$\tan\left(\frac{\sqrt{2ME}\,a}{\hbar}\right) = 0 \qquad E_n = \frac{n^2\pi^2\hbar^2}{2M\,a^2}$$



Quantum Mechanics I

Now, go forth and calculate!!

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