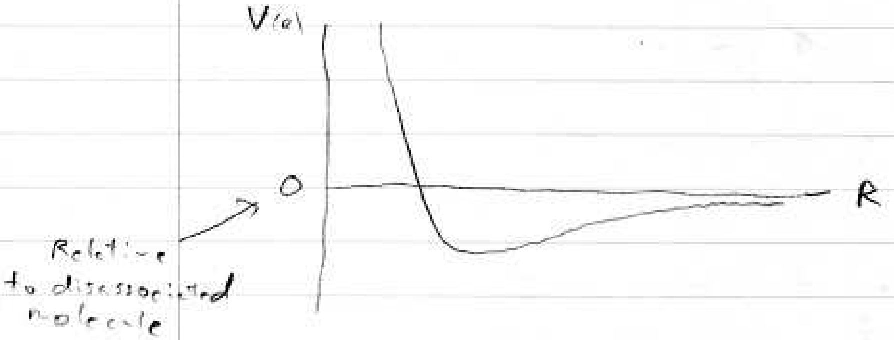
Wed: Prob 11.2 + a bit extra

Lecture 24

Last time, applied variational method to H_2^+

Got estimates for bond length, binding energy

Also got estimate for molecular potential $V(R)$



Standard trick: use this as potential for nuclear motion:

$$H \to -\frac{\hbar^2}{2\mu}\nabla^2\psi(R) + V(R)\psi(R)$$ See Prob 7.10

$\mu = \frac{M}{2}$, M: nuclear mass

Generally attack chemistry problems this way:

Step 1: Solve for electron energy at fixed nuclear positions

Step 2: Use e^- energy as potential for nuclear motion

Only works because electrons are so much lighter = faster

electron state adjusts adiabatically as nuclei move

Called Born-Oppenheimer approximation

Example of where this applies: collision between two atoms

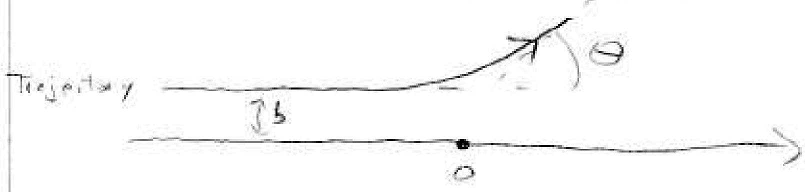
atoms interact via potential $V(r)$: typically complicated

Study how to approach this problem: Chapter 11

Scattering

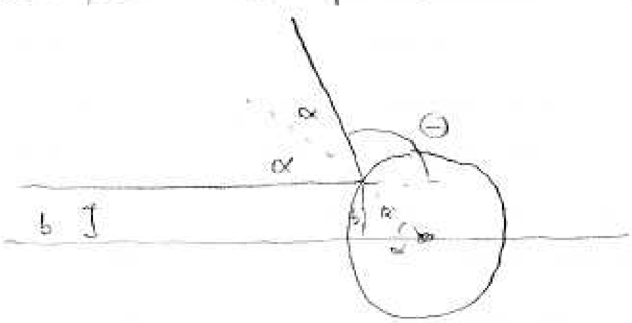
Start with a little classical scattering theory

Assume incident particle moving along z scatters from spherically symmetric potential $V(r)$



Basic classical problem: determine scattering angle Θ as function of impact parameter b

Example: Hard sphere scattering:



Assume elastic collision

See $b = R\sin\alpha$

and $2\alpha + \Theta = \pi$

$$\alpha = \frac{\pi}{2} - \frac{\Theta}{2}$$

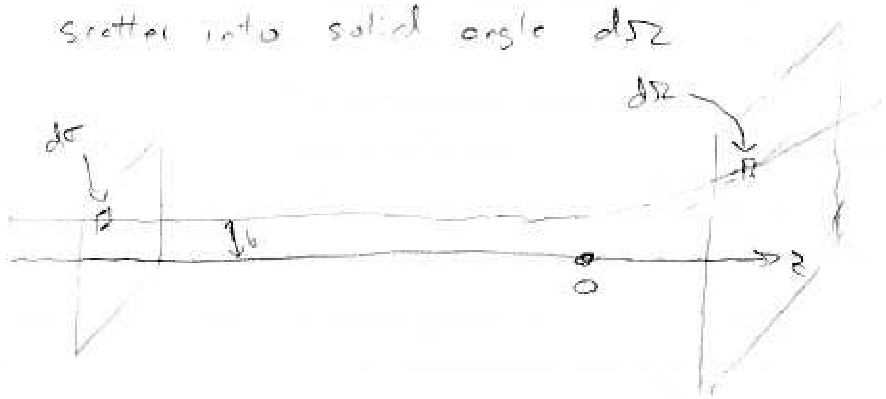
So $b = R\sin\left(\frac{\pi}{2} - \frac{\Theta}{2}\right) = R\cos\frac{\Theta}{2}$

and
$$\Theta = \begin{cases} 2\cos^{-1}\frac{b}{R} & (b \le R) \\ 0 & (b > R) \end{cases}$$

Apply this to problem where we're sending a beam of particles at scatterer.

Then we have a whole range of impact parameters and generalize to 3D:

Particles incident within area $d\sigma$ scatter into solid angle $d\Omega$



$d\Omega = 2\pi \sin\theta \, d\theta$

Of course range of solid angles is proportional to size of incident area

$$d\sigma = D(\theta)\, d\Omega$$

$D(\theta)$ = proportionality constant (only depends on θ for spherically symmetric V)

Can write $d\sigma = 2\pi b\, db = D(\theta)\, 2\pi \sin\theta\, d\theta$

$$\text{So } D(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

For hard sphere, $b = R\cos\frac{\theta}{2}$

$$\frac{db}{d\theta} = -\frac{1}{2} R \sin\frac{\theta}{2}$$

$$D(\theta) = \frac{b}{\sin\theta} \cdot \frac{R}{2}\sin\frac{\theta}{2} = \frac{R^2}{2}\,\frac{\cos\frac{\theta}{2}\sin\frac{\theta}{2}}{\sin\theta}$$

But $\sin\theta = 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$

$$\text{So } D(\theta) = \frac{R^2}{4}$$

Note $D(\theta) = \frac{d\sigma}{d\Omega}$, units of area

Call D = differential cross section
often just write $d\sigma/d\Omega$

If we have a beam of particles with

$L = \frac{\text{\# of particles}}{\text{area} \cdot \text{time}}$ $\equiv$ luminosity or intensity

Then scatter $dN = L\, D(\theta)\, d\Omega$ into solid angle $d\Omega$
per unit time

Makes D pretty easy to measure.

Conventional to define total cross section

$\sigma = \int D(\theta)\, d\Omega$ $\approx$ effective area of target

For hard sphere, $D(\theta) = \frac{R^2}{4}$

$\sigma = \frac{R^2}{4} \int d\Omega = \frac{R^2}{4} \times 4\pi = \pi R^2$

= cross-section area of sphere

Now, that is all completely classical

But ideas carry over into quantum mechanics

Quantum Scattering

Look for solutions to Schr. Eqn with form

$$\psi(\vec{r}) \to A\left\{ \underbrace{e^{ikz}}_{\text{incident plane wave}} + \underbrace{f(\theta)\frac{e^{ikr}}{r}}_{\text{scattered spherical wave}} \right\} \quad (\text{at large } r)$$

Here $k = \frac{\sqrt{2mE}}{\hbar}$ as usual

Relate this to $D(\theta)$: recall $D(\theta) = \frac{1}{L}\frac{dN}{d\Omega}$

$dN = \frac{\#\text{ of particles}}{\text{time}}$ scattered into $d\Omega$

$$= \underbrace{|\psi_{scat}|^2}_{\text{particles per volume}} \times \underbrace{r^2 d\Omega}_{\text{area}} \times \underbrace{v}_{\text{particle velocity}}$$

$$= |A|^2 |f(\theta)|^2 \frac{1}{r^2} r^2 d\Omega\, v$$

L = incident particles / area·time

$$= |\psi_{inc}|^2 \cdot v = |A|^2 v$$

So $\frac{dN}{L\,d\Omega} = \frac{|A|^2 |f(\theta)|^2 d\Omega\, v}{|A|^2 v\, d\Omega} = |f(\theta)|^2$

So $\boxed{D(\theta) = |f(\theta)|^2}$

Get $f(\theta)$ by solving Schr. Eqn.