$$\langle \psi_{0j} | H_1 | \psi_{0i} \rangle + \langle \psi_{0j} | H_0 | \psi_{1i} \rangle$$

$$= E_{1i} \underbrace{\langle \psi_{0j} | \psi_{0i} \rangle}_{\delta_{ij}}$$

$$+ E_{0i} \underbrace{\langle \psi_{0j} | \psi_{1i} \rangle}_{\text{coefficients } c_{1ij}}$$

Say Q is an observable (thus $Q = Q^\dagger$).

$$Q | q \rangle = q | q \rangle$$

where q is an eigenvalue of Q

Say $|\alpha\rangle$ is general

$$\langle \alpha | Q | q \rangle = q \langle \alpha | q \rangle$$

by definition of Hermitian conjugate

$$\langle q | Q^\dagger | \alpha \rangle^* = q \langle q | \alpha \rangle^*$$

Take the complex conjugate

6-32

of both sides

$$\langle q | Q^\dagger | \alpha \rangle = q^* \langle q | \alpha \rangle$$

$= Q$ since Q is an observable

$= q$ since eigvalues are pure real.

$$\langle q | Q | \alpha \rangle = q \langle q | \alpha \rangle$$

$\therefore$ Since $|\alpha\rangle$ is general

$$\boxed{\langle q | Q = q \langle q | = \langle q | q}$$

So $\langle \psi_{0j} | H_0 = \langle \psi_{0j} | E_{0j}$

$$\therefore \langle \psi_{0j} | H_1 | \psi_{0i} \rangle + E_{0j} \langle \psi_{0j} | \psi_{1i} \rangle$$

$$= E_{1i} \delta_{ij}$$

$$+ E_{0i} \langle \psi_{0j} | \psi_{1i} \rangle$$

If $i = j$, we get $E_{1i} = \langle \psi_{0i} | H_1 | \psi_{0i} \rangle$

which is a pretty reasonable result.

The 1^{st} order correction to the energy is given by the diagonal matrix element of H_1 with the unperturbed states.

You might even have guessed this.

if $\langle \psi_{0j}|H_1|\psi_{0i}\rangle = 0$ and $E_{0i} - E_{0j} \neq 0$ then $\langle \psi_{0j}|\psi_{1i}\rangle = 0$ of course. No problem

If $i \neq j$, $\langle \psi_{0j}|H_1|\psi_{0i}\rangle = (E_{0i} - E_{0j})\langle \psi_{0j}|\psi_{1i}\rangle$

If LHS $\neq 0$ and $E_{0i} - E_{0j} = 0$, then $\langle \psi_{0j}|\psi_{1i}\rangle$ diverges and perturbation theory fails.

$$\langle \psi_{0j}|\psi_{1i}\rangle = \frac{\langle \psi_{0j}|H_1|\psi_{0i}\rangle}{E_{0i} - E_{0j}}$$

Especially if there are no other states to consider in perturbation. If there, it is as good as half-way house

If $\langle \psi_{0j}|H_1|\psi_{0i}\rangle = 0$ and $E_{0i} - E_{0j} = 0$, (see p. 6-34b) ~~then $|\psi_{0j}\rangle$ and $|\psi_{0i}\rangle$ are~~ "good" ~~linear~~ combinations ~~(see Gr-258, 259)~~.

But how do we find $\langle \psi_{0j}|\psi_{1i}\rangle$ in this case? For degenerate states matrix H is already diagonal, and so $|\psi_{0i}\rangle$ for degenerate states are the perturbed states.

already. So the $\langle \psi_{0j}|\psi_{1i}\rangle = 0$ works ~~at least~~ ~~is sufficient~~ ~~approximation~~. ??

But since $\{|\psi_{0i}\rangle\}$ is a complete set, we can expand

$$|\psi_{1i}\rangle = \sum_m c_{1im} |\psi_{0m}\rangle$$

$$\therefore \langle\psi_{0j}|\psi_{1i}\rangle = \sum_m c_{1im} \underbrace{\langle\psi_{0j}|\psi_{0m}\rangle}_{\delta_{jm}}$$

$$= c_{1ij}$$

$$\therefore c_{1ij} = \langle\psi_{0j}|\psi_{1i}\rangle = \frac{\langle\psi_{0j}|H_1|\psi_{0i}\rangle}{E_{0i} - E_{0j}}$$

We assumed non-degeneracy and so $E_{0i} \neq E_{0j}$ for $i \neq j$ so no catastrophe

but we have this catastrophe,

$$c_{1ii} = \text{undefined} = \frac{\langle\psi_{0j}|H_1|\psi_{0i}\rangle}{0}$$

but $i \neq j$ by our assumption on p. 6-33

$i \neq j \quad \langle \chi_{0j} | H_1 | \chi_{0i} \rangle = (E_{0i} - E_{0j}) \langle \chi_{0j} | \chi_{1i} \rangle$

If $\langle \chi_{0j} | H_1 | \chi_{0i} \rangle = 0$ and $E_{0i} - E_{0j} \neq 0$,

then $\langle \chi_{0j} | \chi_{1i} \rangle = 0$

and no immediate problem.

If $\langle \chi_{0j} | H_1 | \chi_{0i} \rangle \neq 0$

and $E_{0i} - E_{0j} = 0$ degeneracy

or $|E_{0i} - E_{0j}|$ small near degeneracy

non-degenerate perturbation theory fails for sure

~~for~~ as $|E_{0i} - E_{0j}| \to 0$ at some point the perturbation will not converge and so failure or very slow convergence is ~~must~~ happen.

If $\langle \chi_{0j} | H_1 | \chi_{0i} \rangle = 0$

and $|E_{0i} - E_{0j}| = 0$

6-34c

or is very small.

Well if $E_{0i} - E_{0j} = 0$ exactly

$\langle \Psi_{0j} | \Psi_{1i} \rangle$ is

indeterminate.

Any value satisfies the 1st order equation.

I think we are free to choose (as Milton Friedmann used to say) the ~~there~~ value.

$\langle \Psi_{0j} | \Psi_{1i} \rangle = 0$ is the good choice.

Since higher order perturbation ~~at~~ is affected by lower orders, this choice will affect higher order terms.

Can we arrange $\langle \Psi_{0j} | H_1 | \Psi_{0i} \rangle = 0$

and should we in case of degeneracy. ~~and near-degeneracy.~~

Yes & Yes.

We can diagonalize (to anticipate)

the degenerate or
~~nearly all degenerate~~ sub set
to get new states
which are still eigenstates
of H_0 and still orthonormal.
~~with~~ to all $\{|\psi_{0i}\rangle\}$ and as eigenstates
of H_0 are still degenerate,
but not degenerate as
approximate eigenstates H.

Presumably the energies in
the perturbation series give
the right corrections. Right I think.

Near-degeneracy?
Formally trickier I think.
Diagonalization gives new
states that are mixtures relative
to H_0 ~~and NOT orthogonal~~
~~to~~ still orthogonal to all
other $\{|\psi_{0i}\rangle\}$ states

Not eigenstates of H_0 anymore. but closer to eigenstates of H_0

$\boxed{6\text{-}34e}$

So $\{|\Psi_{0i}\rangle\}_{non-subset}$

and $\{|\Psi_{0i}'\rangle\}_{subset}$ $\left\{ \text{mixtures of } \{|\Psi_{0i}\rangle\}_{subset} \right.$

the diagonalized near degenerate states.

Do they constitute a complete set?

Yes. ~~But not~~

Orthonormal? Yes since all $\{|\Psi_{0i}\rangle\}$ are orthonormal.

$\{|\Psi_{0i}'\rangle\}_{subset}$ Not eigenstates of H_0.

~~Can they be used for the perturbation ex~~

Can $\{|\Psi_{0i}\rangle\}_{non}$ and $\{|\Psi_{0i}'\rangle\}_{subset}$ be used for the expansion series?

Looks tricky. But maybe it could be done.

the degenerate subset $\{|\chi_{0i}\rangle\}_{sub}$
to get new states
that are still
eigenstates of H_0 and still
orthonormal,

$\{|\chi_{0i}\rangle\}_{sub}$ are still degenerate
as ~~diff~~ eigenstates of H_0

One can proceed with ordinary
perturbation theory
and I'd guess that the
perturbation corrections
to energy would lead to
the same energies for the
$\{|\chi_{0i}\rangle\}_{sub}$ that the diagonalization
gives.

$\langle \chi_{0i} | H | \chi_{0j} \rangle$ for states from the subset

$= \langle \chi_{0i} | (H_0 + \lambda H_1) | \chi_{0j} \rangle$

They do. $= E_{0i}\delta_{ij} + \lambda E_{1i}\delta_{ij}$

But what of the near degenerate case?

Here $\{|\psi_{0i}\rangle\}_{subset}$ after diagonalization are such that

$$\langle\psi_{0i}|H_1|\psi_{0j}\rangle = E_{1i}\,\delta_{ij}$$

but $\{|\psi_{0i}\rangle\}_{subset}$ are NOT exact eigenstates of H_0 since there are mixtures of non-degenerate states.

$\{|\psi_{0i}\rangle\}_{subset} + \{|\psi_{0i}\rangle\}_{non-subset}$ are still a complete orthonormal set.

From p. 6-31, one could still write

$$\cancel{\langle\psi_{0j}|H_1|\psi_{0i}\rangle + \langle\psi_{0j}|H_0|\psi_{1i}\rangle = E_{1i}\langle\psi_{0j}|\psi_{0i}\rangle + E_{0i}\langle\psi_{0j}|\psi_{1i}\rangle \quad \delta_{ij}}$$

There must be a formally correct way to treat this case, but darned if I can see it. Maybe it's very finicky.

So $c_{1ij} = \dfrac{\langle \psi_{0j} | H_1 | \psi_{0i} \rangle}{E_{0i} - E_{0j}}$

is only for $i \neq j$

But what is c_{1ii} then?

All the labor on p. 6-17 – 6-25 was to show that normalization of the full perturbed solution requires $c_{1ii} = 0$.

So Now we have the complete 1st order perturbation correction and 1st order corrected quantities

In my view Gr-253 muffs ~~this~~. He shows that you can choose $c_{1ii} = 0$, but NOT ~~that~~ it must be to preserve normalization — Not obviously anyway.

6-36a

$$E_{1i} = \langle \chi_{0i} | H_1 | \chi_{0i} \rangle$$

$$E_i^{1st} = E_0 + \lambda \langle \chi_{0i} | H_1 | \chi_{0i} \rangle$$

mixtures of unperturbed state

$$|\chi_{1i}\rangle = \sum_{\substack{j \\ j \neq i}} \frac{\langle \chi_{0j} | H_1 | \chi_{0i} \rangle}{E_{0i} - E_{0j}} |\chi_{0j}\rangle$$

We note the closer in energy $|\chi_{0j}\rangle$ to $|\chi_{0n}\rangle$ the bigger the ~~eff~~ mixing in general due the denominator

$$|\chi_i^{1st}\rangle = |\chi_{0i}\rangle + \lambda \sum_{j \neq i} \frac{\langle \chi_{0j} | H_1 | \chi_{0i} \rangle}{E_{0i} - E_{0j}} |\chi_{0j}\rangle$$

Note $|\chi_i^{1st}\rangle$ is NOT exactly normalized. It's only normalized to 1st order.

Not i comes first in denominator and second in numerator.

The imposed normalization constraint is for $|\chi_i\rangle$ normalized

The exact perturbed state.

There must be some profound reason why mixing of states decreases with increases in energy separation.

We should reflect on it.

We reflect. Maybe Two things at work expressed by denominator & numerator

a) Recall $\frac{\partial^2 \psi}{\partial x^2} = \kappa^2 \psi$

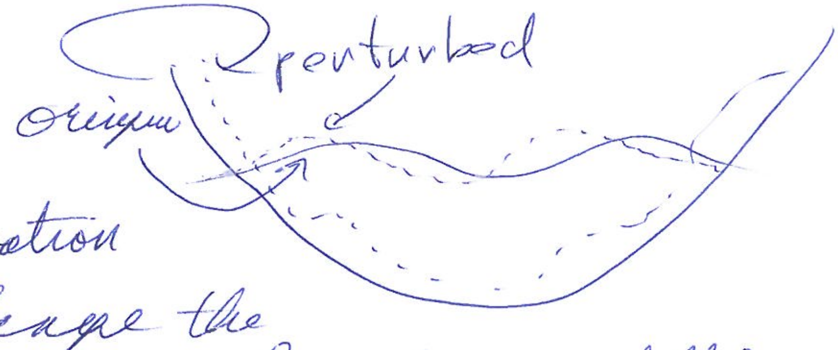
$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V - E)}$$

$\kappa = ik$ if $E > V$

$$k = \sqrt{\frac{2m}{\hbar^2}(E - V)}$$

So E controls local curvature/oscillation.

It seems clear that a small perturbation can only change the shape of the wave function a little.



— So one only needs a bit more or less curvature everywhere and states local in energy space

6-36c

give that.

— remote states in energy give ~~too many~~ lots of wiggles (higher E) or ~~too much~~ lots of smoothing (lower E)

So ultimately it seems like the wave nature dictates the fall off of ~~on~~ mixing with increasing $|E_{0i} - E_{0j}|$.

But what of non-wave function perturbation?

Spin ~~perturba~~ state perturbation?

The same perturbation theory formalism applies.

Well energy still dictates state structure somehow

— more reflection needed.

b) But there is another point.

I think $\langle \Psi_{0j} | H | \Psi_{0i} \rangle$

for $j \neq i$ which are the off-diagonal matrix elements or state couplings in the diagonalization approach

have a <u>tendency</u>

to grow small as $|E_{0i} - E_{0j}|$ increases

For all $|E_{0i} - E_{0j}|$ ~~small or even zero~~

$|\Psi_{0i}\rangle$ and $|\Psi_{0j}\rangle$

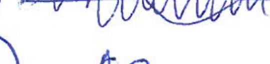
~~for~~ are orthogonal.

But if $|E_{0i} - E_{0j}|$ is small or even zero, that orthogonality is $\left\{ \begin{array}{l} \text{fine-tuned.} \\ \text{global} \end{array} \right\}$

~~But~~ if $|E_{0i} - E_{0j}|$ is large, then $|\Psi_{0i}\rangle$ & $|\Psi_{0j}\rangle$

6-36e

have a very different set
of oscillatory wiggles
and will tend to be
incoherent. → even locally



So even perturbed still tends to be incoherent and near zero. I think.

So $H_1 |\Psi_{0i}\rangle$
distorts $|\Psi_{0i}\rangle$, but tends
in some/often cases to leave as
wiggly as before

$\therefore$ $\langle \Psi_{0j} | H_1 | \Psi_{0i} \rangle$ will

<u>tend</u> to ~~be rather~~

toward zero as $|E_{0i} - E_{0j}|$
grows.

It's just a tendency that can be
overruled by the peculiarities
of $|\Psi_{0i}\rangle$, $|\Psi_{0j}\rangle$, and H_1

— Experience though suggests it is a often/usually
the case I <u>think</u>/guess.

We assumed non-degeneracy, and so our corrections are NOT undefined.

But what if E_{0i} and E_{0j} get very close?
Then the corrections get very big
and
that hints ~~oth~~ that ~~other~~ high orders are needed for accuracy
OR
the series may not converge (in which case perturbation theory is not adequate).

One could say ~~that~~ as $E_{0j} \to E_{0i}$ mixing of the unperturbed states becomes strong and eventually too strong.

That's when the diagonalization approach is Needed (see below)

6) 2^{nd} Order Perturbation

- We only do the 2^{nd} order energy.
- the 2^{nd} order state correction is beyond us. (We could do it. Maybe a good problem.)

From p. 6-29 with $n=2$

$$\sum_{k=1}^{2} H_{2-k} |\psi_{ki}\rangle = \sum_{k=0}^{2} E_{2-k\,i} |\psi_{ki}\rangle$$

$$H_1 |\psi_{1i}\rangle + H_0 |\psi_{2i}\rangle = E_{2i} |\psi_{0i}\rangle + E_{1i} |\psi_{1i}\rangle + E_{0i} |\psi_{2i}\rangle$$

~~We~~ we don't know $|\psi_{2i}\rangle$,
but we can eliminate it
by inner product~~ed~~ with
$|\psi_{0i}\rangle$

$$\langle \psi_{0i}|H_1|\psi_{1i}\rangle + E_{0i}\langle \psi_{0i}|\psi_{2i}\rangle$$
$$= E_{2i} + E_{1i}\langle \psi_{0i}|\psi_{1i}\rangle$$
$$+ E_{0i}\langle \psi_{0i}|\psi_{2i}\rangle$$

These two cancel

E_{1i} and $\langle \psi_{0i}|\psi_{1i}\rangle = 0$

by p. 6-25

$$E_{2i} = \langle \psi_{0i}|H_1|\psi_{1i}\rangle$$

But we know this from p. 6-36

6-40)

So

$$E_{2i} = \langle \chi_{0i} | H_1 | \sum_{\substack{j \\ j \neq i}} \frac{\langle \chi_{0j} | H_1 | \chi_{0i} \rangle}{E_{0i} - E_{0j}} | \chi_{0j} \rangle$$

Note $\langle \chi_{0i} | H_1 | \chi_{0j} \rangle$

$= \langle \chi_{0j} | H_1^{+} | \chi_{0i} \rangle^{*}$ defn. of Hermitian conjugate

$= \langle \chi_{0j} | H_1 | \chi_{0i} \rangle^{*}$ since $H_1 = H_1^{+}$

$$E_{2i} = \sum_{\substack{j \\ j \neq i}} \frac{|\langle \chi_{0j} | H_1 | \chi_{0i} \rangle|^2}{E_{0i} - E_{0j}}$$

$$E_i^{2nd} = E_{0i} + \lambda \langle \chi_{0i} | H_1 | \chi_{0i} \rangle + \lambda^2 \sum_{\substack{j \\ j \neq i}} \frac{|\langle \chi_{0j} | H_1 | \chi_{0i} \rangle|^2}{E_{0i} - E_{0j}}$$

Note as $E_{0j} \to E_{0i}$ we again have an explosion. This suggests that approaching degeneracy ~~[illegible]~~ causes ~~diverges~~ infinities in all order corrections

But I don't know if this is true or not

Note $$E_{2i} = \sum_{\substack{j \\ j\neq i}} \frac{|\langle \psi_{0j}|H_1|\psi_{0i}\rangle|^2}{E_{0i} - E_{0j}}$$

The numerator is always positive.

$\therefore$ If $E_{0i} - E_{0j} > 0$,
there is a positive contribution
to E_{2i}

If $E_{0i} - E_{0j} < 0$, there is
a negative contribution.

So ~~ee~~ E_i^{2nd} is pushed
up by states with $E_{0j} \cancel{<} E_{0i}$
and down by states ~~ø~~
with $E_{0j} > E_{0i}$

~~I think~~ Is this ~~may be an~~ related
phenomenon ~~aspect~~ to the of the "repulsion of
the energy levels" that
turns up with the diagonalization
of the Hamiltonian ~~of~~ with degenerate energy levels.
Probably not — any perturbation would lead to split degeneracy.

6-42

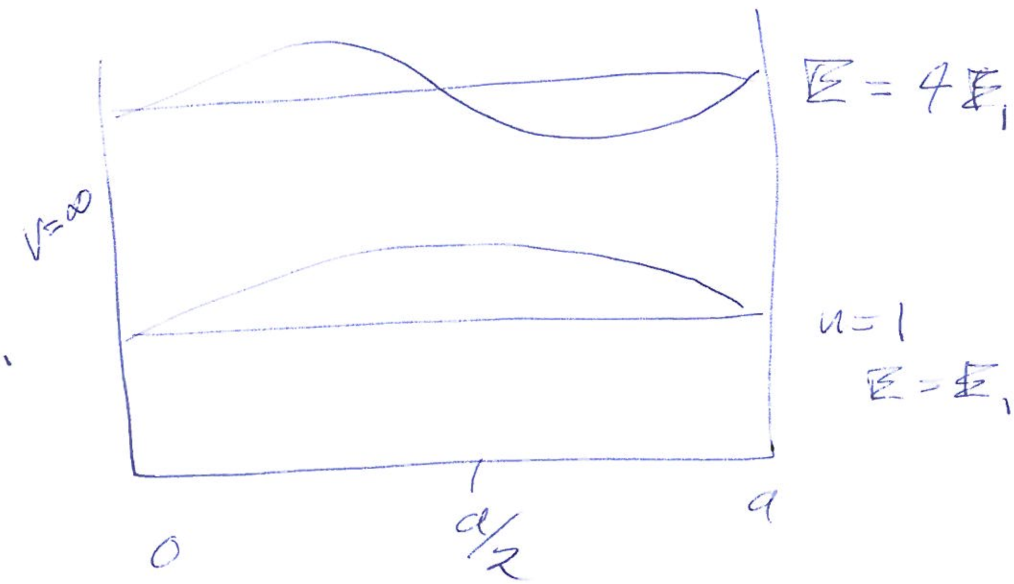
7) Infinite Square Well with A Perturbation (Gr-p.254)

$\psi = \sqrt{\frac{2}{a}} \sin kx$

$ka = n\pi$

$n = 1, 2, 3, \ldots$

quantum numbers



$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 = E_1 n^2$$

The spatial states are non-degenerate, provided we don't add any internal degeneracy like spin

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \qquad \begin{cases} V = 0, & x \in [0, a] \\ V = \infty, & \text{otherwise} \end{cases}$$

Now we add perturbation

$$H_1 = \alpha\, \delta(x - a/2)$$

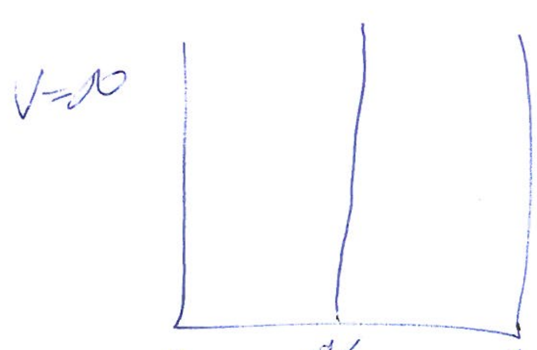
a Dirac delta function potential with α as the potential strength

$$[\alpha] = EL \qquad [\delta(x - \tfrac{a}{2})] = \frac{1}{L}$$

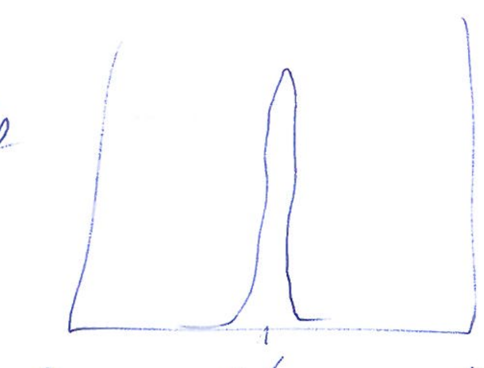
digression

A Dirac Delta function is the limiting form of a sharply peaked function.

One could also think of it as the ~~model~~ ideal model of a sharply peaked function.



models



6-44

— a function that varies rapidly over some distance

interval ~~scale~~ over which ~~that~~ all other behaviors of the system are effectively constant. ~~over that interval.~~

$$\int_a^b f(x)\, \delta(x-x_0)\,dx = \begin{cases} f(x_0), & x_0 \in [a,b] \\ 0, & \text{otherwise} \end{cases}$$

~~Are there any real~~

$$\int_a^b \delta(x-x_0)\,dx = \begin{cases} 1 & x \in [a,b] \\ 0 & \text{otherwise} \end{cases}$$

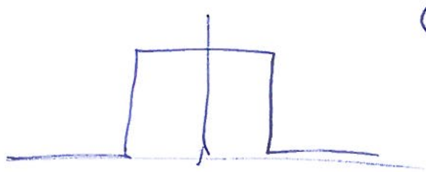
$$\lim_{m\to\infty} \int_a^b f(x)\, \underbrace{\delta_m(x-x_0)}_{\text{a sharply peaked function that grows more sharply peaked as parameter } m \text{ increases}}\,dx$$

Mathematically a Dirac delta function is a limiting process for an integral with a sharply peaked function, A normalized function

There are several common sharply peaked functions that yield Dirac Delta functions as a limiting

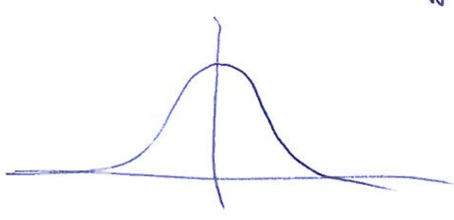
Examples (Arf - 413-414)

a) $$\delta_m = \begin{cases} 0 & x < -\frac{1}{2m} \\ m & -\frac{1}{2m} < x < \frac{1}{2m} \\ 0 & x > \frac{1}{2m} \end{cases}$$



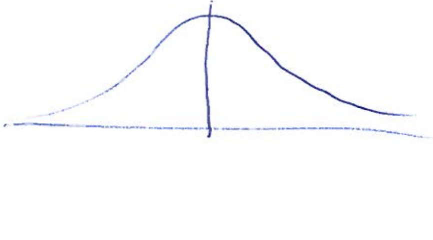
hat function

b) $$\delta_m = \frac{m}{\sqrt{\pi}} e^{-(m^2 x^2)}$$



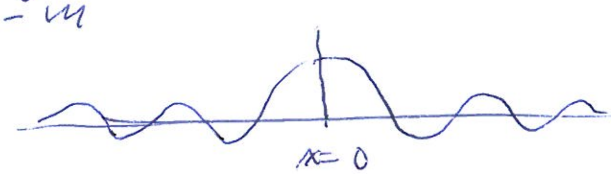
Gaussian

c) $$\delta_m = \frac{m}{\pi} \frac{1}{1+m^2x^2}$$ Lorentzian



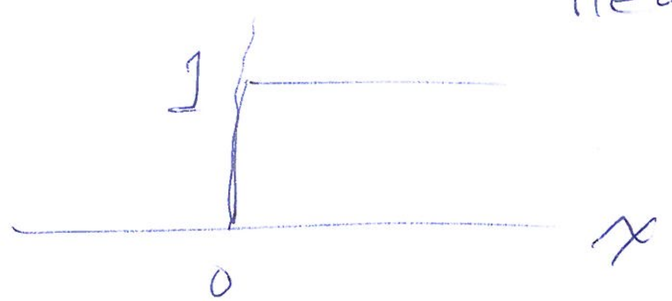
6-46)

d) $S_m = \frac{\sin mx}{\pi x} = \frac{1}{2\pi}\int_{-m}^{m} e^{ixt}\,dt$



Integral of Dirac Delta function

$$\int_{-\infty}^{x} \delta(x')\,dx' = \underbrace{H(x)}_{\text{Heaviside step function}}$$



$$\int_{-\infty}^{x} f(x)\,H(x)\,dx = \int_{0}^{x} f(x)\,dx$$

Derivative of Dirac delta function

$$\int_a^b f(x)\,\frac{d\delta(x)}{dx}\,dx$$

$$= \underbrace{f(x)\,\delta(x)\Big|_a^b}_{=0 \text{ as long as } b\neq 0,\ a\neq 0} - \int_a^b \frac{df}{dx}\,\delta(x)\,dx$$

= 0 as long as $b \neq 0, a \neq 0$ which are undefined cases in general.

$$= \begin{cases} -\frac{df}{dx}(0) & \text{zero in interval } [a,b] \\ 0 & \text{out of interval} \end{cases}$$

This can be generalized ~~too~~

$$\int_a^b f(x)\,\frac{d^n\delta(x)}{dx}\,dx$$

$$= (-1)^n \int_a^b \frac{d^n f}{dx}\,\delta(x)\,dx$$

$$= \begin{cases} (-1)^n \dfrac{d^n f}{dx}(0) & \text{zero in interval } [a,b] \\ 0 & \text{zero out of interval } [a,b] \end{cases}$$

Dirac Delta function of a function

$$\int_a^b f(x)\,\delta(g(x))\,dx$$

Let $y = g(x)$

$dy = g'(x)\,dx$

$$\int_{g(a)}^{g(b)} f(g^{-1}(y))\,\delta(y)\,\frac{dx}{g'(g^{-1}(y))}$$

6-98

$$= \begin{cases} \dfrac{f(g^{-1}(0))}{g'(g^{-1}(0))} & \text{if } 0 \in [g(a), g(b)] \\ 0 & \text{otherwise.} \end{cases}$$

If $g(x) = ax + b$ (a common case),

the $\int_c^d f(x)\, \delta(ax+b)\, dx$

$y = ax + b$

$x = \dfrac{y-b}{a}$

$$= \begin{cases} \dfrac{f(-b/a)}{(-b/a)} & \text{if } 0 \in [ac+b, ad+b] \\ 0 & \text{otherwise.} \end{cases}$$

Real Dirac Delta functions in Nature in some sense?

I don't know.

For many fast varying functions

relative to context,

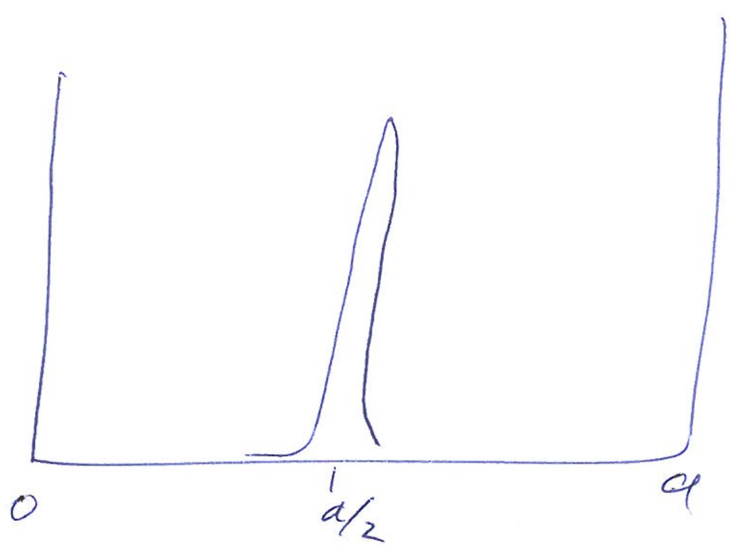
a <u>Dirac Delta function</u> is a good model.

<u>But</u> a real One?

What would it mean?

For the infinite square well,

~~the~~ Dirac Delta function can be



thought of as a model for a sharply peaked function.

Can we guess what such

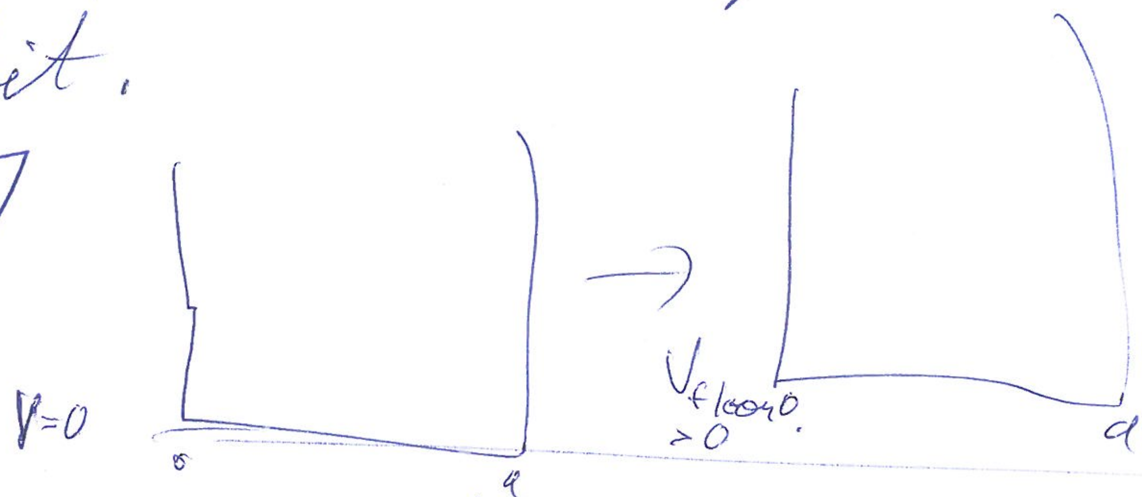
~~peta~~

$\boxed{6\text{-}50}$

perturbation would do to the solutions?

Well raise the energies a bit.

if $\alpha > 0$

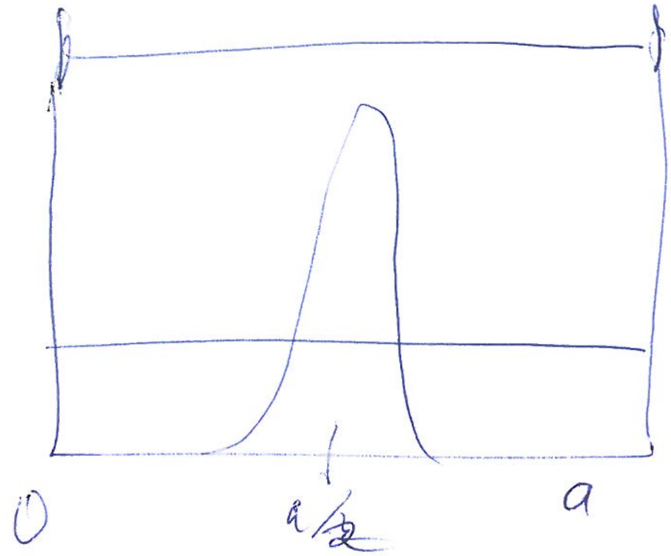


If one raised floor potential of the infinite square well, ~~energy would rise~~ all energies would rise.

So raising a bit of the floor should raise energies one might guess.

What of the stationary states?

6-51



assuming $x > 0$

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

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

$$= k^2 \psi$$

$$k = \begin{cases} \sqrt{\frac{2m}{\hbar^2}(V-E)} & \text{exponential like if } V>E \\ i\sqrt{\frac{2m}{\hbar^2}(E-V)} & \text{oscillatory if } V<E \\ 0 & \text{if } E=V. \end{cases}$$

Well going across the center $x = a/2$ will be less oscillatory.

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This should be true in the limit of the Dirac Delta function.

But more than that it is hard to say.

1st Order

$$E_{1n} = \langle \psi_{0n} | H_1 | \psi_{0n} \rangle$$

$$= \int_0^a \left(\frac{2}{a}\right) \alpha \sin^2 kx \, \delta(x - a/2) \, dx$$

$$= \left(\frac{2}{a}\right) \alpha \sin^2 (k a/2)$$

$$= \left(\frac{2}{a}\right) \alpha \sin^2 \left(\frac{n\pi}{2}\right)$$ (see p. 6-42)

$$= \left(\frac{2}{a}\right) \alpha \left(\frac{1-(-1)^n}{2}\right) \begin{cases} 0 & \text{if } n \text{ is even} \\ 1 & \text{if } n \text{ is odd.} \end{cases}$$

Note $\psi_{0n} = \sqrt{\frac{2}{a}} \sin k_n x$ has a node at $x = a/2$ for all cases on n even and an antinode for n odd, so No 1st order correction to energy

$$|\psi_{1n}\rangle = \sum_{\substack{j \\ j\neq n}} \frac{\langle \chi_{oj} | H_1 | \chi_{on}\rangle}{E_{on} - E_{oj}} |\chi_{oj}\rangle$$

(see p. 6-36)

$$= \left(\frac{2}{a}\right)\frac{\alpha}{E_{01}} \sum_{\substack{j \\ j\neq n}} \frac{\int_0^a \sin k_j x\, \delta(x-a/2) \sin k_n x\, dx}{n^2 - j^2} * |\chi_{oj}\rangle$$

Zeroth order perturbation ground state.

$$\sin k_j a/2 \sin k_n a/2$$

$$= \sin\left(\frac{j\pi}{2}\right) \sin\left(\frac{n\pi}{2}\right)$$

$$= (-1)^{\frac{j-1}{2}}\left(\frac{1-(-1)^j}{2}\right)(-1)^{\frac{n-1}{2}}\left(\frac{1-(-1)^n}{2}\right)$$

$$= (-1)^{\frac{n+j}{2}-1}\left(\frac{1-(-1)^n}{2}\right)\left(\frac{1-(-1)^j}{2}\right)$$

$$l = \frac{j-1}{2}$$

$\therefore\ j = 2l+1$ and as $l = 0, 1, 2, \ldots$

j goes thru all odd numbers

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while l alternates between even and odd.

$$|\psi_{1n}\rangle = \left(\frac{2}{a}\right)\left(\frac{\alpha}{E_{0n}}\right)\sum_{\substack{j \\ j\neq n}}^{\infty}\frac{(-1)^{\frac{n+j-1}{2}}\frac{\left(1-(-1)^n\right)}{2}\frac{\left(1-(-1)^j\right)}{2}}{n^2 - j^2}|\psi_{0j}\rangle$$

The series is infinite.

Does it converge?

Well in the ~~large~~. large j limit $j \gg n$ we have

$$\sum_{j\gg n}^{\infty}|c_j| \le \frac{1}{4}\sum_{l=L}^{\infty}\left|\frac{1}{n^2-(2l+1)^2}\right|$$

$$= \frac{1}{4}\sum_{l=L}^{\infty}\frac{1}{(2l+1)^2-n^2}$$

where $L \gg 2n+1$

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The *integral test for convergence* should work.

(Art-242)

$$\int_L^\infty \frac{1}{(2\cancel{x}+1)^2 - n^2}\, dx$$

let $y = 2x+1$

$dy = 2\cancel{x}\,dx$

$$= \frac{1}{2}\int_{2L+1}^\infty \frac{1}{y^2 - n^2}\, dy$$

$$= \frac{1}{2}\,\frac{1}{\sqrt{1}}\,\ln\left(\frac{y-n}{y+n}\right)\Bigg|_{2L+1}^\infty$$

(Hudson-5)

$$= \frac{1}{2}\ln\left(\frac{2L+1+n}{2L+1-n}\right)$$

The *integral* does converge, and so the series converges (and absolutely converges)

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But the convergence is not real fast it seems.

Example case $n = 1$

So we'll see ~~on~~ how the ~~groundstate~~ ground state is perturbed

1st order correction

$$\psi_{11} = \frac{\left(\frac{2\alpha}{a}\right)}{E_{01}} \sum_{j=2}^{\infty} \frac{(-1)^{\frac{1+j}{2}-1}\frac{\left(1-(-1)^j\right)}{2}}{1 - j^2}\left(\sqrt{\tfrac{2}{a}}\sin k_j x\right)$$

$$= \frac{\left(\frac{2\alpha}{a}\right)}{E_{01}}\Bigg[\frac{(-1)}{1-9}\sqrt{\tfrac{2}{a}}\sin k_3 x - \frac{1}{1-25}\sqrt{\tfrac{2}{a}}\sin k_5 x + \frac{(-1)}{1-49}\sqrt{\tfrac{2}{a}}\sin k_7 x - \dots\Bigg]$$

Gr solution — 154 agrees.

The 1^{st} order state is

$$|\Psi_1^{1st}\rangle = |\Psi_{01}\rangle + \lambda|\Psi_{11}\rangle$$

recall.

2nd Order — just the energy

$$E_{2n} = \sum_{\substack{j \\ j \neq n}} \frac{|\langle\Psi_{0j}|H_1|\Psi_{0n}\rangle|^2}{E_{0n} - E_{0j}}$$

(see p. 6-40)

$$= \frac{\left(\frac{2\alpha}{a}\right)^2}{E_{01}} \sum_{\substack{j \\ j \neq n}} \frac{\left(\frac{1-(-1)^n}{2}\right)^2 \left(\frac{1-(-1)^j}{2}\right)^2}{n^2 - j^2}$$

Now $\left(\frac{1-(-1)^n}{2}\right)^2 = \frac{1-2(-1)^n+1}{4}$

$= \frac{1-(-1)^n}{2}$

Which we should have intuited.

$$E_{2n} = \frac{\left(\frac{2\alpha}{a}\right)^2}{E_{01}} \sum_{\substack{j \\ j \neq n}} \frac{\left(\frac{1-(-1)^n}{2}\right)\left(\frac{1-(-1)^j}{2}\right)}{n^2 - j^2}$$

Converges just as the 1^{st} order state does. See p. 6-54.

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So we had to work reasonably hard even in the simple case of an infinite square well with a central Dirac Delta ~~function~~ potential perturbation.

But it should be ~~known~~ no surprise that QM is tricky.

8) Diagonalization

or Diagonalizing the matrix

or Diagonalizing the Hamiltonian

→ synonyms for solving the Sch. eq. by the matrix method.

— perhaps diagonalization is not a good name, but that's what it is called.

People say let's diagonalize the Hamiltonian not (it seems) ~~the~~ lets solve the Sch. eqn. in ~~the~~ it's matrix form

It is actually an exact method for finite Hilbert space of N dimensions.

→ One solves an N x N matrix.

For infinite dimensions, diagonalization can only be approximate — but

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there is no in principle limit on how accurate you can make it.

You truncate $\infty \times \infty$ to $N \times N$ and if that is not accurate enough increas N until you reach the accuracy you want.

Of course, there practical limitations; e.g., finite computing time, machine accuracy.

Special cases of diagonalization are called degenerate or nearly degenerate perturbation theory.