Lecture 13

Simple 1d solutions of Schrodinger's equation

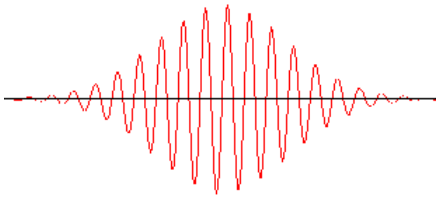
Announcements:

- lectures 12 and 13 are posted
- homework 8 solutions are posted
- homework 9 is due March 30
- reading for this week is:
  - Ch 7 in TZD

Last Time

recall lecture 12:

Schrödinger's equation for ψ(r,t)



- the equation and interpretation:

$P(r,t) = |\psi(r,t)|^2$ – probability density

- free particle: $\psi = e^{i(p\cdot r - Et)/\hbar}$

- observables: $p = -i\hbar\nabla = -i\hbar\dfrac{\partial}{\partial x}$

- measurements: $\langle\psi|O|\psi\rangle = \int d^3r \psi^* O\psi$

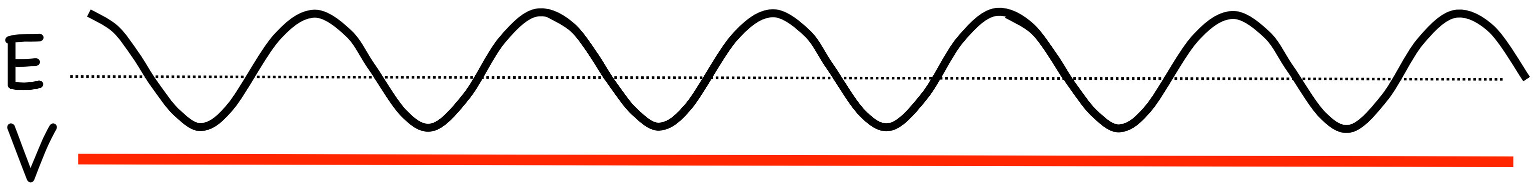
Today

Simple Schrödinger's equation problems in 1d

- mathematical generalities
- free particle
- particle in an infinite square-well
- particle in a finite square-well
- harmonic oscillator
- potential barrier and tunneling

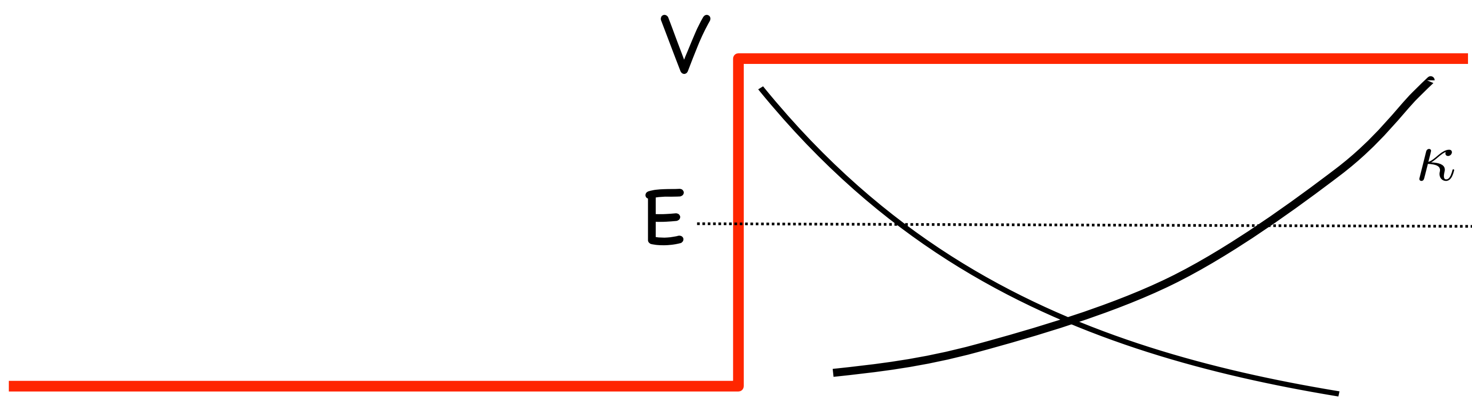
Mathematical background

- simple solutions for constant V : $-\psi'' + V\psi = E\psi$
- solutions are e^{ax} :
  - $\psi_E(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{for } E > V$



$k = \sqrt{E - V}$

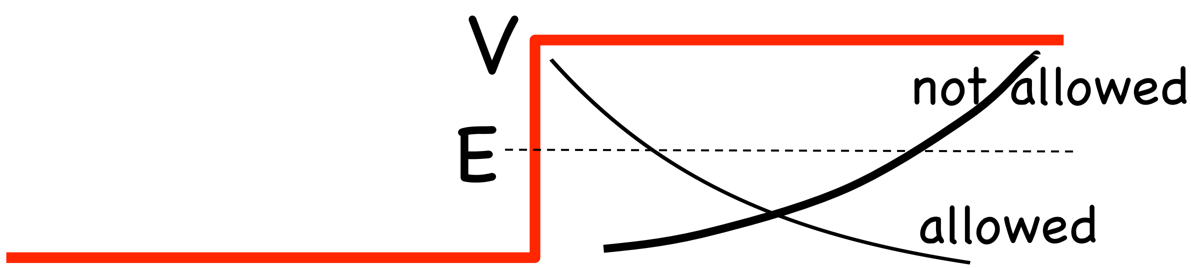
  - $\psi_E(x) = Ae^{\kappa x} + Be^{-\kappa x}, \quad \text{for } E < V$



$\kappa = \sqrt{V - E}$

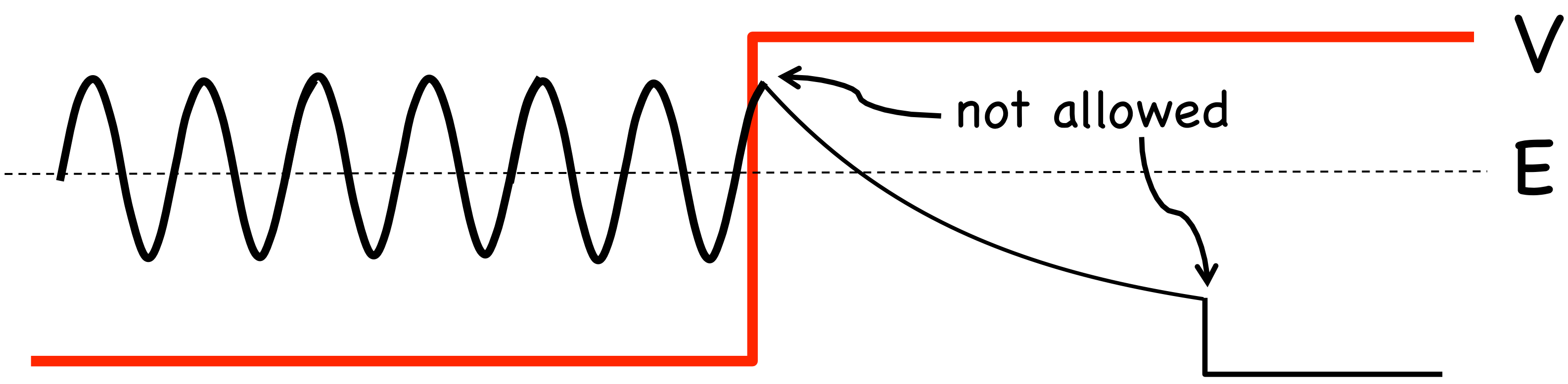
General rules

- legitimate solution must:
  - *satisfy Schrodinger's equation:* $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2}+V(x)\psi_E=E\psi_E$$
  - *satisfy boundary conditions: e.g., cannot diverge*



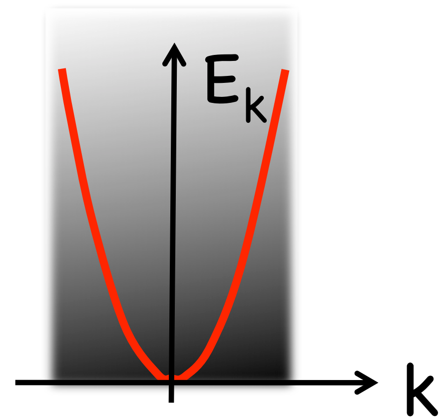
  - *be continuous and have continuous derivatives:*

$\psi(0^-) = \psi(0^+)$, $\psi'(0^-) = \psi'(0^+)$

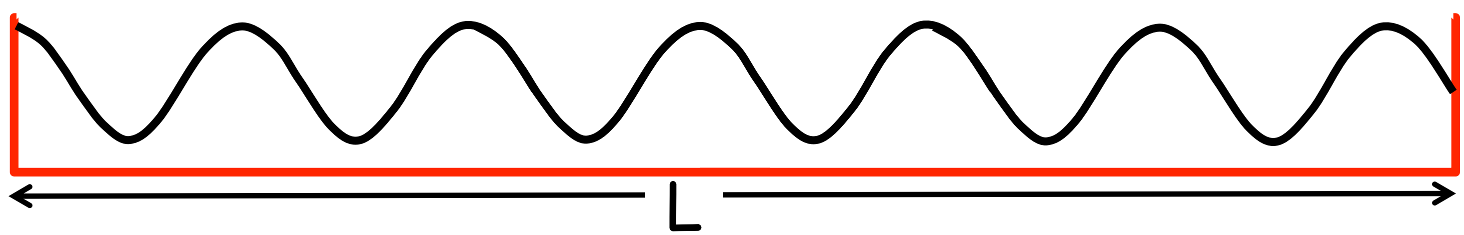


Free particle: V = 0

- $-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2} + V(x)\psi_E = E\psi_E \Longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2} = E\psi_E$
- plane-wave: $\psi_k(x) = A\, e^{ikx}$, with $E_k = \frac{\hbar^2 k^2}{2m}$
- continuum spectrum: E = $p^2/2m$



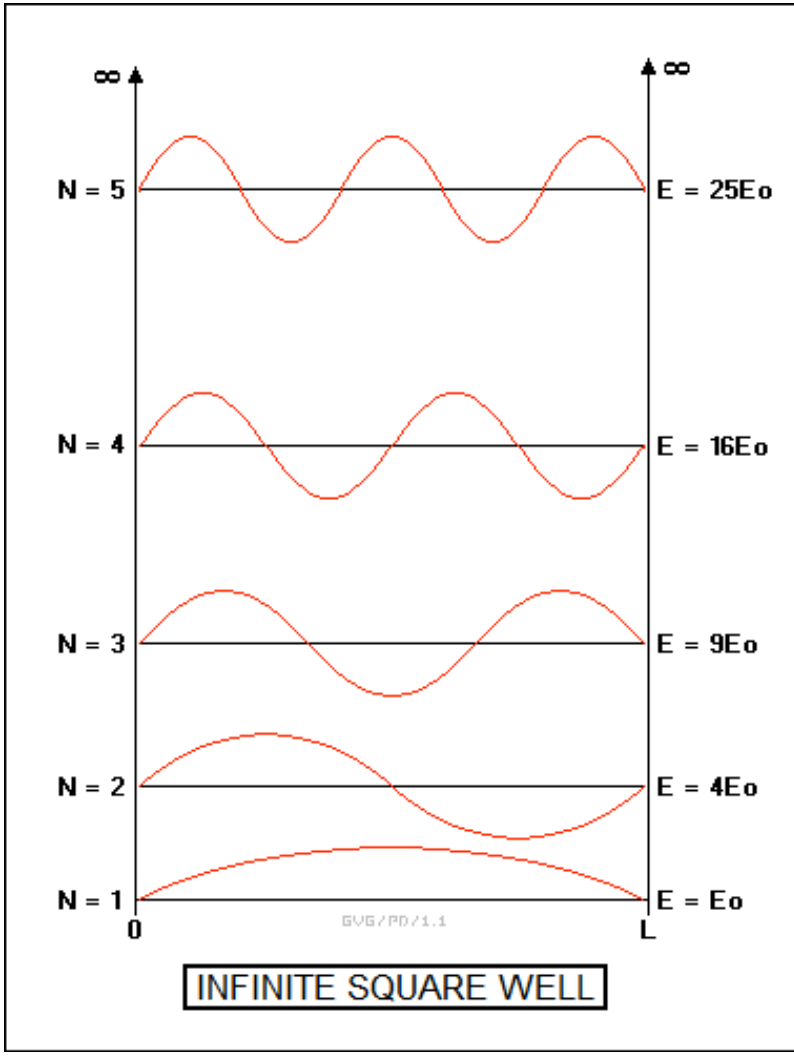
- normalization in a box: *A = ?* *only determined up to a phase* $e^{i\varphi}$



$$1 = \int_{-\infty}^{+\infty} |\psi|^2 = \int_{-L/2}^{+L/2} |A|^2 \Longrightarrow A = 1/\sqrt{L}$$

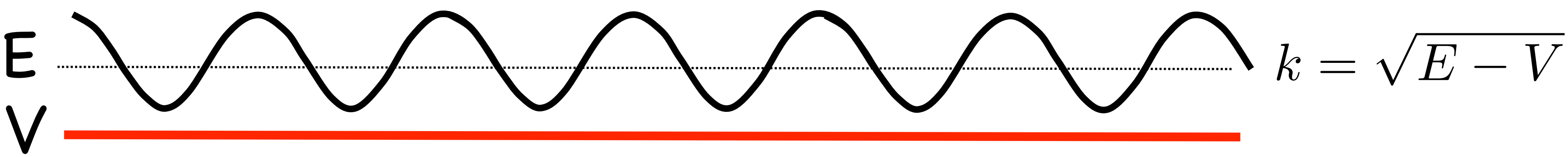
Particle in an infinite square-well

- $V = 0$, for $0 < x < L$, and ∞ outside the well
- $$\psi_k(x) = \sqrt{\frac{2}{L}} \sin k_n x, \quad \text{for } 0 < x < L$$
  $$= 0, \quad \text{otherwise}$$
- with $k_n = n\pi/L$, *n = 1, 2, 3,... (number nodes)*
- discrete spectrum: $E_n = \dfrac{\hbar^2 \pi^2}{2mL^2} n^2$
- no degeneracy in 1d, one state at each E
- $$P_n(x) = |\psi_n(x)|^2, \quad = \frac{2}{L}\sin^2\frac{\pi n x}{L}, \quad \text{for } 0 < x < L$$
- "crude" path to solution: $p \approx n\, h/L$ and minimize $E(x)$ over x

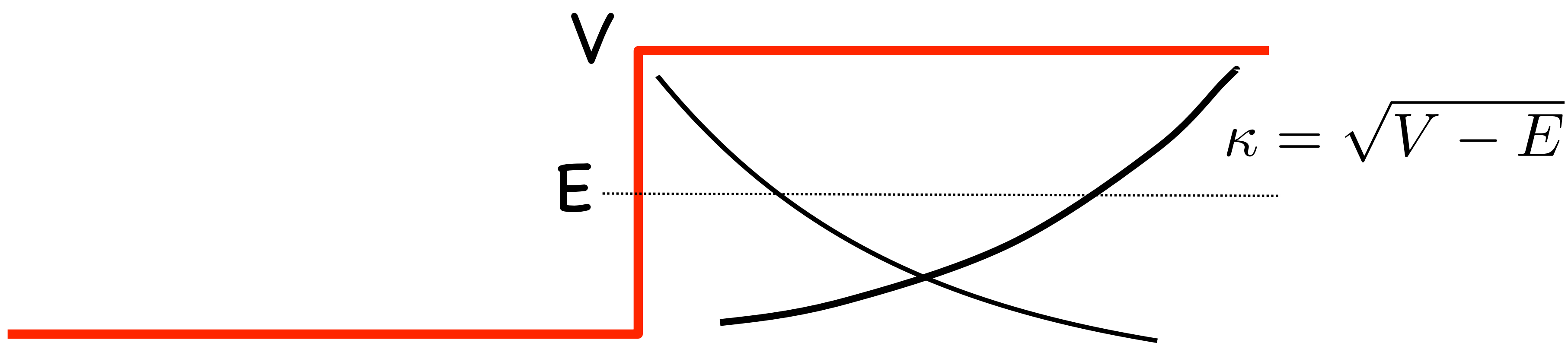


General solutions reminder

- simple solutions for constant V : $-\psi'' + V\psi = E\psi$
- solutions are:
  - $\psi_E(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{for } E > V$

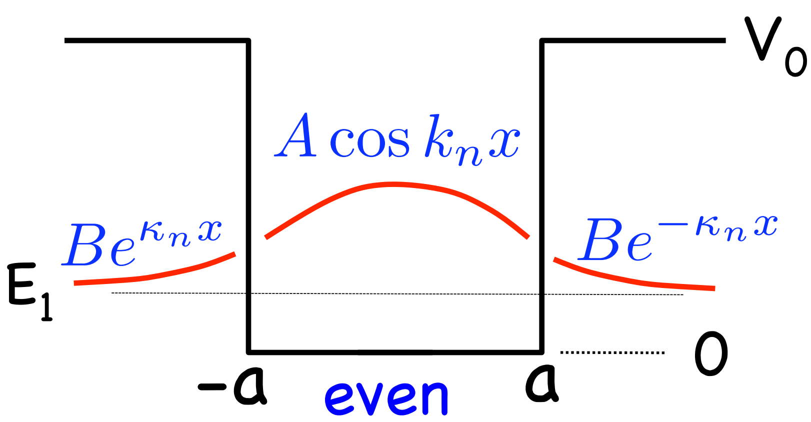


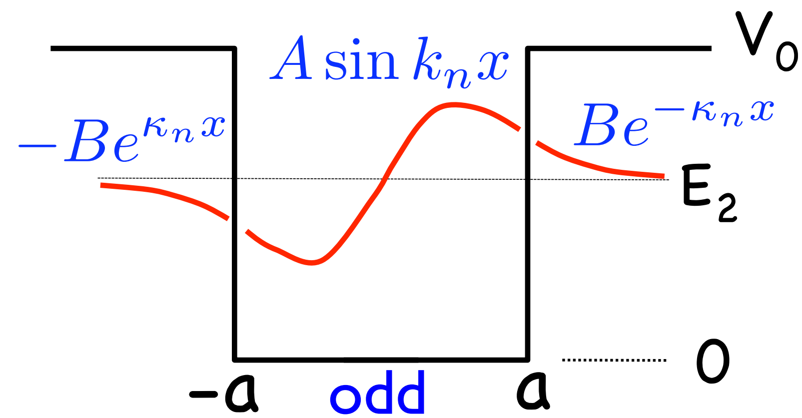
  - $\psi_E(x) = Ae^{\kappa x} + Be^{-\kappa x}, \quad \text{for } E < V$



Particle in a finite square-well

- $V = 0$, for $-a < x < a$, and V_0 outside the well





- A, B, $k = \sqrt{2mE/\hbar^2}, \kappa = \sqrt{2m(V_0 - E)/\hbar^2}$

  are determined by normalization, continuity and finiteness:

  $\psi_{inside}(a) = \psi_{outside}(a)$ $\quad\quad$ $\psi'_{inside}(a) = \psi'_{outside}(a)$

- even: $A\cos ka = Be^{-\kappa a}$ $\quad\quad$ $-Ak\sin ka = -B\kappa e^{-\kappa a}$

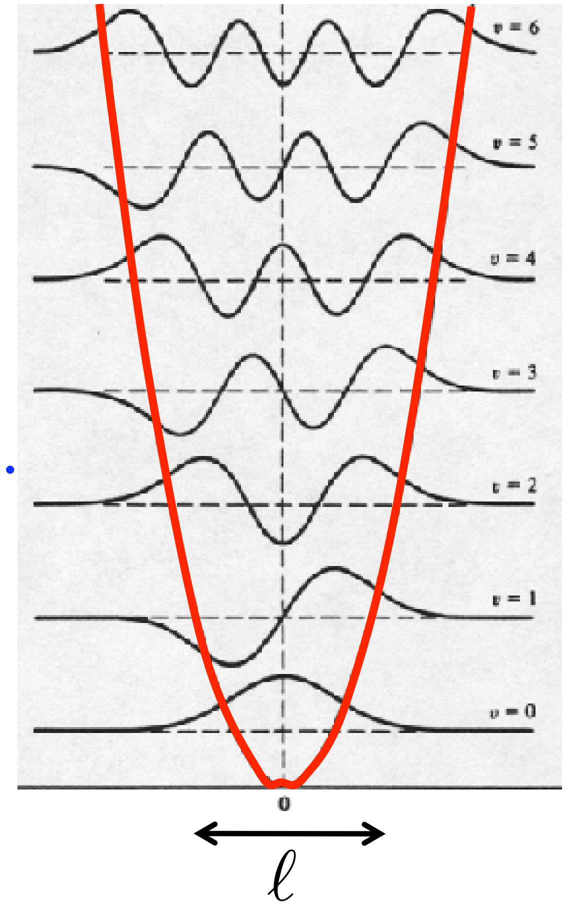
  $$\longrightarrow \boxed{k\tan ka = \kappa} \longleftarrow$$

- odd: $A\sin ka = Be^{-\kappa a}$ $\quad\quad$ $Ak\cos ka = -B\kappa e^{-\kappa a}$

  $$\longrightarrow \boxed{k\cot ka = -\kappa} \longleftarrow$$

- solve together with $k^2 + \kappa^2 = 2mV_0/\hbar \rightarrow E_n$
- there is also a continuum part of spectrum for $E > V_0$

Harmonic oscillator



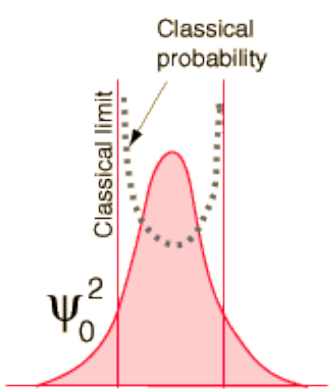
- S.Eqn: $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2}+\frac{1}{2}m\omega_0^2x^2\psi_E=E\psi_E$$

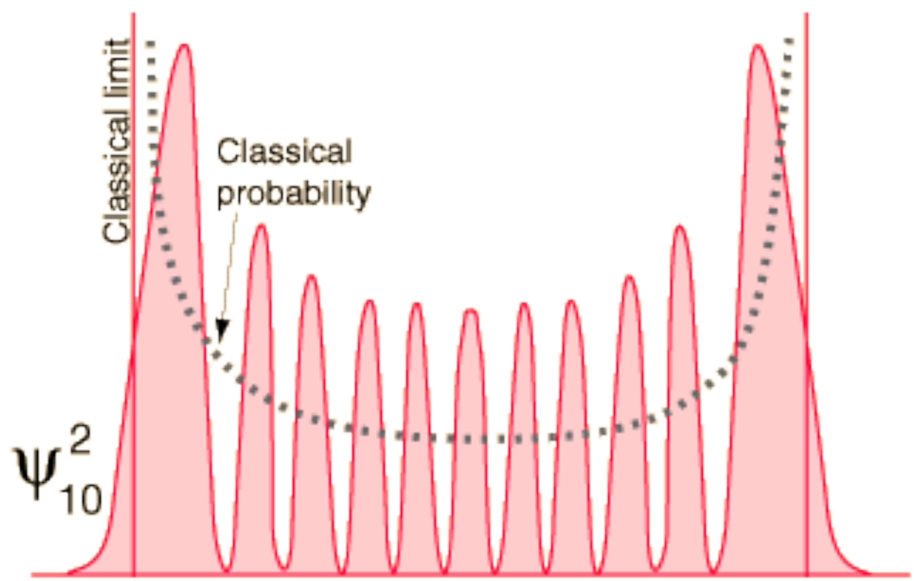
- spectrum: $E_n=\hbar\omega_0(n+1/2),\quad n=0,1,2,\ldots$

- eigenstates: $\psi_n(x)=H_n(x/\ell)e^{-x^2/2\ell^2},\ \ell=\sqrt{\frac{\hbar}{m\omega_0}}$

$$\begin{aligned}\psi_0(x) &= e^{-\hat{x}^2/2},\quad E_0=\frac{1}{2}\hbar\omega_0,\\ \psi_1(x) &= \hat{x}e^{-\hat{x}^2/2},\quad E_1=\frac{3}{2}\hbar\omega_0,\\ \psi_2(x) &= (1-2\hat{x}^2)e^{-\hat{x}^2/2},\quad E_2=\frac{5}{2}\hbar\omega_0\end{aligned}$$

- classical limit:





- "crude" path to solution: p ≈ n h/x and minimize E(x) over x

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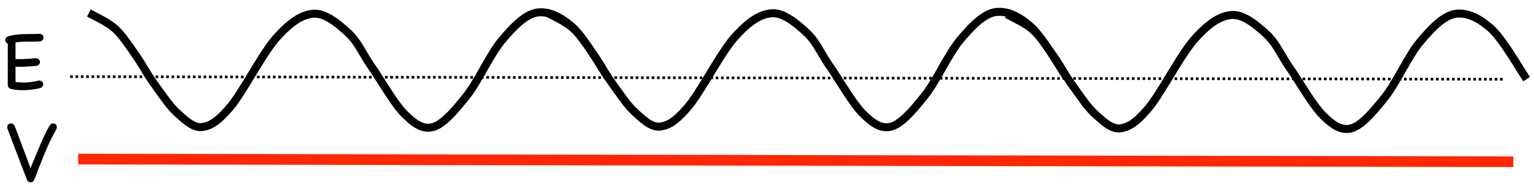

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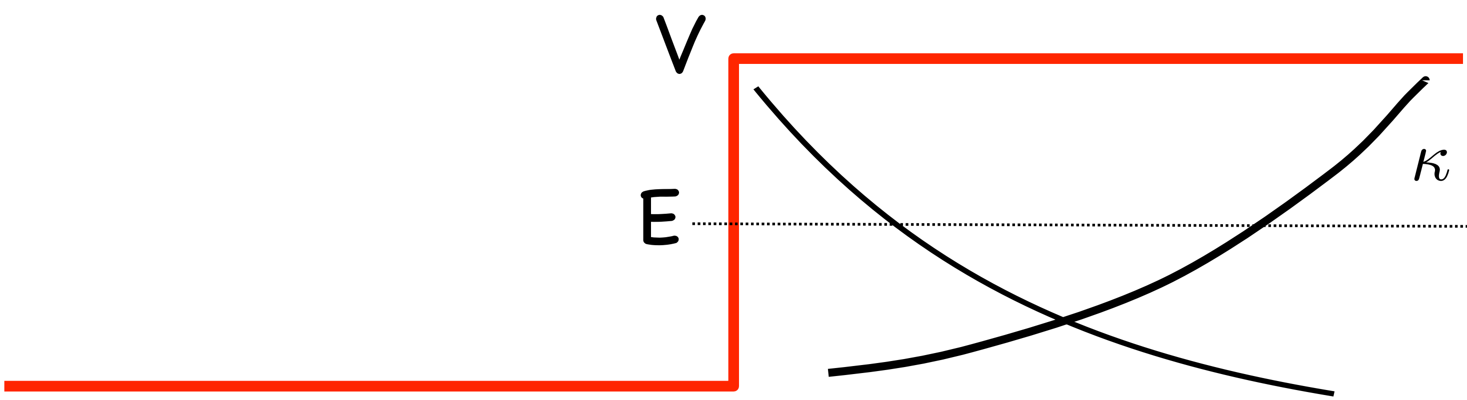
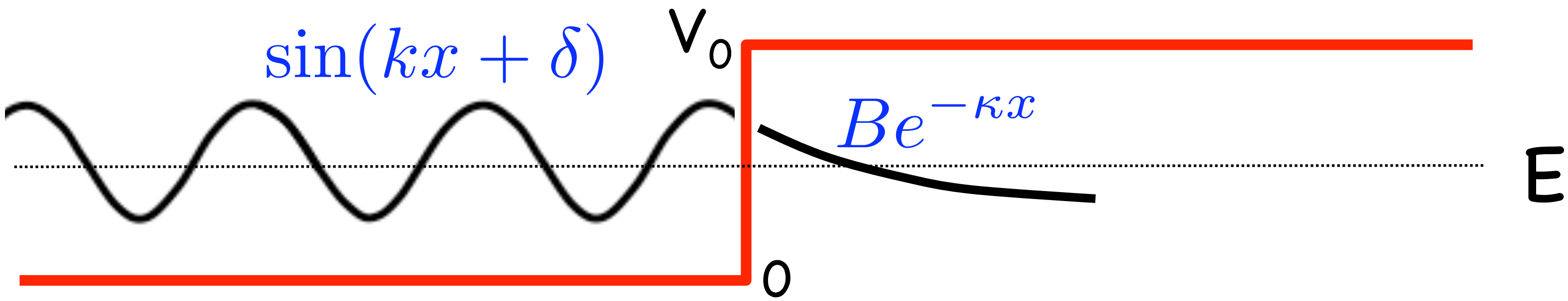


$$\kappa = \sqrt{V - E}$$

Step potential

- E < V_0



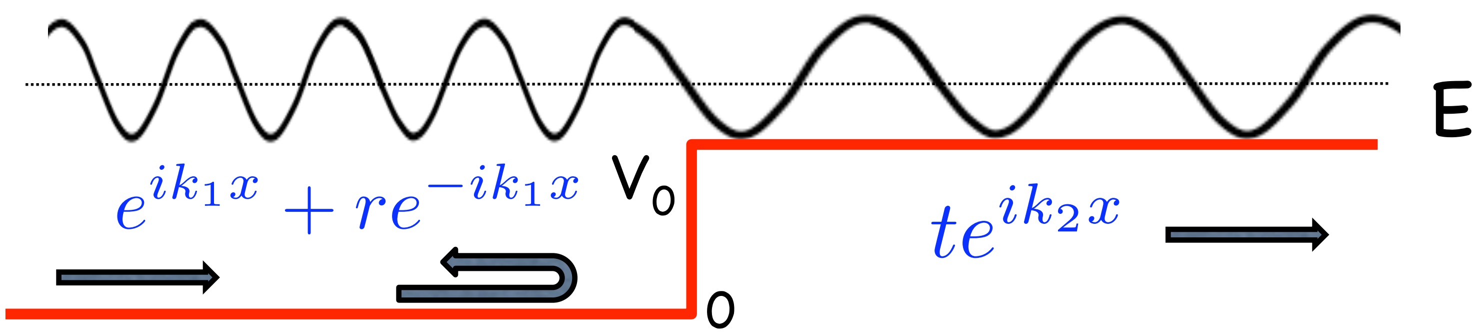
- $k = \sqrt{2mE/\hbar^2}, \kappa = \sqrt{2m(V_0 - E)/\hbar^2}$
- δ, B are determined by continuity across interface:

$\psi_<(0) = \psi_>(0)$ $\qquad$ $\psi'_<(0) = \psi'_>(0)$

$\sin(\delta) = B$ $\qquad$ $k\cos(\delta) = -\kappa B$

$$\tan(\delta) = -k/\kappa$$

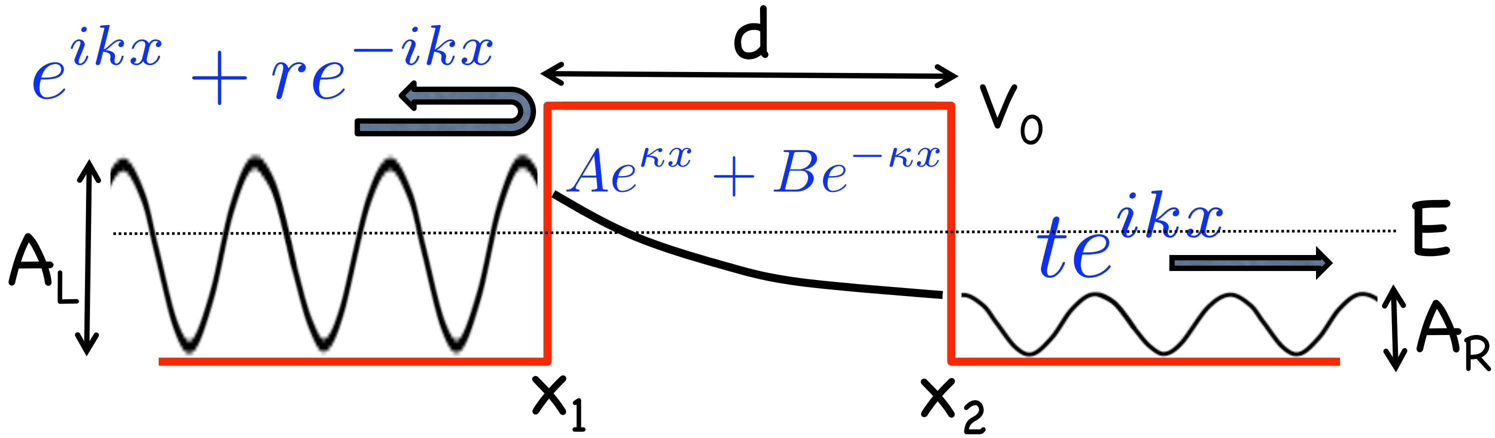
- E > V_0



nonclassical reflection even for E > V_0

Potential barrier: tunneling

- $E < V_0$



- reflection (r), transmission (t): $|r|^2 + |t|^2 = 1$

- exponentially weak tunneling: $t \approx A_R/A_L \approx e^{-\kappa x_2}/e^{-\kappa x_1} \approx e^{-\kappa d}$

$$P = |t|^2$$

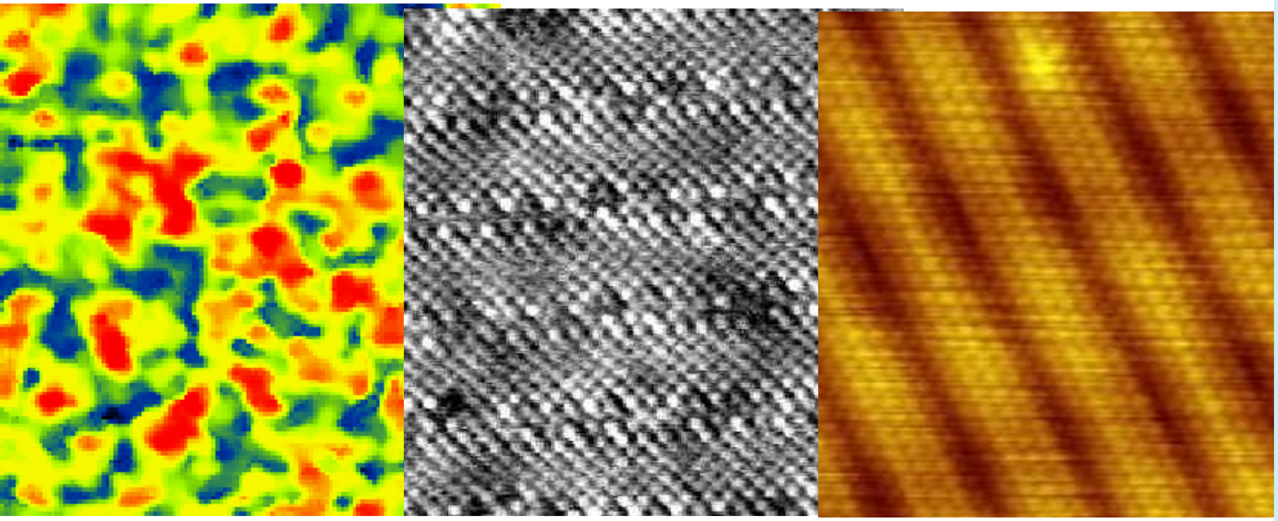
- controlled by thickness (d), height (V_0): $\kappa d = d\sqrt{2m(V_0 - E)/\hbar^2}$

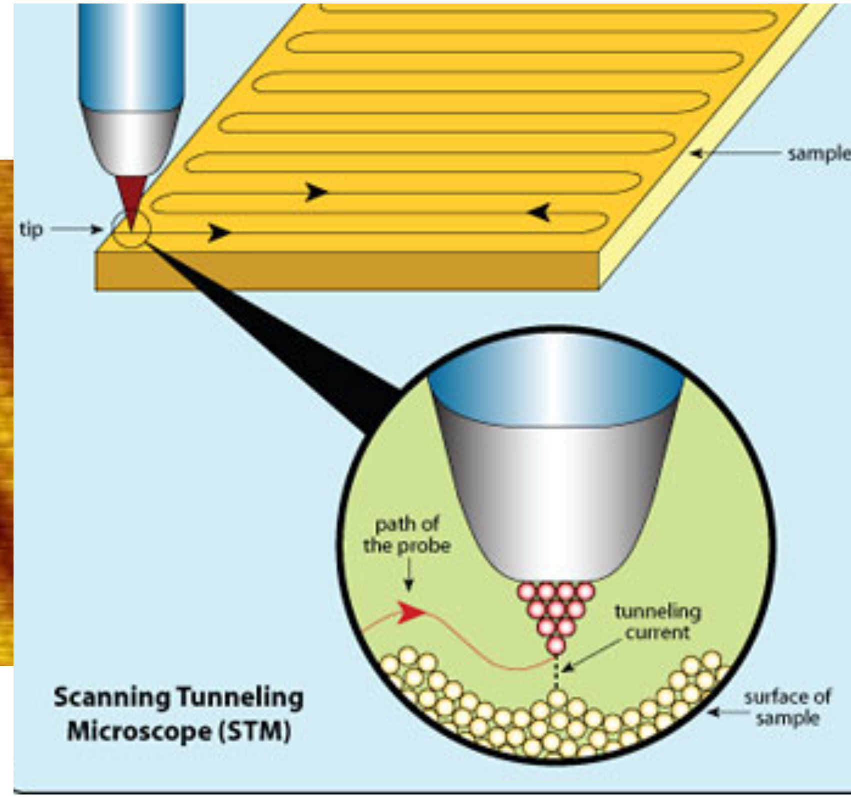
- many applications: α-decay, scanning tunneling microscope (STM)

  flash memory, microelectronics,...

Tunneling applications:

- scanning tunneling microscope (STM):





- α−decay (George Gamow, 1928):