Lecture 12

Schrodinger's Equation

Announcements:

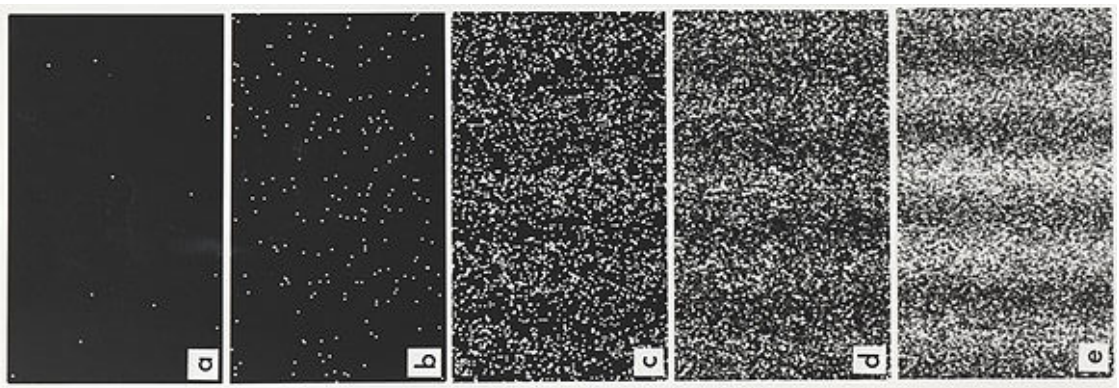
- lecture 11 is posted
- homework 7 solutions are posted
- homework 8 is due Fri, March 11
- reading for this week is:
  - Ch 6, 7 in TZD

Last Time

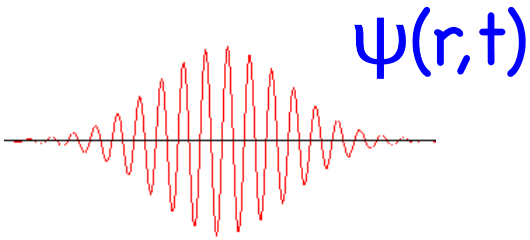
recall lecture 11:

Wave nature of matter:

- electron diffraction Davisson-Germer experiment



- deBroglie matter waves



- wavefunction and its interpretation

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

- Heisenberg uncertainty principle $\Delta x \Delta p > \frac{\hbar}{2}$ $\Delta E \Delta t > \frac{\hbar}{2}$

Today

Schrödinger's equation

- the equation
- free particle
- general properties

Erwin Schrödinger
(1887 – 1961)

clicker question

Imaginary number i

Q: *What is the correct expression for i^{65}*

a) +1

b) -1

c) $\boxed{+i}$

d) -i

e) +65 I

A: *(c) because every multiple of 4 i's gets you back to 1*

($i^1 = i$, $i^2 = -1$, $i^3 = -i$, $i^4 = 1$)

clicker question

Complex numbers

Q: *What is the correct expression for:*

$$(6 + 7\,i) \times (2 - 3\,i)\ ?$$

a) $+8 + 4\,i$

b) $\boxed{+33 - 4\,i}$

c) $-8 - 4\,I$

d) $+12 + 14\,I$

e) none of the above

A: *(b) any complex number can be expressed as $(a + i\,b)$:*

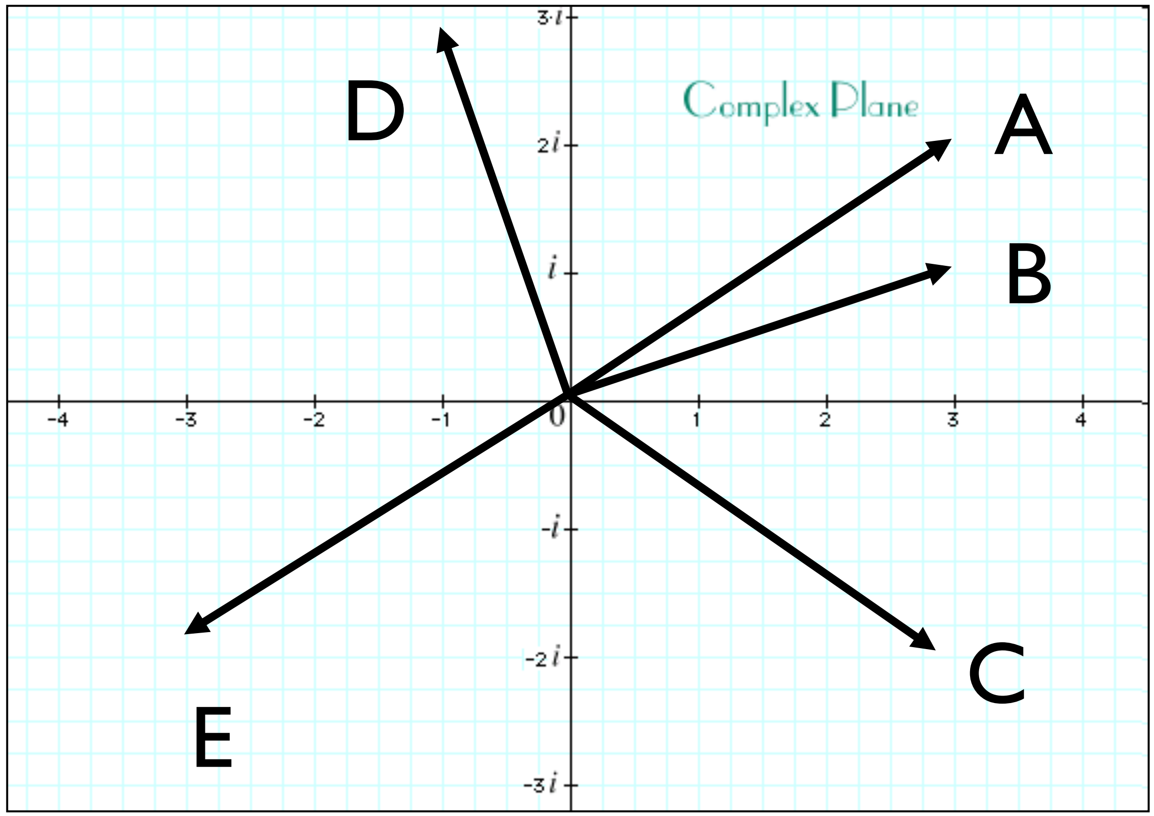
$(6 + 7\,i) \times (2 - 3\,i) = 12 - 18\,i + 14\,i - 21\,i^2$

clicker question

Complex numbers

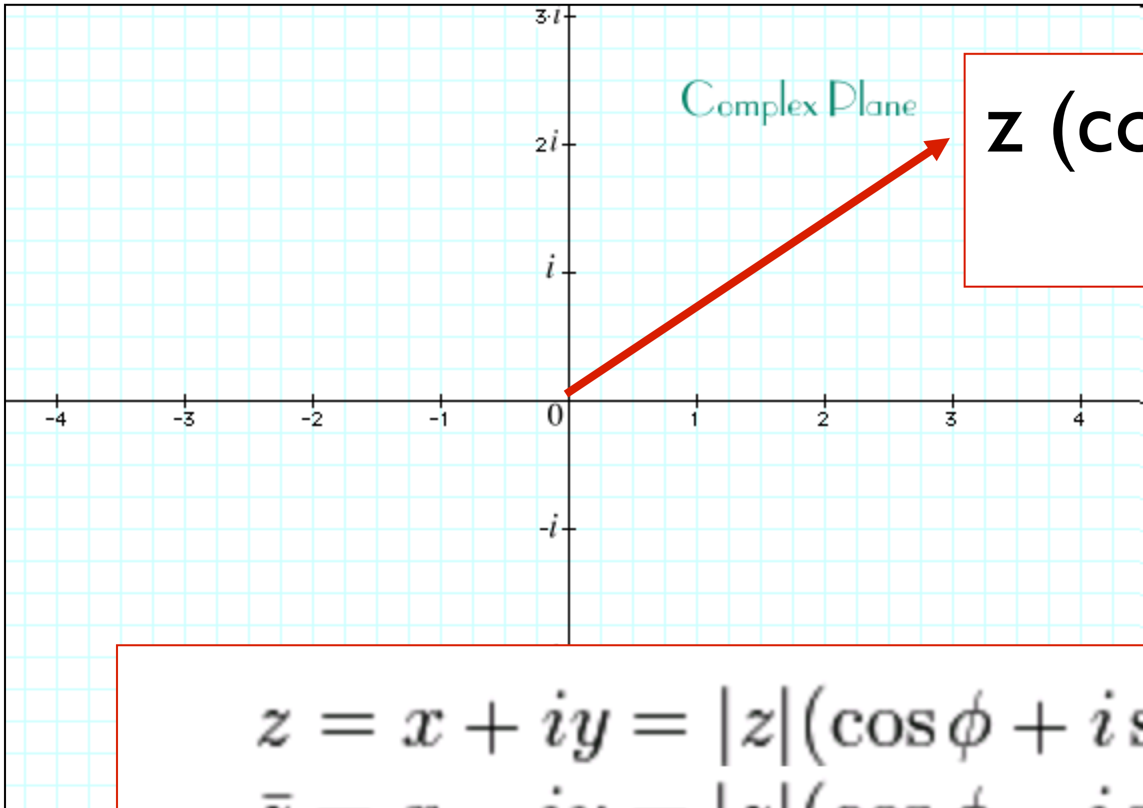
Q: *One can draw complex numbers in the complex plane. Which is the correct for the complex conjugate of*

3 – 2 i ?



A: *(a) complex conjugate is 3 + 2 i , obtained by changing i → –i*

Complex numbers summary



z (complex number)
= 3 + 2i

$$z = x + iy = |z|(\cos\phi + i\sin\phi) = |z|e^{i\phi}$$
$$\bar{z} = x - iy = |z|(\cos\phi - i\sin\phi) = |z|e^{-i\phi}$$

where

$x = \mathrm{Re}\{z\}$ the real part

$y = \mathrm{Im}\{z\}$ the imaginary part

$|z| = \sqrt{x^2 + y^2}$ the magnitude of z

$\phi =$ atan2(y, x)

Plane waves in different forms

- solutions to EM wave equation: $$\frac{\partial^2 \vec{E}}{\partial t^2} = c^2 \frac{\partial^2 \vec{E}}{\partial x^2}$$

- real forms: $$\begin{aligned} E_1(x,t) &= A\cos(kx - \omega t) + B\cos(kx + \omega t) \\ E_2(x,t) &= A\sin(kx - \omega t) + B\sin(kx + \omega t) \end{aligned}$$

- complex form: $$E_3(x,t) = Ce^{i(kx - \omega t)} + De^{i(-kx - \omega t)}$$

(just reshuffling of coefficients)

- plug into wave equation to get: $\omega^2 = c^2 k^2 \Longleftrightarrow E^2 = c^2 p^2$
- relativistic dispersion for a massless particle (photon)

Schrödinger's equation

Erwin Schrödinger
(1887 – 1961)

- ingredients:
  - *free particle: $E = p^2/2m$, with* $\psi = e^{i(p\cdot r - Et)/\hbar}$
    instead of E = pc (for photon)
  - *linear in $\psi(r,t)$ (superposition):*
    if ψ_1 and ψ_2 are solutions so is $\psi = c_1\psi_1 + c_2\psi_2$

- Schrodinger's wave equation: $i\hbar\dfrac{\partial\psi}{\partial t} = H\psi$
  - *where* $H = \dfrac{p^2}{2m} + V(r)$ *is the Hamiltonian of the system*

$$= -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

kinetic energy + potential energy

  - *1d:*

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

compare to EM wave eqn:

$$\frac{\partial^2\vec{E}}{\partial t^2} = c^2\frac{\partial^2\vec{E}}{\partial x^2}$$

Compare Schrodinger's and EM waves

- $$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$ vs $$\frac{\partial^2\vec{E}}{\partial t^2} = c^2\frac{\partial^2\vec{E}}{\partial x^2}$$

- *both are linear equations → superposition/interference*

- *$E = p^2/2m$ (dispersion/spreads) vs $E = pc$*

$$i\hbar\frac{\partial}{\partial t} \rightarrow E, \quad -i\hbar\frac{\partial}{\partial x} \rightarrow p_x$$ → *that's why one time and two space derivatives*

- *$|\psi|^2$ = probability density for finding a particle at x,t*

- *$|E|^2$ = light intensity = probability density of finding a photon at x,t*

- *ψ complex single function vs **E** is a real 3 component vector*

Operators and observables in QM

- Operators O:
  - *position:* x
  - *momentum:* $p = -i\hbar\nabla = -i\hbar\frac{\partial}{\partial x}$
  - *energy:* $$\begin{aligned} H &= \frac{p^2}{2m} + V(r) \\ &= -\frac{\hbar^2}{2m}\nabla^2 + V(r) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(r) \end{aligned}$$
- Observables of O in state ψ: $\langle\psi|O|\psi\rangle = \int d^3r\psi^* O\psi$
  - $\langle\psi|x|\psi\rangle = \int dx\psi^* x\psi = \int dx x|\psi|^2$
  - $\langle\psi|p|\psi\rangle = -i\int dx\psi^* \frac{d}{dx}\psi$

Single vs ensemble measurements

- $\psi(x,t)$ is deterministically determined by $V(x)$ from S. Eqn

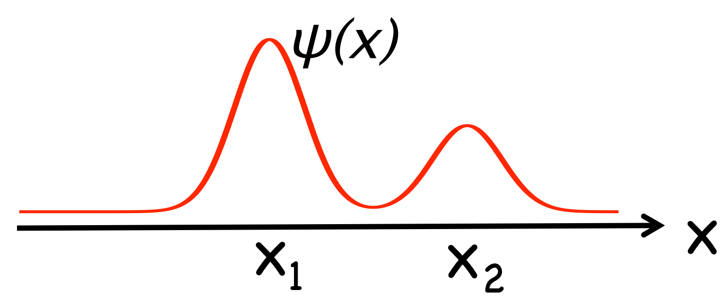
... BUT ...

- measurement of O in a single experiment:

(interaction with a classical system)

can essentially be anything (any of the eigenvalues of O) allowed by nonzero $\psi(x)$

e.g., for $\psi(x)$, measurement of x can find any value, but most likely value is x_1 and $\langle x \rangle \approx (x_1+x_2)/2$



- measurement of O in an ensemble of (many) experiments:

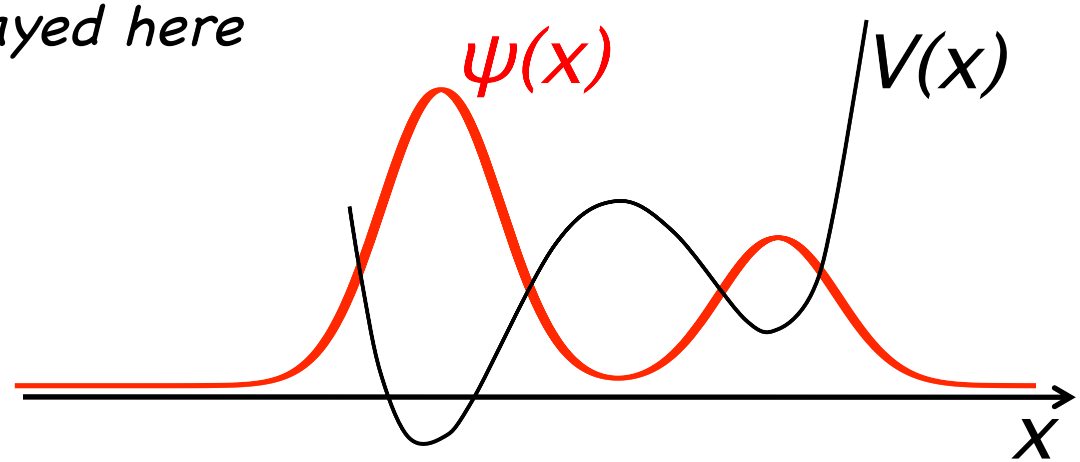
obtain average value of O using $P(x) = |\psi(x)|^2$

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

clicker question

Wave-function interpretation

Q: *What is not true about a particle in a potential well (black) described by the wave-function (red) displayed here*



a) more likely to be found in the left than in the right well

b) in a measurement can in principle be found in any position

c) probability of being found at some x is 1

d) cannot be found on top of the hill since it does not have enough energy and energy is conserved

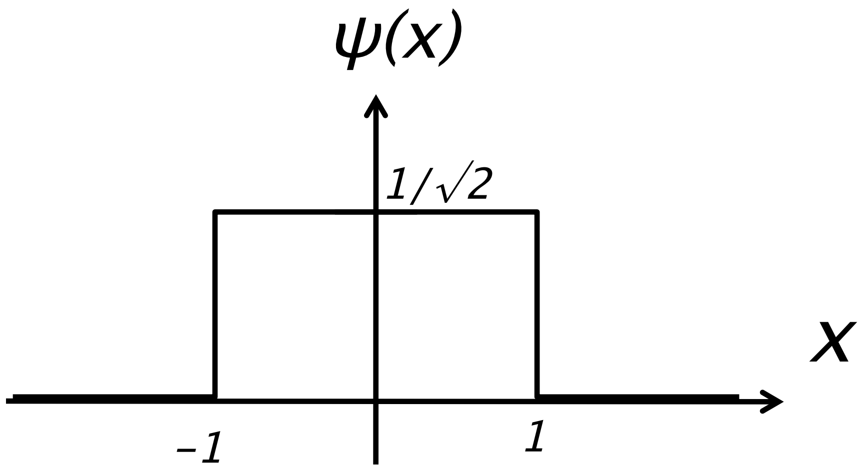
e) if it is found to be in the right well, a little later it can be found in the left well

A: *(d) Although the probability (after many many measurements) is low, in any one measurement it can indeed be found anywhere $\psi \neq 0$*

clicker question

Value of observables

Q: *For a particle described by a wavefunction below what is the average value of the potential energy $V(x) = V_0\, x^2$ found after many measurements*



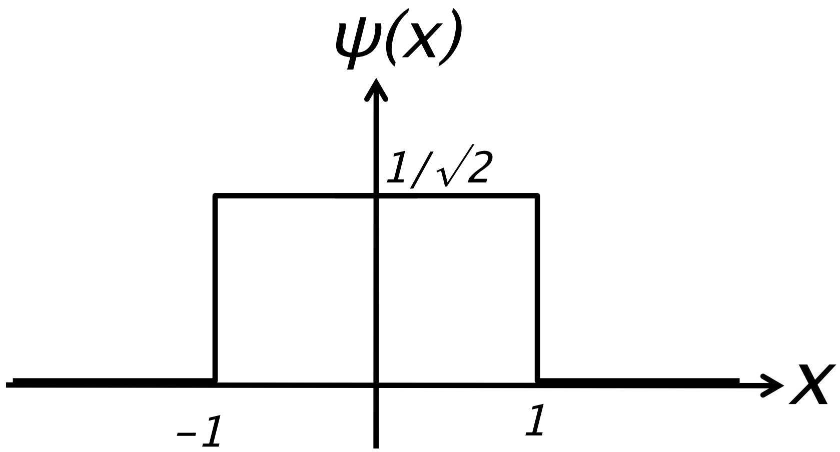
(a) V_0 , (b) 0, (c.) 10 V_0 , $\boxed{\text{(d) } V_0/3}$, (e) $V_0/2$, (f) none

A: *(d) The probability density is constant, $P = |\psi|^2 = ½$, which when used to average (integrate from $-1 < x < 1$) $V_0\, x^2$ gives* $V_0/3$.

clicker question

Value of observables

Q: *For a particle described by a wavefunction below what is the highest value of potential energy $V(x) = V_0\, x^2$, that can be found in any one measurement of $V(x)$ via a measurement of x ?*



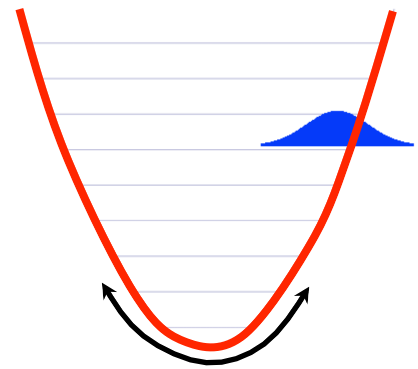
(a) V_0 ,   (b) 0,   (c.) 10 V_0 ,   (d) $V_0/3$,   (e) $V_0/2$,   (f) none

A: *(d) In any one measurement, the value of $V(x)$ observable can be anything allowed by the wavefunction. Thus, the maximum one that can be found is for $x=1$, giving $V(1) = V_0$.*

Two classes of problems

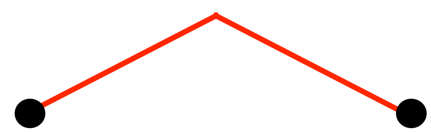
- *Time evolution* of ψ(r,t) with initial ψ(r,0) noneigenstate:
  - *evolves according to time dependent Schrodinger's Eqn*

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$



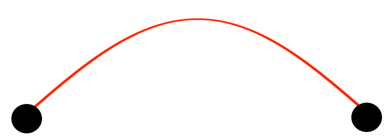
  - *e.g., particle oscillating in a well:*

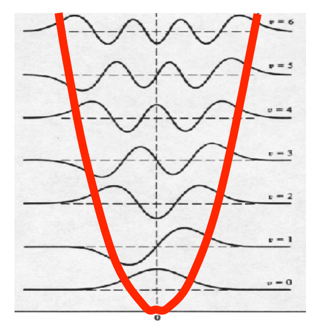
cf randomly plucking a string:



- *Eigenstates:*

cf plucking a single note:





- take $\psi(r,t) = e^{-iEt/\hbar}\psi_E(r)$
- $\Longrightarrow$ *time-independent* *Schrodinger Eqn:* $E\psi_E = H\psi_E$
- from $\psi_E(r)$, we then obtain ψ(r,t) (if needed)

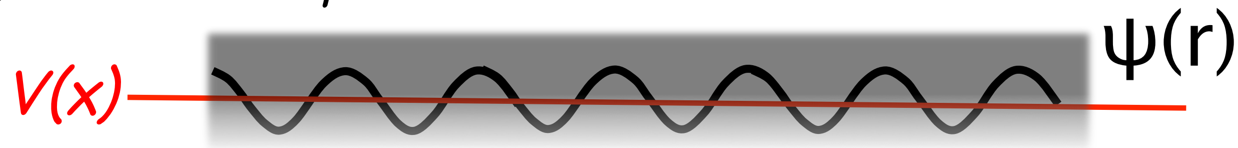
Two types of eigenstate problems

Possible states given by:

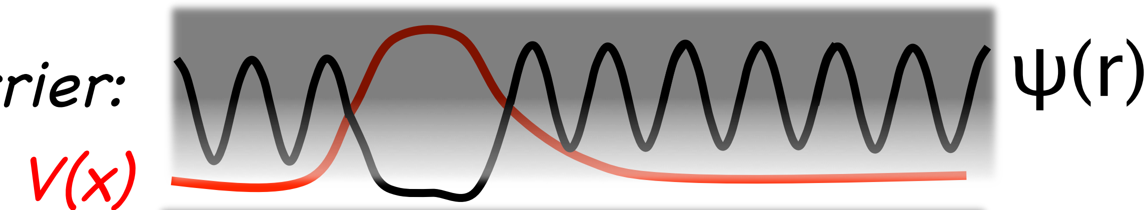
specified by V(x)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2}+V(x)\psi_E=E\psi_E$$

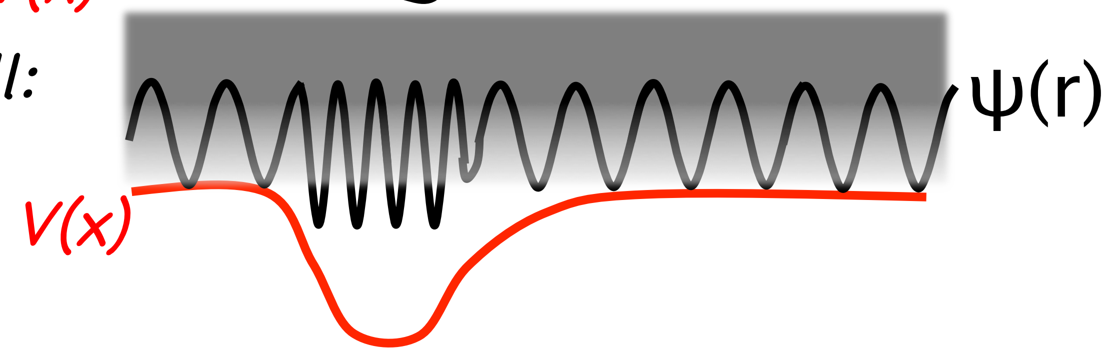
- **Extended states:** *V(x) that allows particle → x = ∞*
  - *free particle, (V=0):*



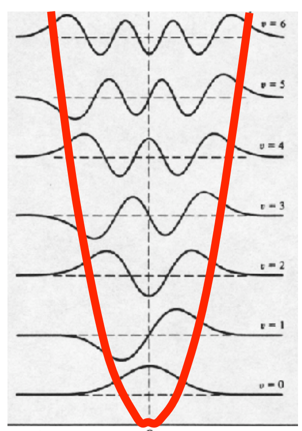
  - *particle moving near a barrier:*



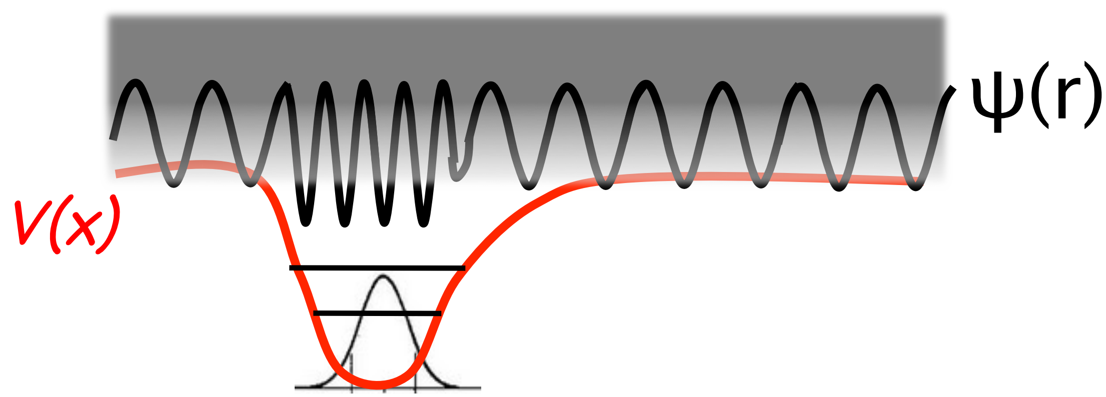
  - *particle moving above a well:*



- **Bound states:** *confined*
  - *potential well:*



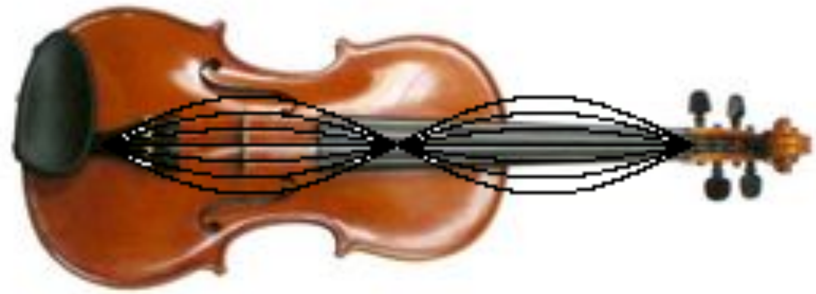
Some V(x) allow both extended and bound states:



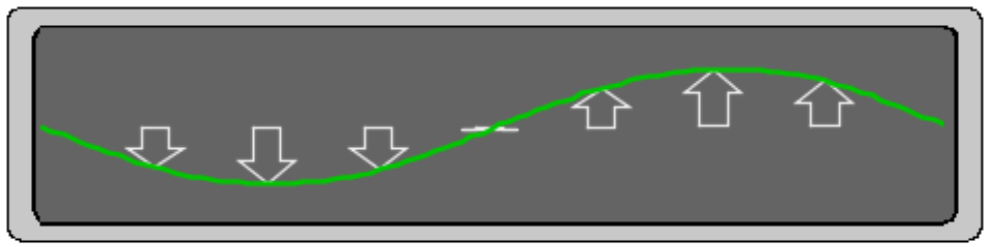
Discrete eigenstates (standing waves)

- standing waves on a violin string:

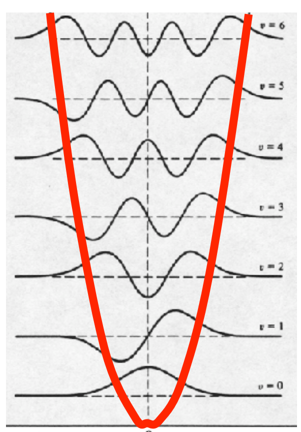
  only certain values of k=πn/L and ω are allowed due to boundary conditions (location of nodes of clamped ends); same for other musical instruments

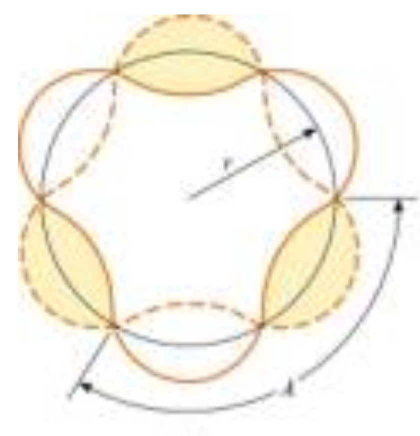


- standing EM waves in a microwave oven:



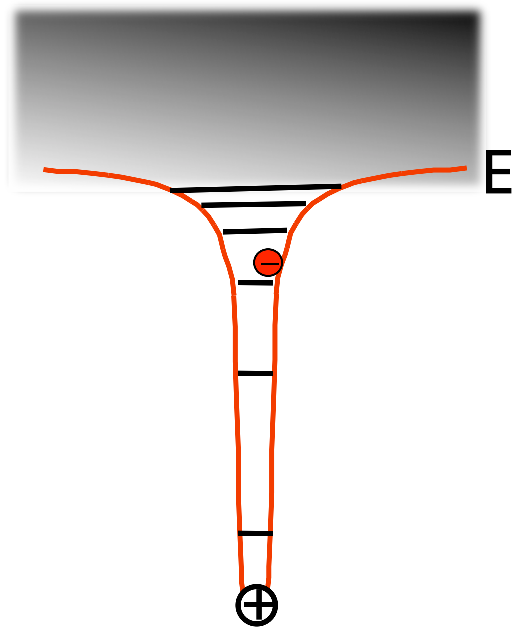
- standing Schrodinger matter waves in a potential well:





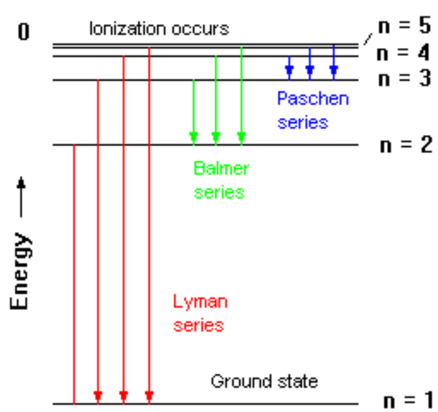
Standing vs free waves

electron bound in atom:

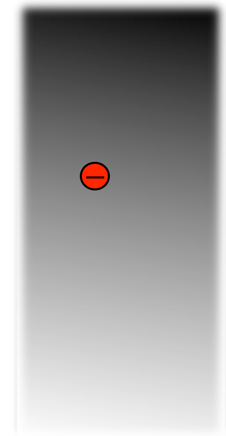


boundary conditions
⇒ standing waves

only certain energies allowed quantized energies



free electron:

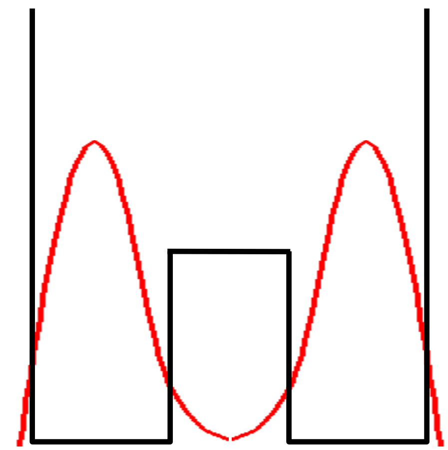


no boundary conditions
⇒ traveling waves

any energy allowed
continuum of energies

Schrodinger's cat: macroscopic QM

- particle in double-well potential: *in superposition of left and right wells, $\psi=\psi_L + \psi_R$*



- "cat" in a superposition of a dead and alive states: *have been created in a number of systems*