Lecture 2

Quantum mechanics in one dimension

Quantum mechanics in one dimension

- Schrödinger equation for **non-relativistic quantum particle**:

$$i\hbar\partial_t\Psi(\mathbf{r}, t) = \hat{H}\Psi(\mathbf{r}, t)$$

where $\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})$ denotes quantum Hamiltonian.

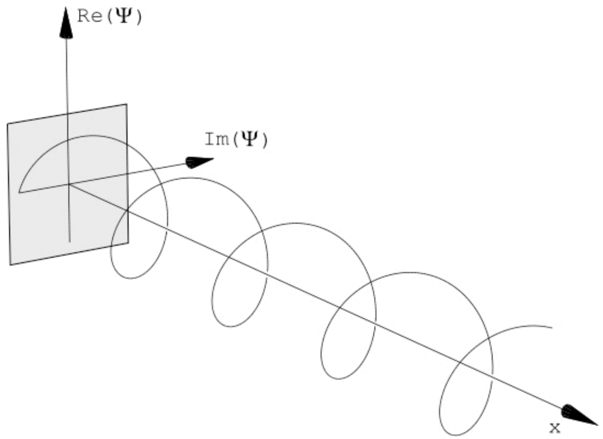
- To acquire intuition into general properties, we will review some simple and familiar(?) applications to one-dimensional systems.

- Divide consideration between potentials, $V(x)$, which leave particle free (i.e. unbound), and those that bind particle.

Quantum mechanics in 1d: Outline

1. Unbound states
   - Free particle
   - Potential step
   - Potential barrier
   - Rectangular potential well
2. Bound states
   - Rectangular potential well (continued)
   - δ-function potential
3. Beyond local potentials
   - Kronig-Penney model of a crystal
   - Anderson localization

Unbound particles: free particle



$$i\hbar\partial_t\Psi(x,t) = -\frac{\hbar^2\partial_x^2}{2m}\Psi(x,t)$$

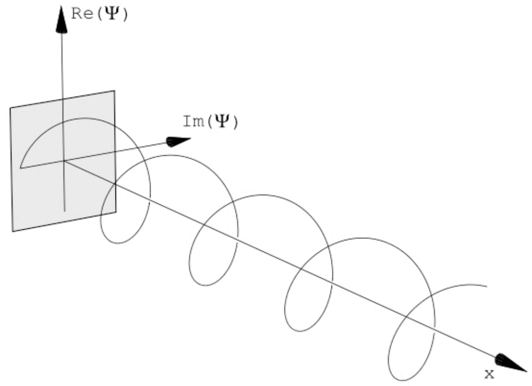
- For $V = 0$ Schrödinger equation describes travelling waves.

$$\Psi(x,t) = A\,e^{i(kx-\omega t)}, \qquad E(k) = \hbar\omega(k) = \frac{\hbar^2 k^2}{2m}$$

  where $k = \frac{2\pi}{\lambda}$ with λ the wavelength; momentum $p = \hbar k = \frac{h}{\lambda}$.

- Spectrum is continuous, semi-infinite and, apart from $k = 0$, has two-fold degeneracy (right and left moving particles).

Unbound particles: free particle



$$i\hbar\partial_t\Psi(x,t) = -\frac{\hbar^2\partial_x^2}{2m}\Psi(x,t) \qquad \Psi(x,t) = A\, e^{i(kx-\omega t)}$$

- For infinite system, it makes no sense to fix wave function amplitude, A, by normalization of total probability.
- Instead, fix particle flux: $j = -\dfrac{\hbar}{2m}\left(i\Psi^*\partial_x\Psi + \text{c.c.}\right)$

$$j = |A|^2\frac{\hbar k}{m} = |A|^2\frac{p}{m}$$

- Note that definition of j follows from continuity relation,

$$\partial_t|\Psi|^2 = -\nabla\cdot\mathbf{j}$$

Preparing a wave packet

- To prepare a **localized** wave packet, we can superpose components of different wave number (cf. Fourier expansion),

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k)\, e^{ikx}\, dk$$

where Fourier elements set by

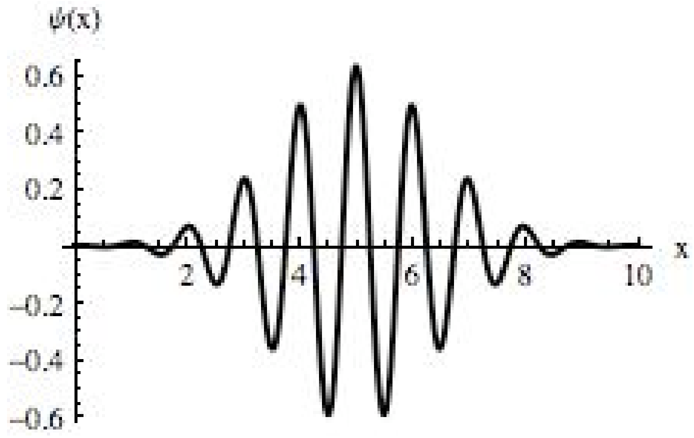
$$\psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx\,.$$

- Normalization of $\psi(k)$ follows from that of $\psi(x)$:

$$\int_{-\infty}^{\infty} \psi^*(k)\psi(k)dk = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$$

- Both $|\psi(x)|^2 dx$ and $|\psi(k)|^2 dk$ represent probabilities densities.

Preparing a wave packet: example



- The Fourier transform of a normalized Gaussian wave packet,

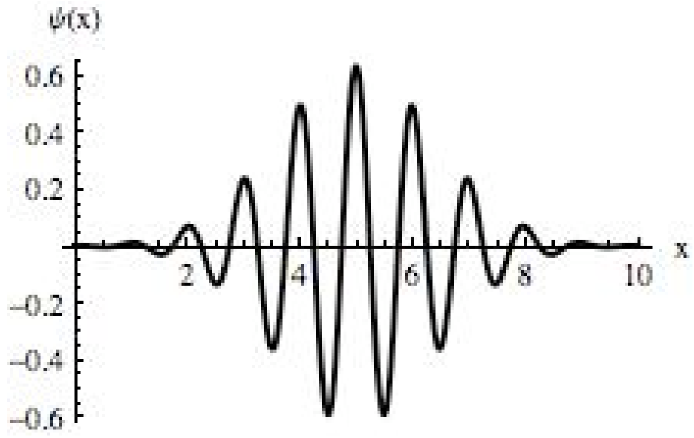
$$\psi(x) = \left(\frac{1}{2\pi\alpha}\right)^{1/4} e^{ik_0 x} e^{-\frac{x^2}{4\alpha}} .$$

  (moving at velocity $v = \hbar k_0/m$) is also a Gaussian,

$$\psi(k) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha(k-k_0)^2} ,$$

- Although we can localize a wave packet to a region of space, this has been at the expense of having some width in k.

Preparing a wave packet: example



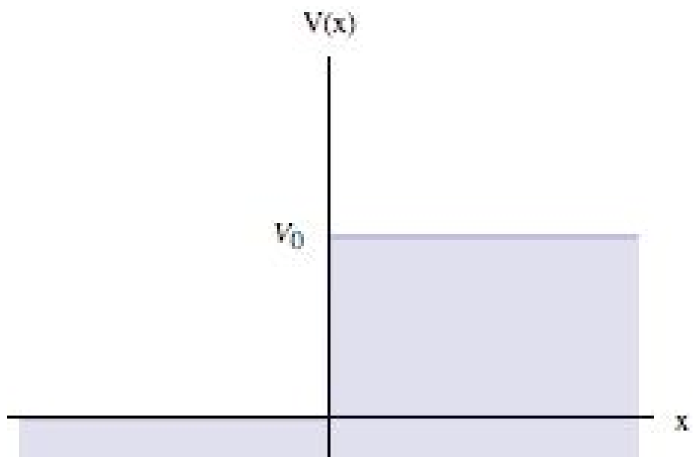
- For the Gaussian wave packet,

$$\Delta x = \left\langle [x - \langle x \rangle]^2 \right\rangle^{1/2} \equiv \left[\langle x^2 \rangle - \langle x \rangle^2 \right]^{1/2} = \sqrt{\alpha}, \qquad \Delta k = \frac{1}{\sqrt{4\alpha}}$$

- i.e. $\Delta x \, \Delta k = \frac{1}{2}$, constant.
- In fact, as we will see in the next lecture, the Gaussian wavepacket has **minimum uncertainty**,

$$\boxed{\Delta p \, \Delta x = \frac{\hbar}{2}}$$

Unbound particles: potential step

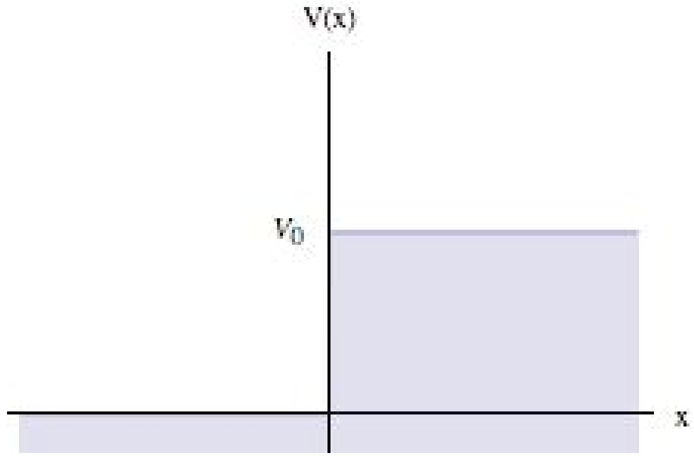


- Stationary form of Schrödinger equation, $\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$:

$$\boxed{\left[-\frac{\hbar^2\partial_x^2}{2m} + V(x)\right]\psi(x) = E\psi(x)}$$

- As a linear second order differential equation, we must specify **boundary conditions on both ψ and its derivative, $\partial_x\psi$.**
- As $|\psi(x)|^2$ represents a probablility density, it must be everywhere finite $\Rightarrow$ $\psi(x)$ is also finite.

Unbound particles: potential step



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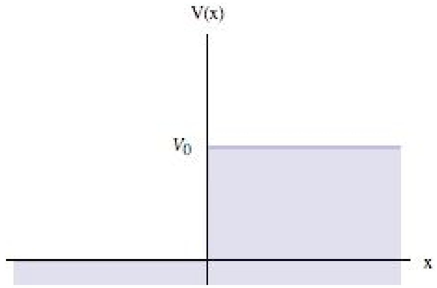
- Since $\psi(x)$ is finite, and E and $V(x)$ are presumed finite, so $\partial_x^2\psi(x)$ must be finite.
- $\Rightarrow$ **both $\psi(x)$ and $\partial_x\psi(x)$ are continuous functions of x** (even if potential $V(x)$ is discontinous).

Unbound particles: potential step

$$\left[-\frac{\hbar^2\partial_x^2}{2m} + V(x)\right]\psi(x) = E\psi(x)$$



- Consider beam of particles (energy E) moving from left to right incident on potential step of height V_0 at position $x = 0$.
- If beam has unit amplitude, reflected and transmitted (complex) amplitudes set by r and t,

$$\begin{array}{ll} \psi_<(x) = e^{ik_< x} + r\, e^{-ik_< x} & x < 0 \\ \psi_>(x) = t\, e^{ik_> x} & x > 0 \end{array}$$

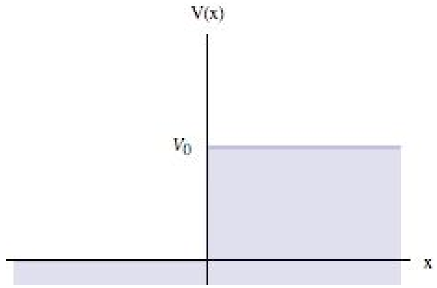
where $\hbar k_< = \sqrt{2mE}$ and $\hbar k_> = \sqrt{2m(E - V_0)}$.

- Applying continuity conditions on ψ and $\partial_x\psi$ at $x = 0$,

$$\begin{array}{ll} (a) & 1 + r = t \\ (b) & ik_<(1-r) = ik_> t \end{array} \quad \Rightarrow \quad r = \frac{k_< - k_>}{k_< + k_>}, \qquad t = \frac{2k_<}{k_< + k_>}$$

Unbound particles: potential step

$$\left[-\frac{\hbar^2\partial_x^2}{2m} + V(x)\right]\psi(x) = E\psi(x)$$



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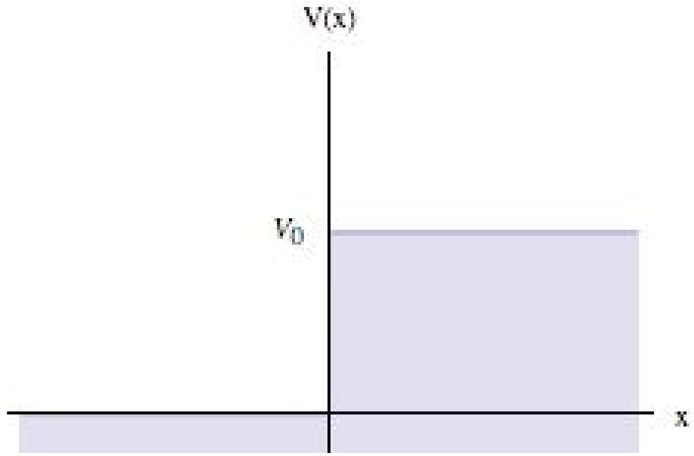
Unbound particles: potential step



- For $E > V_0$, both $\hbar k_<$ and $\hbar k_> = \sqrt{2m(E - V_0)}$ are real, and

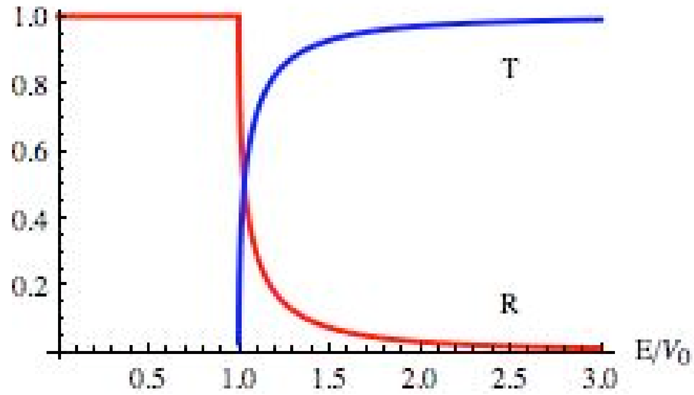
$$j_{\rm i} = \frac{\hbar k_<}{m}, \qquad j_{\rm r} = |r|^2 \frac{\hbar k_<}{m}, \qquad j_{\rm t} = |t|^2 \frac{\hbar k_>}{m}$$

- Defining reflectivity, R, and transmittivity, T,

$$R = \frac{\text{reflected flux}}{\text{incident flux}}, \qquad T = \frac{\text{transmitted flux}}{\text{incident flux}}$$

$$R = |r|^2 = \left(\frac{k_< - k_>}{k_< + k_>}\right)^2, \quad T = |t|^2 \frac{k_>}{k_<} = \frac{4k_< k_>}{(k_< + k_>)^2}, \quad R + T = 1$$

Unbound particles: potential step



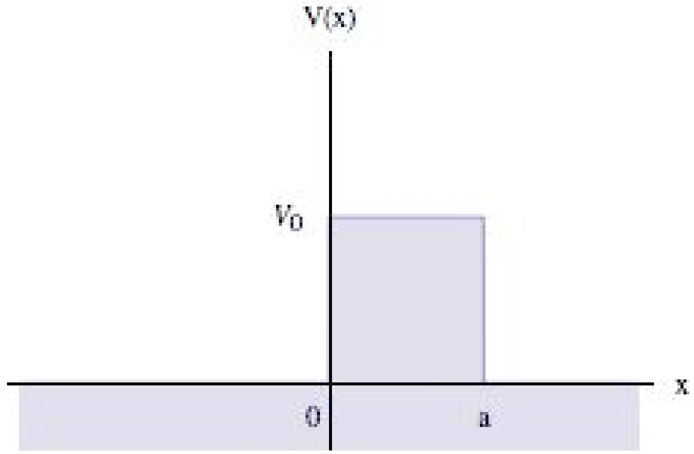
- For $E < V_0$, $\hbar k_> = \sqrt{2m(E - V_0)}$ becomes pure imaginary, wavefunction, $\psi_>(x) \simeq t e^{-|k_>|x}$, decays evanescently, and

$$j_{\rm i} = \frac{\hbar k_<}{m}, \qquad j_{\rm r} = |r|^2 \frac{\hbar k_<}{m}, \qquad j_{\rm t} = 0$$

- Beam is completely reflected from barrier,

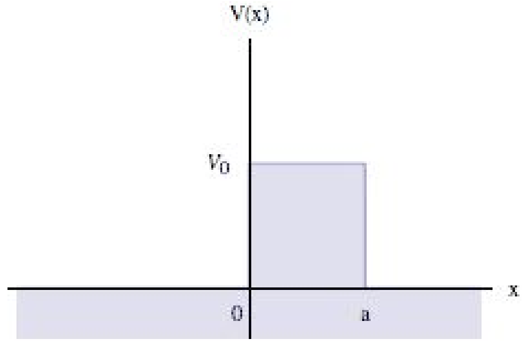
$$R = |r|^2 = \left| \frac{k_< - k_>}{k_< + k_>} \right|^2 = 1, \quad T = 0, \quad R + T = 1$$

Unbound particles: potential barrier



- Transmission across a potential barrier – prototype for generic **quantum scattering** problem dealt with later in the course.
- Problem provides platform to explore a phenomenon peculiar to quantum mechanics – **quantum tunneling**.

Unbound particles: potential barrier



- Wavefunction parameterization:

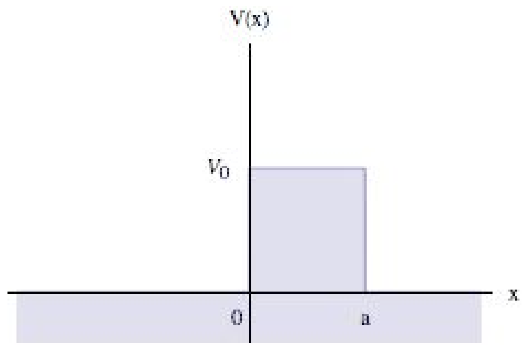
$$\begin{array}{ll} \psi_1(x) = e^{ik_1x} + r\,e^{-ik_1x} & x \leq 0 \\ \psi_2(x) = A\,e^{ik_2x} + B\,e^{-ik_2x} & 0 \leq x \leq a \\ \psi_3(x) = t\,e^{ik_1x} & a \leq x \end{array}$$

where $\hbar k_1 = \sqrt{2mE}$ and $\hbar k_2 = \sqrt{2m(E - V_0)}$.

- Continuity conditions on ψ and $\partial_x \psi$ at $x = 0$ and $x = a$,

$$\left\{ \begin{array}{l} 1 + r = A + B \\ Ae^{ik_2a} + Be^{-ik_2a} = te^{ik_1a} \end{array} \right. , \qquad \left\{ \begin{array}{l} k_1(1 - r) = k_2(A - B) \\ k_2(Ae^{ik_2a} - Be^{-ik_2a}) = k_1 te^{ik_1a} \end{array} \right.$$

Unbound particles: potential barrier



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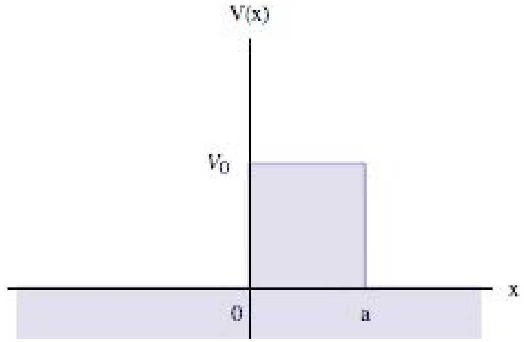
Unbound particles: potential barrier



- Solving for transmission amplitude,

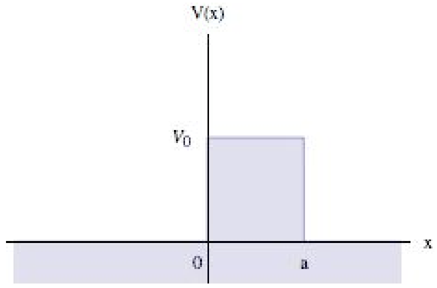
$$t = \frac{2k_1 k_2 e^{-ik_1 a}}{2k_1 k_2 \cos(k_2 a) - i(k_1^2 + k_2^2)\sin(k_2 a)}$$

which translates to a transmissivity of

$$T = |t|^2 = \frac{1}{1 + \frac{1}{4}\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)^2 \sin^2(k_2 a)}$$

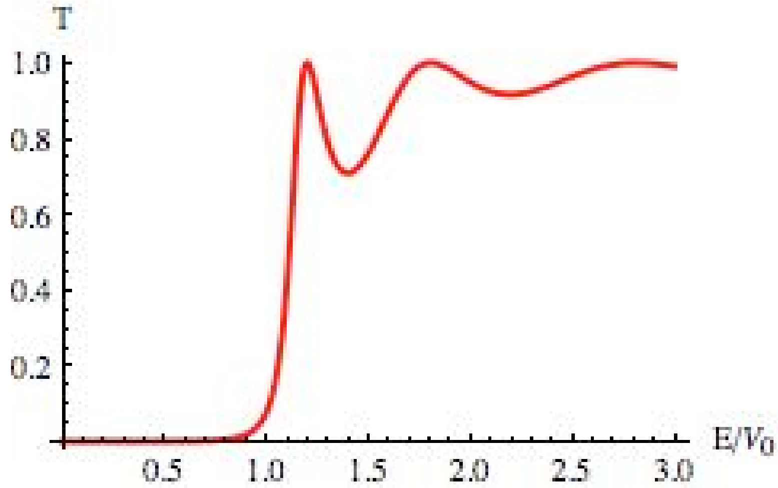
and reflectivity, $R = 1 - T$ (particle conservation).

Unbound particles: potential barrier



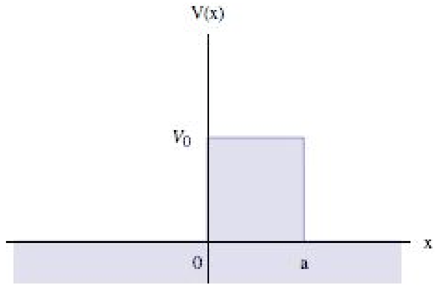
$$T = |t|^2 = \frac{1}{1 + \frac{1}{4}\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)^2 \sin^2(k_2 a)}$$

- For $E > V_0 > 0$, T shows oscillatory behaviour with T reaching unity when $k_2 a \equiv \frac{a}{\hbar}\sqrt{2m(E - V_0)} = n\pi$ with n integer.



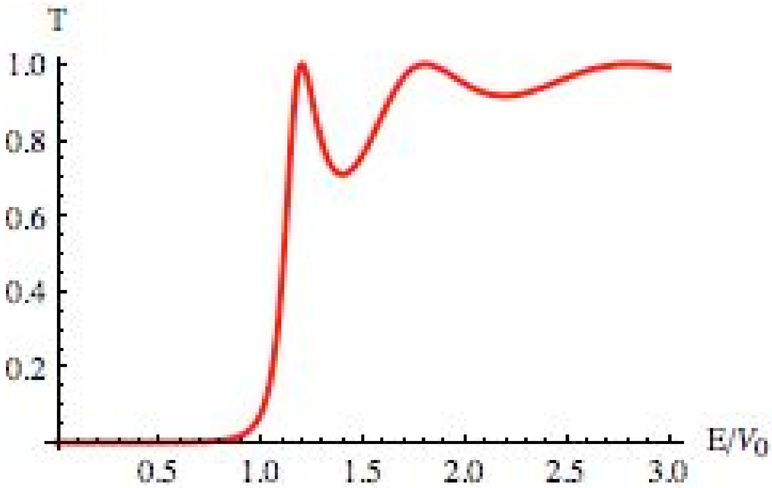
- At $k_2 a = n\pi$, fulfil **resonance** condition: interference eliminates altogether the reflected component of wave.

Unbound particles: potential barrier



$$T = |t|^2 = \frac{1}{1 + \frac{1}{4}\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)^2 \sin^2(k_2 a)}$$

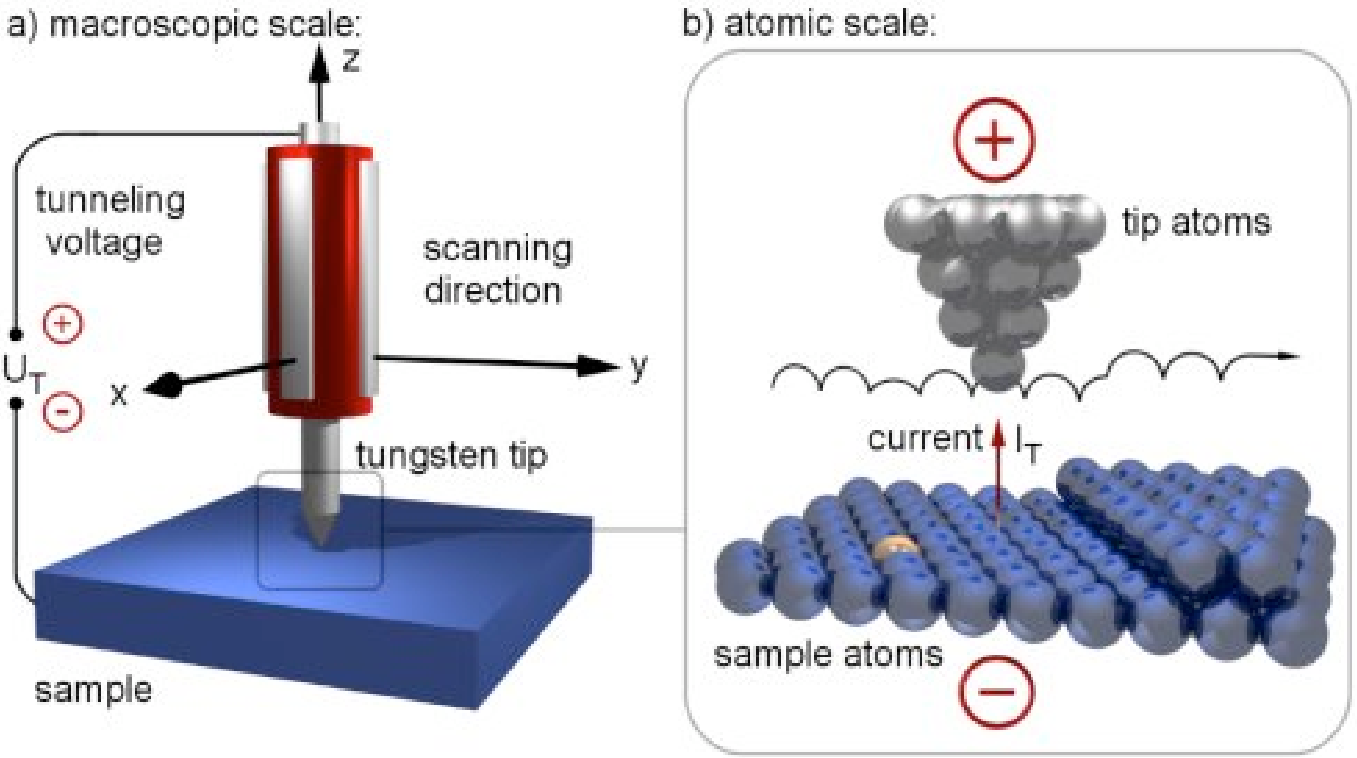
- For $V_0 > E > 0$, $k_2 = i\kappa_2$ turns pure imaginary, and wavefunction decays within, but penetrates, barrier region – **quantum tunneling**.



- For $\kappa_2 a \gg 1$ (weak tunneling), $T \simeq \frac{16 k_1^2 \kappa_2^2}{(k_1^2 + \kappa_2^2)^2} e^{-2\kappa_2 a}$.

Unbound particles: tunneling

- Although tunneling is a robust, if uniquely quantum, phenomenon, it is often difficult to discriminate from thermal activation.
- Experimental realization provided by **Scanning Tunneling Microscope (STM)**



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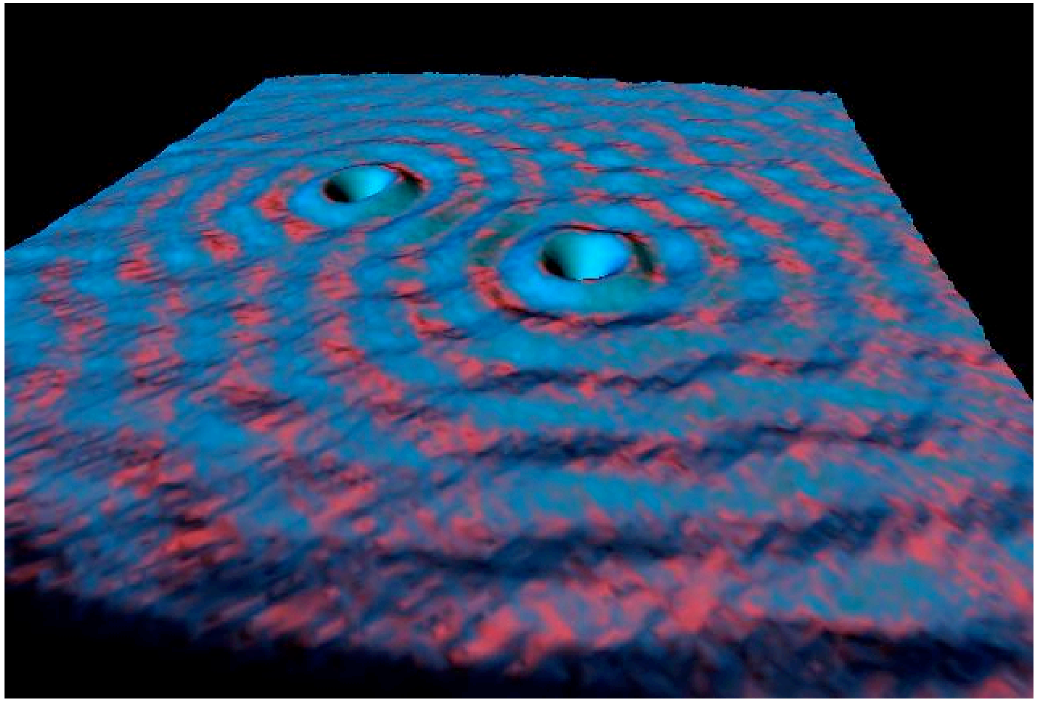
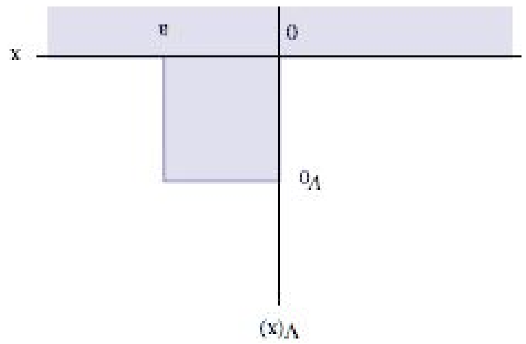


e.g. Friedel charge density oscillations from impurities on a surface.

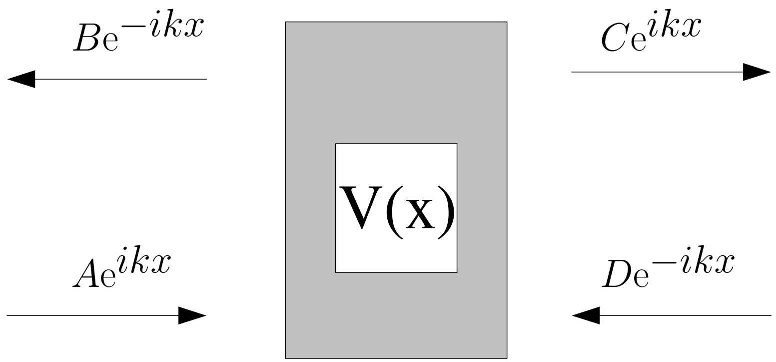
Unbound particles: potential well

$$T = |t|^2 = \frac{1}{1 + \frac{1}{4}\left(\frac{k_1}{k_2} - \frac{k_2}{k_1}\right)^2 \sin^2(k_2 a)}$$



- For scattering from potential well ($V_0 < 0$), while $E > 0$, result still applies – continuum of unbound states with resonance behaviour.
- However, now we can find **bound states** of the potential well with $E < 0$.
- But, before exploring these bound states, let us consider the general scattering problem in one-dimension.

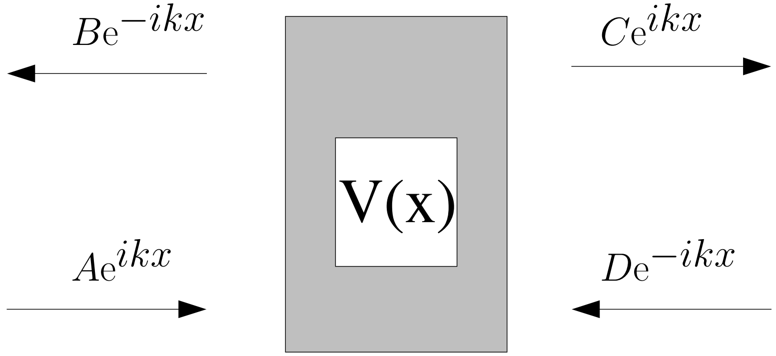
Quantum mechanical scattering in one-dimension



- Consider **localized** potential, $V(x)$, subject to beam of quantum particles incident from left and right.
- Outside potential, wavefunction is plane wave with $\hbar k = \sqrt{2mE}$.
- Relation between the incoming and outgoing components of plane wave specified by scattering matrix (or **S-matrix**)

$$\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} \quad \Longrightarrow \quad \Psi_{\rm out} = S\Psi_{\rm in}$$

Quantum mechanical scattering in one-dimension



- With $j_{\rm left} = \frac{\hbar k}{m}(|A|^2 - |B|^2)$ and $j_{\rm right} = \frac{\hbar k}{m}(|C|^2 - |D|^2)$, particle conservation demands that $j_{\rm left} = j_{\rm right}$, i.e.

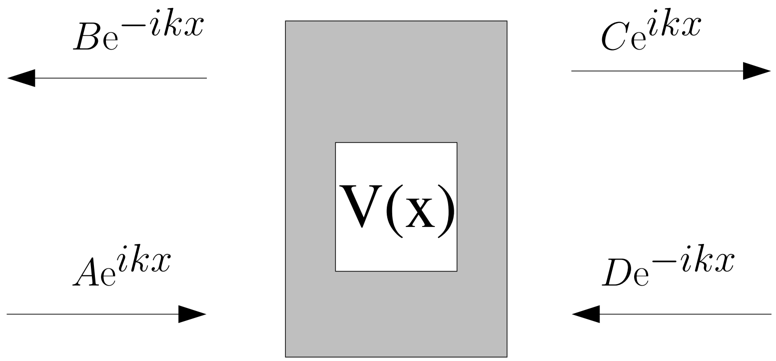
$$|A|^2 + |D|^2 = |B|^2 + |C|^2 \qquad \text{or} \qquad \Psi_{\rm in}^\dagger \Psi_{\rm in} = \Psi_{\rm out}^\dagger \Psi_{\rm out}$$

- Then, since $\Psi_{\rm out} = S\Psi_{\rm in}$,

$$\Psi_{\rm in}^\dagger \Psi_{\rm in} \stackrel{!}{=} \Psi_{\rm out}^\dagger \Psi_{\rm out} = \Psi_{\rm in}^\dagger \underbrace{S^\dagger S}_{\stackrel{!}{=}\mathbb{I}} \Psi_{\rm in}$$

and it follows that S-matrix is **unitary**: $S^\dagger S = \mathbb{I}$

Quantum mechanical scattering in one-dimension



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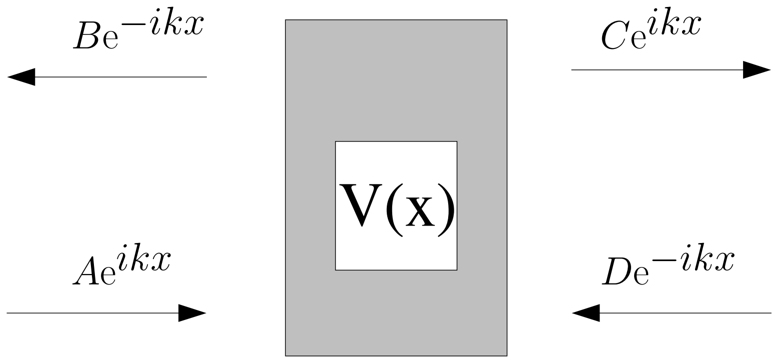


- For matrices that are unitary, eigenvalues have unit magnitude.

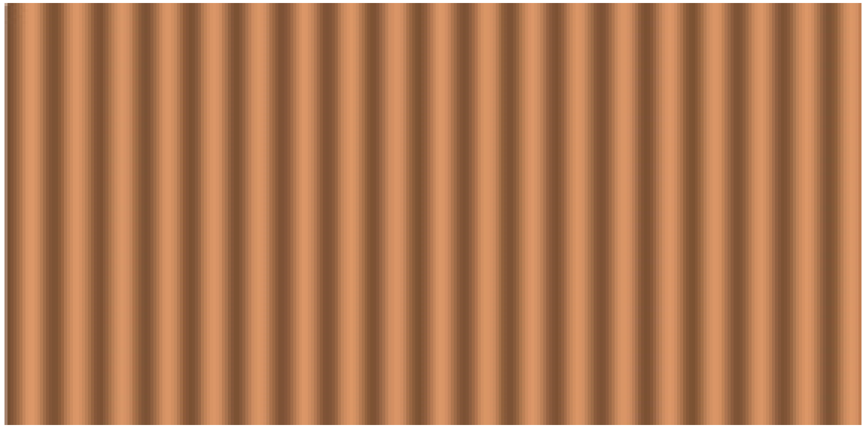
  Proof: For eigenvector $|v\rangle$, such that $S|v\rangle = \lambda|v\rangle$,

  $$\langle v|S^\dagger S|v\rangle = |\lambda|^2\langle v|v\rangle = \langle v|v\rangle$$

  i.e. $|\lambda|^2 = 1$, and $\lambda = e^{i\theta}$.

- S-matrix characterised by two **scattering phase shifts**, $e^{2i\delta_1}$ and $e^{2i\delta_2}$, (generally functions of k).

Quantum mechanical scattering in three-dimensions

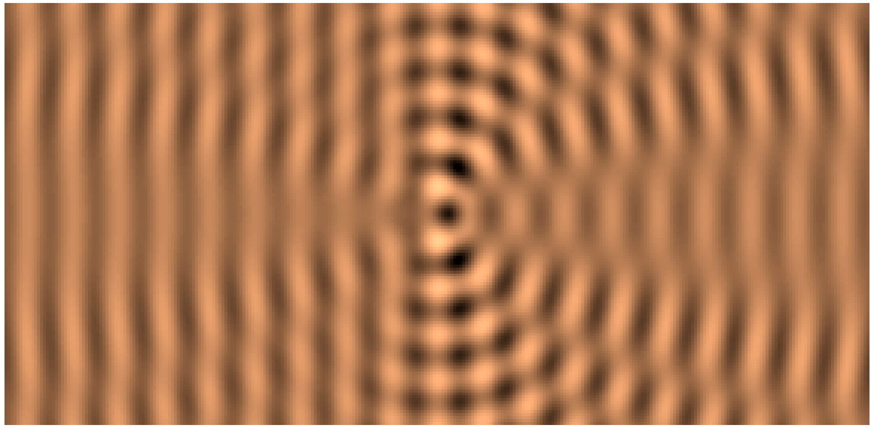


- In three dimensions, plane wave can be decomposed into superposition of incoming and outgoing spherical waves:
- If $V(\mathbf{r})$ short-ranged, scattering wavefunction takes *asymptotic* form,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{i}{2k}\sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)\left[\frac{e^{-i(kr-\ell\pi/2)}}{r} - S_\ell(k)\frac{e^{i(kr-\ell\pi/2)}}{r}\right]P_\ell(\cos\theta)$$

where $|S_\ell(k)| = 1$ (i.e. $S_\ell(k) = e^{2i\delta_\ell(k)}$ with $\delta_\ell(k)$ the phase shifts).

Quantum mechanical scattering in three-dimensions



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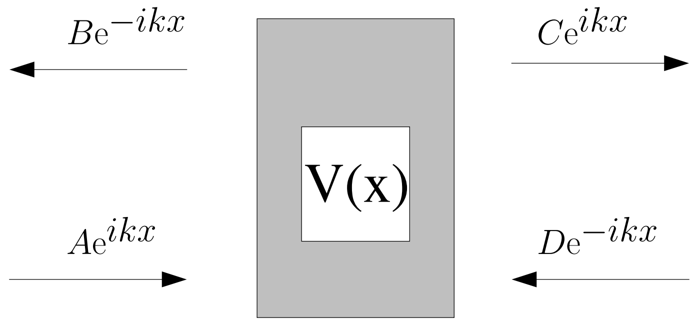


- For a symmetric potential, $V(x) = V(-x)$, S-matrix has the form

$$S = \begin{pmatrix} t & r \\ r & t \end{pmatrix}$$

  where r and t are complex reflection and transmission amplitudes.

- From the unitarity condition, it follows that

$$S^\dagger S = \mathbb{I} = \begin{pmatrix} |t|^2 + |r|^2 & rt^* + r^*t \\ rt^* + r^*t & |t|^2 + |r|^2 \end{pmatrix}$$

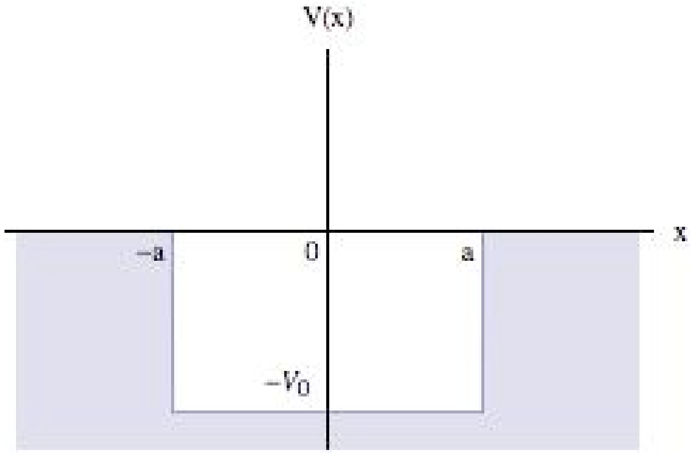
  i.e. $rt^* + r^*t = 0$ and $|r|^2 + |t|^2 = 1$ (or $r^2 = -\frac{t}{t^*}(1 - |t|^2)$).

- For application to a δ-function potential, see problem set I.

Quantum mechanics in 1d: bound states

1. Rectangular potential well (continued)
2. δ-function potential

Bound particles: potential well



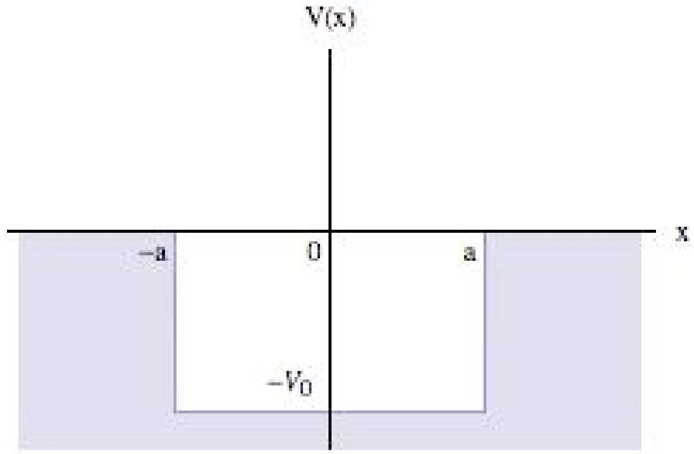
- For a potential well, we seek bound state solutions with energies lying in the range $-V_0 < E < 0$.
- Symmetry of potential $\Rightarrow$ states separate into those symmetric and those antisymmetric under parity transformation, $x \to -x$.
- Outside well, (bound state) solutions have form

$$\psi_1(x) = Ce^{\kappa x} \quad \text{for } x > a, \qquad \hbar\kappa = \sqrt{-2mE} > 0$$

- In central well region, general solution of the form

$$\psi_2(x) = A\cos(kx) \text{ or } B\sin(kx), \qquad \hbar k = \sqrt{2m(E+V_0)} > 0$$

Bound particles: potential well



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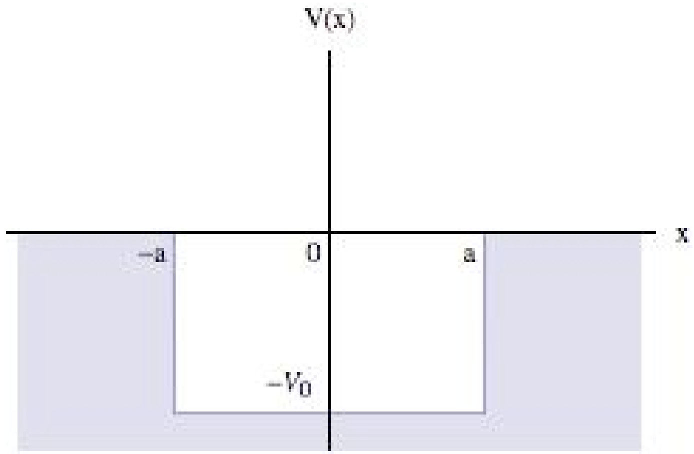
Bound particles: potential well

- Applied to even states,
  $\psi_1(x) = Ce^{-\kappa x}$, $\psi_2(x) = A\cos(kx)$,
  continuity of ψ and $\partial_x \psi$ implies

$$Ce^{-\kappa a} = A\cos(ka)$$
$$-\kappa Ce^{-\kappa a} = -Ak\sin(ka)$$

  (similarly odd).



- Quantization condition:

$$\kappa a = \begin{cases} ka\tan(ka) & \text{even} \\ -ka\cot(ka) & \text{odd} \end{cases}$$

$$\kappa a = \left(\frac{2ma^2 V_0}{\hbar^2} - (ka)^2 \right)^{1/2}$$

- $\Rightarrow$ at least one bound state.

Bound particles: potential well

- Applied to even states, $\psi_1(x) = Ce^{-\kappa x}$, $\psi_2(x) = A\cos(kx)$, continuity of ψ and $\partial_x\psi$ implies

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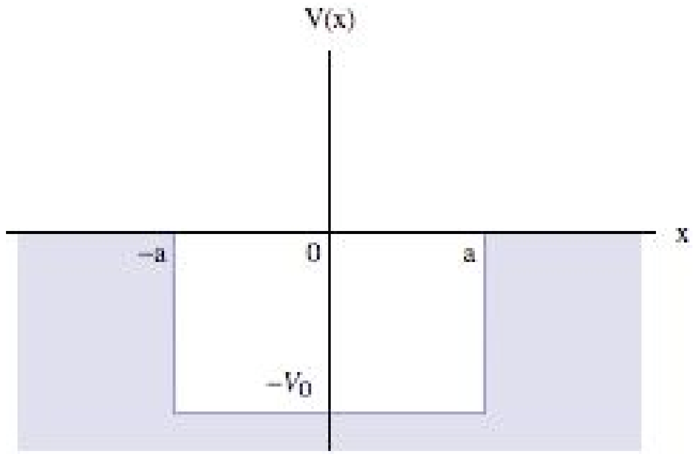

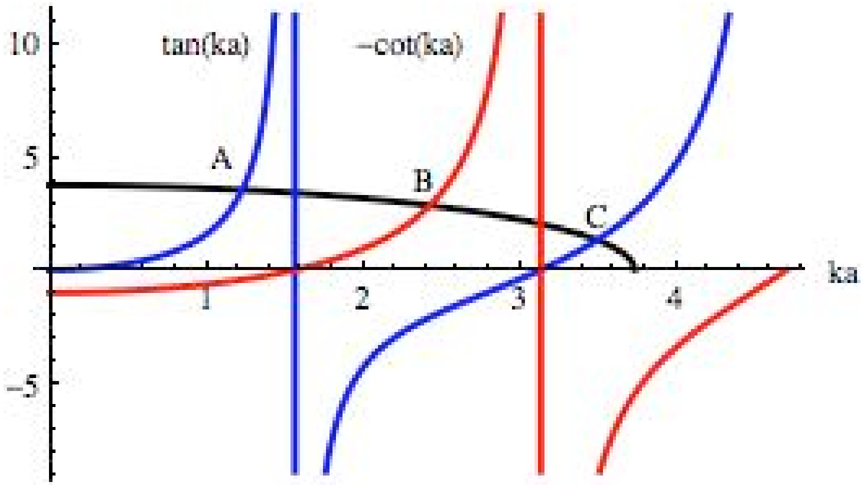

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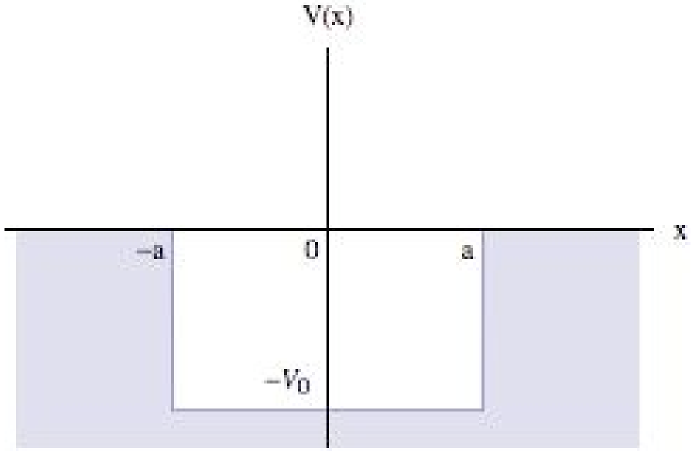
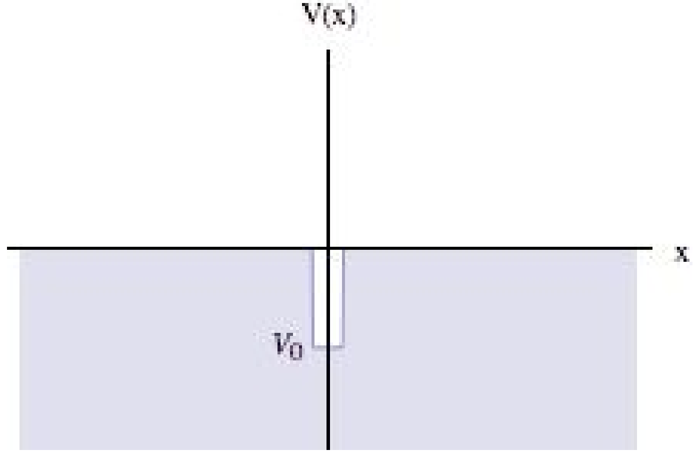
- $\Rightarrow$ **at least one bound state.**

Bound particles: potential well



- Uncertainty relation, $\Delta p \Delta x > h$, shows that confinement by potential well is balance between narrowing spatial extent of ψ while keeping momenta low enough not to allow escape.
- In fact, one may show (exercise!) that, in one dimension, **arbitrarily weak binding always leads to development of at least one bound state**.
- In higher dimension, potential has to reach critical strength to bind a particle.

Bound particles: δ-function potential

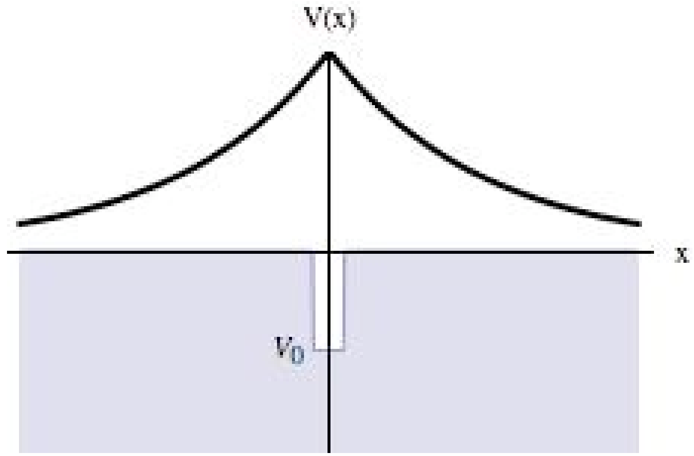


- For δ-function potential $V(x) = -aV_0\delta(x)$,

$$\boxed{\left[-\frac{\hbar^2\partial_x^2}{2m} - aV_0\delta(x)\right]\psi(x) = E\psi(x)}$$

- (Once again) symmetry of potential shows that stationary solutions of Schrödinger equation are eigenstates of parity, $x \to -x$.
- States with odd parity have $\psi(0) = 0$, i.e. insensitive to potential.

Bound particles: δ-function potential



$$\left[-\frac{\hbar^2\partial_x^2}{2m} - aV_0\delta(x)\right]\psi(x) = E\psi(x)$$

- Bound state with even parity of the form,

$$\psi(x) = A\begin{cases} e^{\kappa x} & x < 0 \\ e^{-\kappa x} & x > 0 \end{cases}, \qquad \hbar\kappa = \sqrt{-2mE}$$

- Integrating Schrödinger equation across infinitesimal interval,

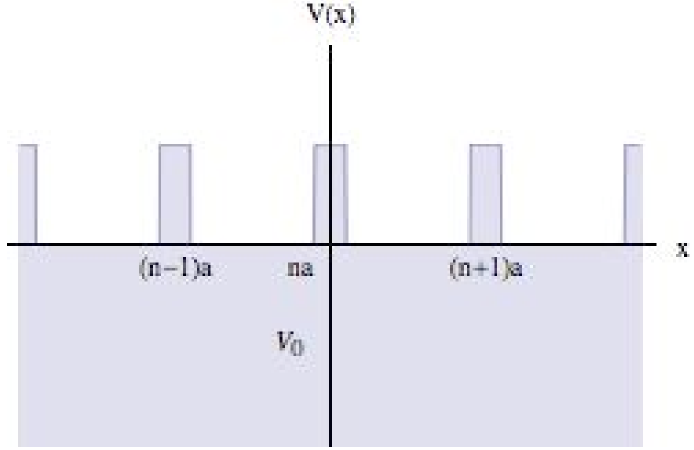
$$\partial_x\psi|_{+\epsilon} - \partial_x\psi|_{-\epsilon} = -\frac{2maV_0}{\hbar^2}\psi(0)$$

find $\kappa = \dfrac{maV_0}{\hbar^2}$, leading to bound state energy $E = -\dfrac{ma^2V_0^2}{2\hbar^2}$

Quantum mechanics in 1d: beyond local potentials

1. Kronig-Penney model of a crystal
2. Anderson localization

Kronig-Penney model of a crystal

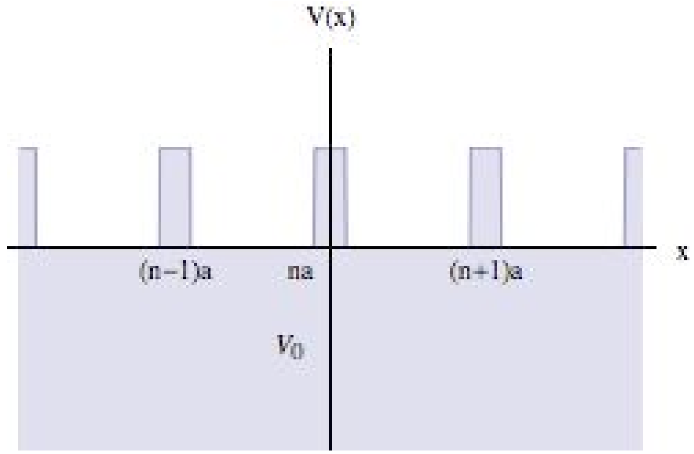


- **Kronig-Penney model** provides caricature of (one-dimensional) crystal lattice potential,

$$V(x) = aV_0 \sum_{n=-\infty}^{\infty} \delta(x - na)$$

- Since potential is repulsive, all states have energy $E > 0$.
- Symmetry: translation by lattice spacing a, $V(x + a) = V(x)$.
- Probability density must exhibit same translational symmetry, $|\psi(x + a)|^2 = |\psi(x)|^2$, i.e. $\psi(x + a) = e^{i\phi}\psi(x)$.

Kronig-Penney model of a crystal



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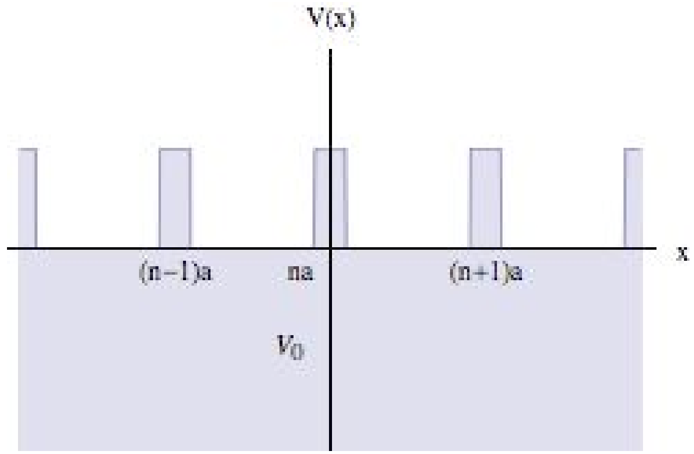


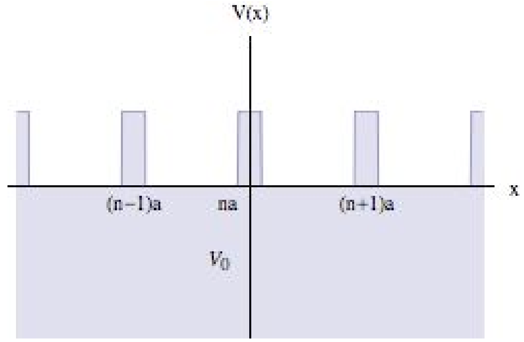
- In region $(n-1)a < x < na$, general solution of Schrödinger equation is plane wave like,

$$\psi_n(x) = A_n \sin[k(x-na)] + B_n \cos[k(x-na)]$$

with $\hbar k = \sqrt{2mE}$

- Imposing boundary conditions on $\psi_n(x)$ and $\partial_x \psi_n(x)$ and requiring $\psi(x+a) = e^{i\phi}\psi(x)$, we can derive a constraint on allowed k values (and therefore E) similar to quantized energies for bound states.

Kronig-Penney model of a crystal



$$\psi_n(x) = A_n \sin[k(x - na)] + B_n \cos[k(x - na)]$$

- Continuity of wavefunction, $\psi_n(na) = \psi_{n+1}(na)$, translates to

$$B_{n+1} \cos(ka) = B_n + A_{n+1} \sin(ka) \qquad (1)$$

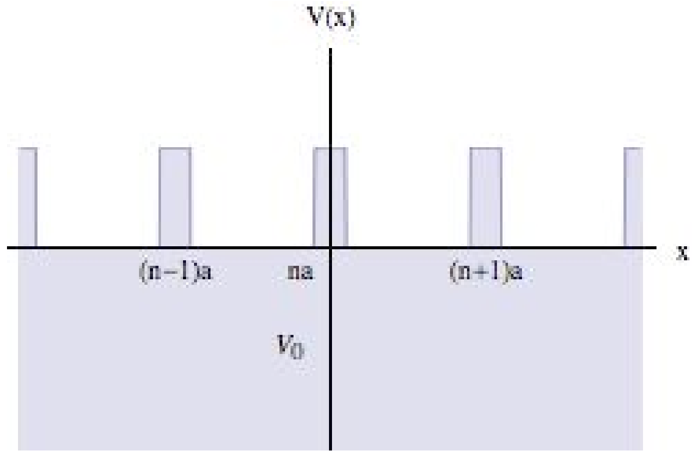
- Discontinuity in first derivative,

$$\partial_x \psi_{n+1}|_{x=na} - \partial_x \psi_n|_{na} = \frac{2maV_0}{\hbar^2} \psi_n(na)$$

leads to the condition,

$$k\left[A_{n+1} \cos(ka) + B_{n+1} \sin(ka) - A_n\right] = \frac{2maV_0}{\hbar^2} B_n \qquad (2)$$

Kronig-Penney model of a crystal

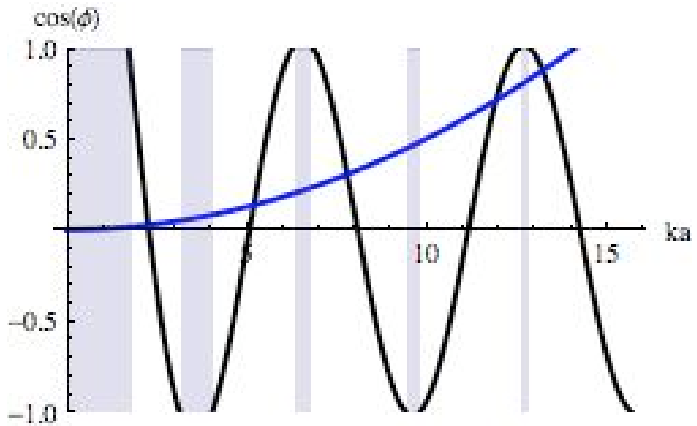


- Rearranging equations (1) and (2), and using the relations $A_{n+1} = e^{i\phi} A_n$ and $B_{n+1} = e^{i\phi} B_n$, we obtain

$$\cos\phi = \cos(ka) + \frac{maV_0}{\hbar^2 k}\sin(ka)$$

- Since $\cos\phi$ can only take on values between -1 and 1, there are allowed "bands" of k with $E = \frac{\hbar^2 k^2}{2m}$ and gaps between those bands.
- Appearance of energy bands separated by energy gaps is hallmark of periodic lattice potential system $\Rightarrow$ **metals and band insulators**

Kronig-Penney model of a crystal



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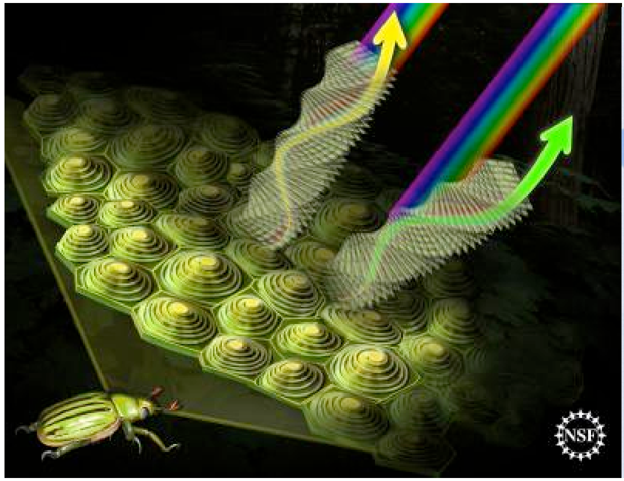
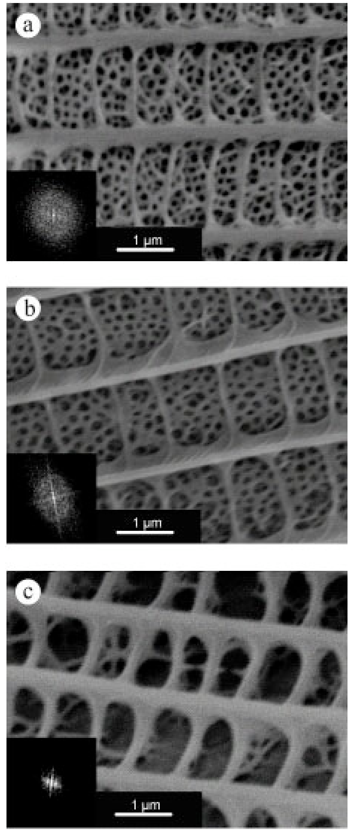
Example: Naturally occuring photonic crystals

- “Band gap” phenomena apply to any wave-like motion in a periodic system including light traversing dielectric media,

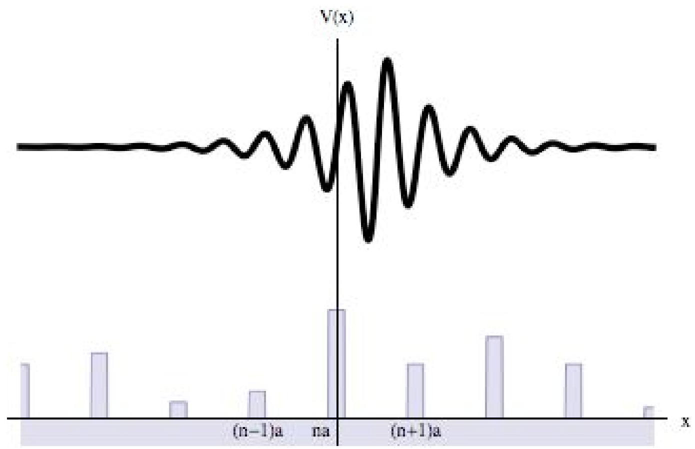
e.g. photonic crystal structures in beetles and butterflies!





- Band-gaps lead to perfect reflection of certain frequencies.

Anderson localization



- We have seen that even a weak potential can lead to the formation of a bound state.
- However, for such a confining potential, we expect high energy states to remain unbound.
- Curiously, and counter-intuitively, in 1d a weak **extended disorder potential** always leads to the exponential localization of all quantum states, no matter how high the energy!
- First theoretical insight into the mechanism of localization was achieved by Neville Mott!

Summary: Quantum mechanics in 1d

- In one-dimensional quantum mechanics, **an arbitrarily weak binding potential leads to the development of at least one bound state.**
- For quantum particles incident on a spatially localized potential barrier, the scattering properties are defined by a unitary S-matrix, $\psi_{\rm out} = S\psi_{\rm in}$.
- The scattering properties are characterised by eigenvalues of the S-matrix, $e^{2i\delta_i}$.
- For potentials in which $E < V_{\rm max}$, particle transfer across the barrier is mediated by **tunneling.**
- For an extended periodic potential (e.g. Kronig-Penney model), the spectrum of allow energies show **"band gaps" where propagating solutions don't exist.**
- For an extended random potential (however weak), **all states are localized, however high is the energy!**

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