Scattering theory in quantum mechanics - 3D. (potential scat.)

1. Basic concepts, why scattering happens in QM.

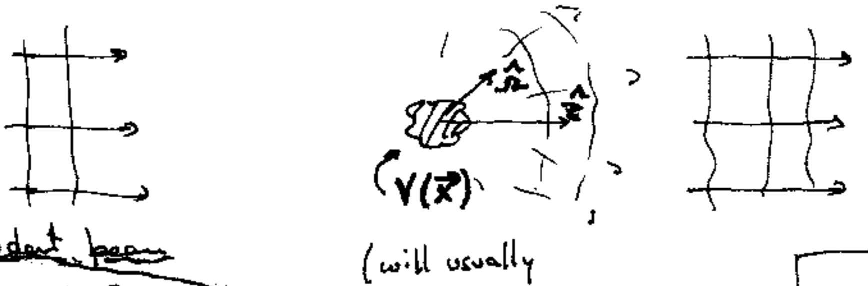
2. Perturbative treatment of the scattered wfn: Born series.

3. Partial wave decomposition of scat. amps: phase shifts. Examples.

4. Integral eqns for scattering, exact relations.

QM, basic scattering theory

"Vanilla scat. theory : $V(\vec{x})$ only, single particle.
no explicit time dep; implicit factor of $e^{-i\omega t} = e^{-iEt/\hbar}$
on all wfns. $\psi(\vec{x},t) = \psi(\vec{x})e^{-i\omega t}$



(will usually be $V(r)$ for nuclear scat.)

$$\psi = e^{i\vec{k}\cdot\vec{x}} + \underbrace{f(\hat{\Omega})}\frac{e^{+ikr}}{r}$$

($\frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{x}}$ if correctly normalized)

(large r) outgoing spherical wave with angular dependence $f(\Omega)$

corresp. flux outgoing $\vec{j}\cdot\hat{r} = \frac{\hbar k}{mr^2}|f(\Omega)|^2$

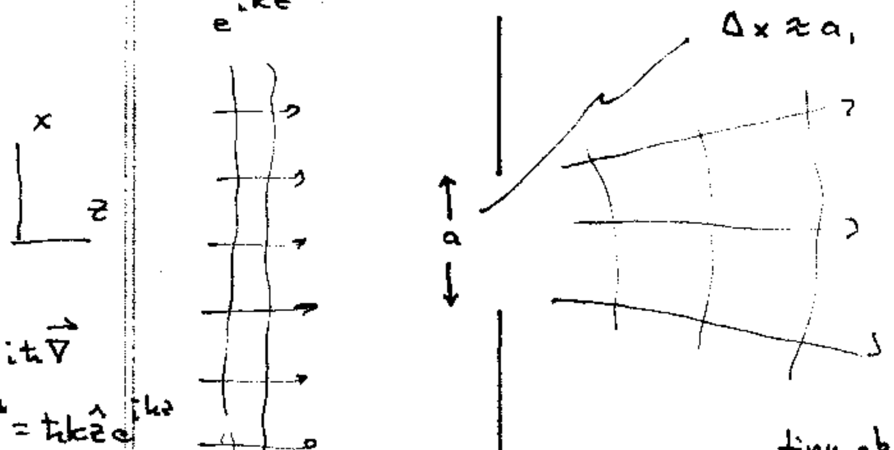
1^{st}, general question : why is there scattering at all?

Uncertainty princ.

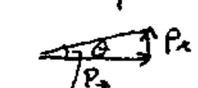
Consider scat through an aperture :

$\Delta x \approx a$, so $\Delta p_x \approx h/a$

e^{ikz}



we then expect the beam to spread through an angle



$\tan\theta \approx \theta = \frac{p_x}{p_z}$

$$\theta \sim \frac{p_x}{p_z} \sim \frac{h}{p_z a} = \frac{h}{\hbar k_z a} = \frac{\lambda}{a}$$

tiny objects are hard scatterers

$\vec{p} = -i\hbar\vec{\nabla}$

$\vec{p}\,e^{ikz} = \hbar k\hat{z}\,e^{ikz}$

$p_x = 0$, $p_z = \hbar k$, comp. deloc. in x & z.

"diffraction limited optics" , "quantum limit"

e.g. human pupil, $a \sim \frac{1}{2}$ cm $= 0.5$ [cm]

$\lambda \sim 5000\,\text{Å} = 0.5\ [\mu m] = 0.5 \cdot 10^{-4}$ [cm]

$$\theta \sim 10^{-4}\ [\text{rad}]$$

↳ in theory you might be able to resolve these dots at 10 [m]. I have trouble at 2 [m]. (Recall also there are vague factors of 2π in this estimate.)

Similarly, for small-angle scattering from an object of extent a we expect a scattered beam width of $\theta \sim \frac{\lambda}{a}$.

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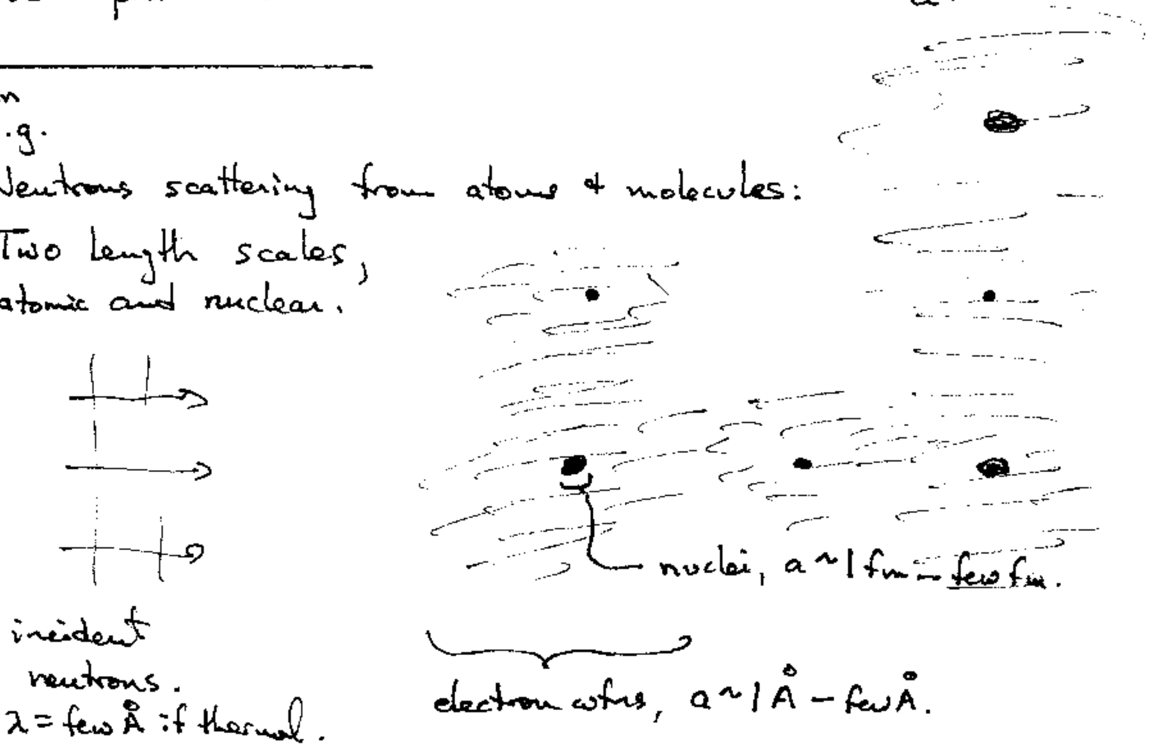
an e.g.

Neutrons scattering from atoms + molecules:

Two length scales, atomic and nuclear.



$\theta_{\substack{\text{atomic}\\ \text{wfns}}} \sim \frac{\lambda}{a} \sim \frac{\text{few Å}}{\text{few Å}} \sim 1$, so this will fill up solid angle (typically forward) in an interesting and measurable way.

$\theta_{\substack{\text{nuclear}\\ \text{wfns}}} \sim \frac{\lambda}{a} \sim \frac{\text{few Å}}{\text{few fm}} \sim 10^5$. What?!

This just means
1) small angle approx fails
2) low E scat from nuclei is spread uniformly over all angles, "isotropic"

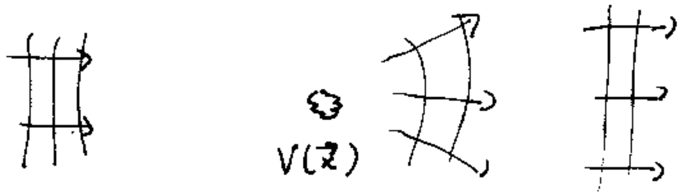
≈ spherical scattered wave

$1 \cdot \frac{e^{ikr}}{r}$

Scattering & perturbation theory.

Given a $V(\vec{x})$ and an incident beam of particles, what is the scattered particle intensity? $\underset{\sim}{\dfrac{d\sigma}{d\Omega}}$ (also called $W(\theta)$ or $I(\theta)$ sometimes).

$$\psi(\vec{x}) = \underbrace{\psi_{inc}(\vec{x})}_{e^{ikz}} + \underbrace{\psi_{scat}(\vec{x})}_{\approx f(\hat{\Omega})\frac{e^{ikr}}{r}} \quad \text{at large } r$$



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

$E \to \dfrac{\hbar^2 k^2}{2m}$

since must be valid everywhere including $z \to -\infty$ where $V=0$.

assume $\psi_{scat}(\vec{x})$ is a perturbation due to the presence of $V(\vec{x})$.

$$\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]\left(\cancel{\psi_{inc}(\vec{x})} + \psi_{scat}(\vec{x})\right)$$

$$= V(\vec{x})\left(\psi_{inc}(\vec{x}) + \psi_{scat}(\vec{x})\right)$$

$$\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]\underbrace{\psi_{scat}(\vec{x})}_{\therefore\, \mathcal{O}(V)} = \underbrace{V(\vec{x})\psi_{inc}(\vec{x})}_{\mathcal{O}(V)} + \underbrace{V(\vec{x})\psi_{scat}(\vec{x})}_{\therefore\, \mathcal{O}(V^2)}$$

to keep track of powers of V. will set =1 later

We can formalize this by writing: $V \to \lambda V$

$$\psi(\vec{x}) = \underbrace{\psi_{inc}(\vec{x})}_{\psi^{(0)}(\vec{x})} + \underbrace{\psi_{scat}(\vec{x})}_{\lambda\psi^{(1)}(\vec{x}) + \lambda^2\psi^{(2)}(\vec{x}) + \cdots}$$

then subst in the Schrödinger equation & find

λ^0: $$\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]\psi^{(0)}(\vec{x}) = 0 \qquad \psi^{(0)}(\vec{x}) = e^{ikz}$$

λ^1: $$\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]\underbrace{\psi^{(1)}(\vec{x})}_{\text{"1st Born approx" to the wfn.}} = V(\vec{x})\,\psi^{(0)}(\vec{x})$$ → known functions

Just solve for $\psi^{(1)}(\vec{x})$.

λ^2: $$\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]\underbrace{\psi^{(2)}(\vec{x})}_{\text{"2nd Born approx".}} = V(\vec{x})\,\psi^{(1)}(\vec{x}) \quad \text{etc}$$

(Usually stop at 1st.)

etc

$$\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]\psi^{(1)}(\vec{x}) = V(\vec{x})\,\psi^{(0)}(\vec{x})$$

solve this for $\psi^{(1)}(\vec{x})$. How? Easy:

$$\psi^{(1)}(\vec{x}) = \left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]^{-1} V(\vec{x})\,\psi^{(0)}(\vec{x})$$

What??? Divide by an operator???
whatever does this mean?

formally it's an infinite series of gradients,

$$\left[E + \frac{\hbar^2}{2m}\nabla^2\right]^{-1} = \frac{1}{E}\left[1 + \frac{\hbar^2}{2mE}\nabla^2\right]^{-1} = \frac{1}{E}\left\{1 - \frac{\hbar^2}{2mE}\nabla^2 + \left(\frac{\hbar^2}{2mE}\right)^2\nabla^4 - \left(\frac{\hbar^2}{2mE}\right)^3\nabla^6 + \cdots\right\}$$

Hence maybe it's not surprising it's equivalent to a nonlocal kernel (smearing):

$$\Big[\underbrace{E}_{\frac{\hbar^2 k^2}{2m}} + \frac{\hbar^2}{2m}\vec{\nabla}^2\Big]^{-1} f(\vec{x}) = \int d^3x' \, \underbrace{K(\vec{x}-\vec{x}')}\, f(\vec{x}')$$

this nonlocal smearing function can be found by Fourier transforming everything in sight and is

"Kernel" or "Green function" for free Schrödinger eqn.

$$\underbrace{\Big[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\Big] K(\vec{x}-\vec{x}') \equiv \delta(\vec{x}-\vec{x}')}$$

$$\boxed{K(\vec{x}-\vec{x}') = -\frac{m}{2\pi\hbar^2}\,\frac{e^{i\overset{\sqrt{2mE}}{k}|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}}$$

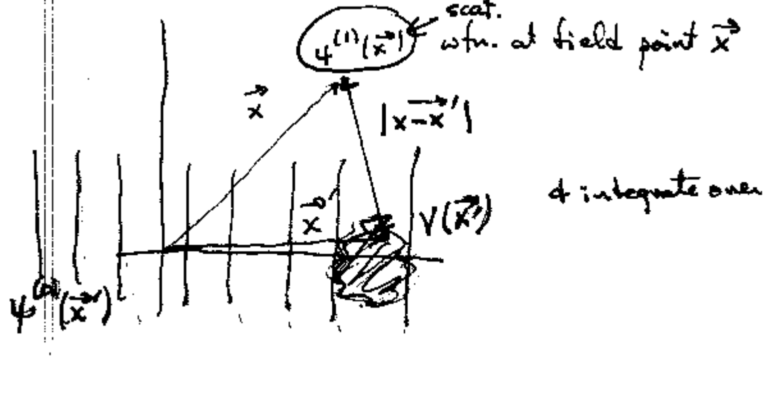
this G.F. is a function only of the sep. $|\vec{x}-\vec{x}'|$ between two points, not angles, because the operator $\Big[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\Big]$ is isotropic & trans. invar.

and so the 1st Born approx is

$$\underbrace{\psi^{(1)}(\vec{x})}_{O(V)} = \int d^3x' \, \underbrace{K(\vec{x}-\vec{x}')}_{\text{known}} \, \underbrace{V(\vec{x}')}_{\text{given}} \, \underbrace{\psi^{(0)}(\vec{x}')}_{\text{that plane wave}}$$

fine, but it looks like the cure is worse than the disease! :

$$\psi^{(1)}(\vec{x}) = -\frac{m}{2\pi\hbar^2}\int d^3x' \, \frac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \, V(\vec{x}')\,\psi^{(0)}(\vec{x}')$$



& integrate over all $\vec{x}'$!?

Actual correct 1st Born approx.

...and if we were really insane we could continue and iterate this to higher Born order,

$$\underbrace{\psi^{(n)}(\vec{x})} = \underbrace{\left\{\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]^{-1} V(\vec{x})\right\}\left\{\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]^{-1} V(\vec{x})\right\} \cdots \left\{\left[E + \frac{\hbar^2}{2m}\vec{\nabla}^2\right]^{-1} V(\vec{x})\right\}}_{n \text{ such factors}} \psi^{(0)}(\vec{x})$$

$$= \int\!\cdots\!\int d^3x_1\, d^3x_2 \ldots d^3x_n \;\; K(\overrightarrow{x - x_1})\, V(\vec{x}_1)\; K(\overrightarrow{x_1 - x_2})\, V(\vec{x}_2)$$

$$\ldots \; K(\overrightarrow{x_{n-1} - x_n})\, V(\vec{x}_n)\, \psi^{(0)}(\vec{x}_n)$$

which combining all $\psi^{(n)}(\vec{x})$ gives the exact solution of the scattering problem,

$$\psi(\vec{x}) = \sum_{n=0}^{\infty} \psi^{(n)}(\vec{x}).$$

So now 1^{st} Born order doesn't look so bad! We can now make it look even easier.

{ n.b. when is it accurate? Weak potentials, far from bound states. Faster preferred.

First note you've seen something like this before:

electrostatics

~~$\rho(\vec{x}')$ given~~

$\uparrow$ find $\varphi(\vec{x})$

$$\left(\varphi(\vec{x}) = \sum_i \frac{q_i}{|\overrightarrow{x - x_i}|} \right)$$

$$\varphi(\vec{x}) = \int d^3x' \; \frac{\rho(\vec{x}')}{|\overrightarrow{x - x'}|}$$

$\leftarrow \frac{1}{R}$ for each charge $dq = \rho(\vec{x}')\,dv$

solves Poisson's eqn $\quad \nabla^2 \varphi(\vec{x}) = -4\pi \rho(\vec{x})$

Our case, set $k=0$ $(E=0)$, $\frac{\hbar^2}{2m}=1$, we are solving

$$\vec\nabla^2 \underbrace{\psi^{(1)}(\vec x)}_{\text{"}\varphi\text{"}} = \underbrace{V(\vec x)\,\psi^{(0)}(\vec x)}_{\text{"}-4\pi\rho\text{"}}$$

soln is

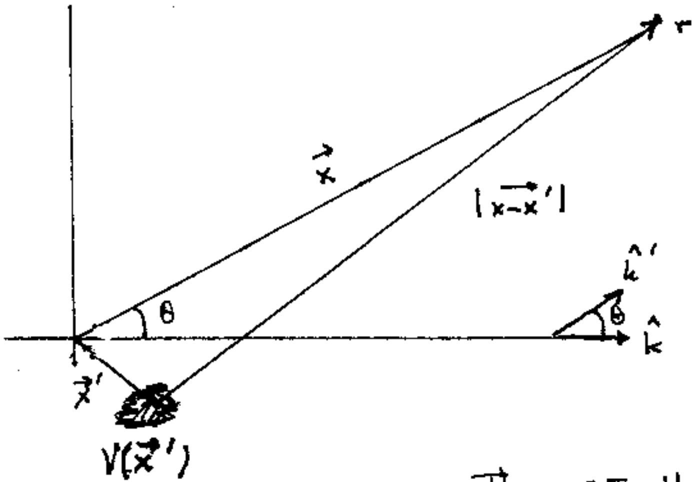
$$\underbrace{\psi^{(1)}(\vec x)}_{\varphi} = -\frac{1}{4\pi}\cdot\underbrace{\left(\frac{2m}{\hbar^2}\right)}_{1}\cdot\int d^3x' \frac{1}{|\vec x-\vec x'|}\underbrace{\psi(\vec x')\,\psi^{(0)}(\vec x')}_{-4\pi\rho}$$

$$\varphi(\vec x) = \int d^3x' \frac{\rho(\vec x')}{|\vec x-\vec x'|}$$ ✓ Coulomb problem

OK now let's solve it.

Crucial step is to ask what is the far-field $\psi^{(1)}(\vec x)$.

[After all it's a scattering experiment, that's all we care about.]



(n.b. $\vec x \equiv \vec r$ and $\vec x' \equiv \vec r'$)

$$|\vec x-\vec x'| = \left(r^2+r'^2-2\vec x\cdot\vec x'\right)^{1/2} = r - \hat r\cdot\vec r' + O(r'^2/r)$$

$$= r - \hat k'\cdot\vec r' \quad \text{as } r\to\infty$$

The GF then becomes $\propto$

$$\frac{e^{ik|\vec x-\vec x'|}}{|\vec x-\vec x'|} \to \frac{e^{ikr}}{r}\cdot e^{-i\vec k'\cdot\vec r'}$$

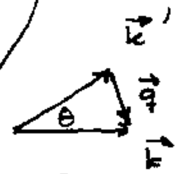
and we find

$$\lim_{r\to\infty} \psi^{(1)}(\vec{x}) = -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3x'\, e^{-i\vec{k}'\cdot\vec{x}'}\, V(\vec{x}')\,\underbrace{\psi^{(0)}(\vec{x}')}_{e^{ikz'} = e^{i\vec{k}\cdot\vec{x}'}}$$

the prev $\dfrac{e^{ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$

$$= -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3x'\, V(\vec{x}')\, e^{i\vec{q}\cdot\vec{x}'}$$

$\vec{q} \equiv \vec{k} - \vec{k}'$ "momentum transfer"



$\vec{q}^{\,2} = 2k^2(1-\cos\theta)$
$= 4k^2\sin^2(\theta/2)$

In 1st Born approx, scattered wfn. is $\propto$ the 3D F.T. of the potential $V(\vec{x})$.

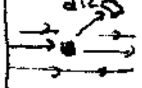
Note also since we anticipated $\psi^{(1)}(\vec{x}) = f(\hat{\Omega})\dfrac{e^{ikr}}{r}$ (far field)
we have

$$\underline{f(\hat{\Omega}) = -\frac{m}{2\pi\hbar^2}\int d^3x'\, V(\vec{x}')\, e^{i\vec{q}\cdot\vec{x}'}}$$

n.b. for a $V(r)$ only this will give a $f(|\vec{q}|)$ only. (no preferred direction) Hence will depend on length $\underline{\vec{q}^{\,2}} = \underline{4k^2\sin^2(\theta/2)}$

This is very useful, since the differential scattering cross section is for elastic, potential scattering

$$\underline{\frac{d\sigma}{d\Omega} = |f(\hat{\Omega})|^2}$$



$dN\big|^{\text{part.}}$ /sec into $d\Omega$

$= \Phi \cdot \dfrac{d\sigma}{d\Omega} \cdot d\Omega$

$\frac{\text{part}}{\text{cm}^2\cdot\text{sec}} \cdot \text{cm}^2$

& from there

$$\underline{\sigma = \int |f(\hat{\Omega})|^2\, d\Omega}$$

We haven't checked units recently!
Let's see if they still work.

$$\frac{d\sigma}{d\Omega} = |f|^2 \quad \text{so} \quad [f] = [\text{cm}] \quad \text{we hope!}$$

$$f(\vec{x}) = \underbrace{-\frac{m}{2\pi\hbar^2}}_{\left[\frac{\text{gm}}{\text{erg}^2\cdot\text{sec}^2}\right]} \int d^3x' \, V(\vec{x}') \, e^{i\vec{q}\cdot\vec{x}'}$$

$$\left[\frac{\text{gm}}{\text{erg}^{2}\cdot\text{sec}^2}\right]\cdot[\text{cm}^3]\cdot[\cancel{\text{erg}}] = \frac{[\cancel{\text{gm}}\cdot\text{cm}^3]}{[\cancel{\text{gm}}\cdot\text{cm}^2\,\cancel{\text{sec}^{-2}}\cdot\cancel{\text{sec}^2}]} = [\text{cm}] \checkmark$$