

Review Model Problems

Particle—no potential

Wave solution—continuous wavelength/Energy

Since only $(T=H)$ $KE = [H,p] = 0$

And particle has conserved momentum (Classical no Force)

INSERT EQN

Add potential – E, no longer continuous quantization from B.C. (restrict motion)

1.

$V = \text{Const.}$ But restricted in space:

-- box-artificial but good model to illustrate

E – number of wavelengths in box (curvature)

Must be half integral ($\psi(0) = \psi(L) = 0$) so quantize

-- circular box ψ same picture but integer wavelength ψ continuous first de??? or no double value $\psi(2) = \psi(???)$

Becomes eigen function Lz

--multidimensional box ψ final degeneracy as a function of symmetry

[if $x=y$ then excitation along x and y must have the same impact]

provides great example of separation of variables summed $H, E = \text{product}$ ψ works because coordinates are independent

Now if potential not infinite still have B.C. lent these are ones related to first postulate in that ψ must be continuous etc., and $\psi^*y = N$

Also expect continuity between problem with $V =$ and $V =$ very large ψ steady change as walls???

Atkins 2.3 and 2.5

1. General aspects of Schrödinger's Eqn

INSERT EQN

ψ derived to correspond to classical mech, not contain “pure gin” prop such as spin

ψ also no relativistic connection

Now looking at time dependence—not a wave eqn

From classical point of view wave equation time/space both second de??? form is diffusion equation

(does tell us what particle does in moving)

for $H = H(t)$

Separation: $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$

Time indep part: $H = E = \psi(x)$ – standing wave equation

i.e. wave equation from spatial point

Time dep part: just a phase $e^{-iEt/\hbar}$

Trick here is to remember that all measurement use $|\psi|^2$ (prob) \times (prob. meas.)

So phase cancels: $e^{iEt/\hbar} \times e^{-iEt/\hbar} = 1$

So have $\psi(x,t) = \psi(x) f(t)$ – stationary state

2. Quantization – big difference from classical – Energy not continuous (??)

rearrange: **INSERT EQN** curvature

-- $V=E$ on $\psi = 0$ – no curvature **INSERT DRAWING**

-- $\psi = 0$, curvature $\sim V-E$ – sign change:

all of this makes the function oscillate (wave) so the potential – causes the wave behavior

but also leads to the bounds because $\int \psi^2 dx = N$

INSERT GRAPH

In order to get the $\psi = 0$ behavior

Slope at x for $V-E \sim$ must be limited—not all shapes

Only a few will give $\psi = 0$ both sides potential contains the ???????? particle

Particle in a finite well: **INSERT GRAPH**

INSERT EQN

at boundary $\psi(0)$, $E < V_0$ so have change from $E > V$ to $E < V$

– curvature must change at wall from (-) to (+) from $\psi(0)$

– Restriction to be finite $\psi \sim e^{+kx}$ ($x < 0$) damp

– in II – (+), $(V - E)$ – curvature

INSERT GRAPH

Now at $\psi(L)$ – change sign curvature again to (+) quantization ψ only contain $\psi(L)$

values lead to proper damping ψ other integral # 's fit

$\psi = 0$ – zero curve so opp curve (+) and (-)

Putting together the sides of I II, and II III requires finding the amplitude of the function

at $x = 0$ and $x = L$ – $\psi(0) = \psi(L) : C = A$

INSERT EQN

Now what is unusual is that the constants are functions of the energy levels – πb – only of L

so ratioing **INSERT EQN**

give a complex function that could be solved for E

INSERT EQN

Point: this solved only for certain values of E

Handout

Kangman, p. 191, figure plot both sides find intersection

– regular spacing violated – πb – expand $\sim k^2$, have $\sim \text{const}$ (amide)

– number of levels limited: **INSERT EQN** (max level)

– $E > V$ get continuum, unbound states

What about inverting the problem – tunnelling?

INSERT GRAPH

so now particle in Region I can approach II and see a wall (V_0)

INSERT EQN

INSERT EQN

so have plane wave solution in each part:

$$\psi_p = A_p e^{+ikx} + B_p e^{-ikx} \quad p = I, II, III$$

INSERT EQN

INSERT EQN

now if $E < V_0$ – classically particle bounces back and does not penetrate barrier (stays on one side)

but $k_{II} = \text{imaginary} = iK$ **INSERT EQN**

$$\psi_{II} = A_{II} e^{-Kx} + B_{II} e^{+Kx}$$

so in barrier – function decays and grows exp but does not oscillate

as width on height increases – $B_{II} \rightarrow 0$ since clearly $\psi_{II} \rightarrow 0$ (inside barrier)

but – thin barrier not yet zero and if thin enough will be some probability on other side (tunnel)

ex 1eV electron in 2V barrier

decays $\sim e^{-5.12(x/nm)}$ so decays $\sim 1/e$ in 0.2 nm

Thin barrier $B_{II} \rightarrow 0$ since rising function stays finite inside

$$X = 0: A_I + B_I = A_{II} + B_{II} \quad Ae^{ikl} + Be^{-ikl} = A_E e^{-kl} + B_{II} e^{-kl}$$

now have 4 eqn and 6 unknowns _ if assume specific case of particle approaching barrier from left (momentum right)

Then know $B_{III} = 0$ (i.e. particles right of barrier only to risk) but cannot set $B_I = 0$ since could reflect.

Now: **INSERT EQN** _ probability of reflection
INSERT EQN _ probability of penetration (tunnel)

Transmission probi/Ag **INSERT EQN** turns out

Correspondence with classical:

How work:

1. as V increase _ $G \sim Ve$ **INSERT EQN** _ , and $P \sim 0$

So high barrier _ no transmission

2. as L increase _ $G \sim e^{KL}$ _ , $P \sim 0$, so wide barrier _ no transmission

3. note: as m increase, G inc we^{tm} and $P \sim 0$

4. as E increases _ $G \sim$ **INSERT EQN** _ 0, so very high energy $P \sim$ non zero
(eg. Like bullet on better particle)

so if E suff and V,L small oscillary (line mom.) mave/ part ????? strike wall from left,
part penetrate damp, rearrange with reduced amplitude A_{III}

antitunnelling (analogy to reflection when change indep)

for $E > V$ classically $P = 1$ but with QM $P < 1$, some reflection due to V