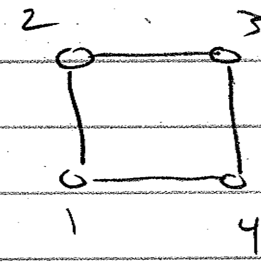
H9

Connection with Heisenberg model material:

Recall that for Heisenberg model matrix for $\hat{H}$

was block diagonal



16 dim Hilbert space

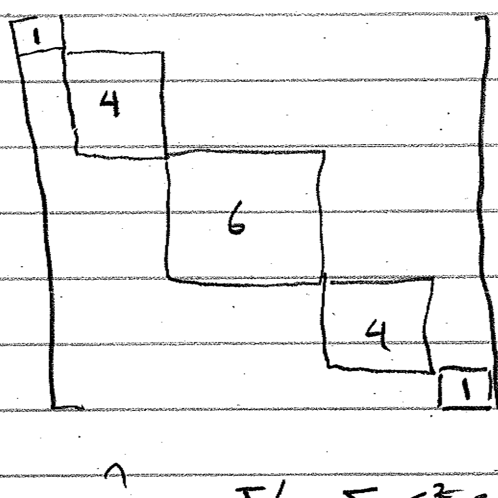
$\hat{H}|{+}{+}{+}{+}\rangle = J|{+}{+}{+}{+}\rangle$

$\hat{H}|{+}{+}{+}{-}\rangle = J/2\,|{-}{+}{+}{+}\rangle + J/2\,|{+}{+}{-}{+}\rangle$

$\hat{H}|{+}{+}{-}{+}\rangle =$

$\hat{H}|{+}{-}{+}{+}\rangle =$

$\hat{H}|{-}{+}{+}{+}\rangle =$



Q Why?!

A!: $$\hat{H} = J/\hbar^2 \underbrace{\sum S^z_\ell S^z_{\ell+1}}_{\substack{\text{doesn't change}\\ \text{vector}\\ \text{(all } S^z_\ell \text{ same)}}} + J/2\hbar^2 \underbrace{\sum \left(S^+_\ell S^-_{\ell+1} + S^-_\ell S^+_{\ell+1}\right)}_{\substack{\text{doesn't change}\\ \text{total } S^z_\ell}}$$

A2: More formally $[\hat{H}, \underbrace{\sum_e \hat{S}_e^z}_{\hat{S}^z_{TOT}}] = \phi$

$\Rightarrow$ Search eigenstates of $\hat{H}$ in list of eigenstates of $\hat{S}^z_{TOT}$.

Precisely same idea here with $\hat{H}$ for any central force and $\hat{L}^2, \hat{L}^z$ operators!

4.1)

To solve "radial eqn" guess $R(r) = cr^s$

as $r \to 0$

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right]R(r) = ER(r)$$

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r^{s+1} + \frac{\ell(\ell+1)\hbar^2}{2mr^2}r^s + V(r)r^s = ER(r)$$

$$-\frac{\hbar^2}{2m}s(s+1)r^{s-2} + \frac{\hbar^2}{2m}\ell(\ell+1)r^{s-2} + V(r)r^s = ER(r)$$

likewise! $\sim r^s$

if $V(r) \sim 1/r$
This is r^{s-1} which vanishes faster than r^{s-2} near $r=0$ so neglect

$\therefore$ $s = \ell$ or $s = -(\ell+1)$

not possible (diverges at $r \to 0$)

So $R(r) = cr^\ell$ near $r = 0$

We will skip much of the details of what follows:

To solve full radial eqn

(1) Define $u(r) = r R(r)$

$$\left[-\hbar^2/2m \, d^2/dr^2 + \ell(\ell+1)/2mr^2 + V(r) \right] u(r) = E\, u(r)$$

(gets rid of funny $1/r \; d^2/dr^2 \; r$!)

(2) Dimensionless units $\rho = r/a_0$

$a_0 = \hbar^2/me^2$ Bohr radius (0.52 Å)

$\lambda^2 = -E/(e^2/2a_0) \leftarrow$ Rydberg (13.6 eV)

$$\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{2}{\rho} - \lambda^2 \right] u(\rho) = 0$$

(3) Asymptotics $\rho \to \infty$

$$\left[d^2/d\rho^2 - \lambda^2 \right] u(\rho) = 0 \qquad u \sim e^{-\lambda\rho}$$

$\therefore \; u(\rho) = e^{-\lambda\rho}\, \gamma(\rho)$

H13

(4) $$\left[\frac{d^2}{d\rho^2} - 2\lambda\frac{d}{d\rho} + \frac{2}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right] y(\rho) = 0$$

$$Y(\rho) = \rho^{\ell+1}\sum_{q=0}^{\infty} c_q \rho^q$$

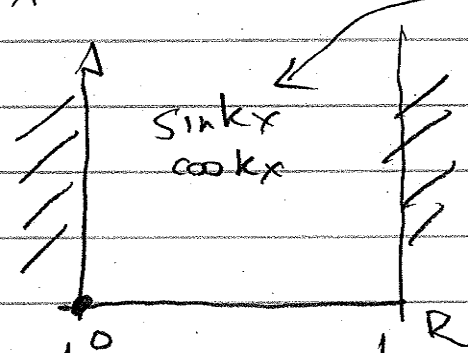
known behavior at $\rho \to 0$ $(r \to 0)$ Recall $u = rR \to r^{\ell}$

(5) Plug in and do algebra

In a nutshell: get a recursion reln relating c_q to c_{q-1}. If series doesnt terminate can show $Y(\rho) \sim e^{2\lambda\rho}$ which, even with $e^{-\lambda\rho}$ blows up at $\rho \to \infty$. So series must terminate at $q_{max} \equiv k$. This quantizes Energy levels (series will only terminate for certain special discrete Energy values)

Analogy: ∞ square well

solns of $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi$



$\psi(x) = 0$ here

Boundary condition $\Rightarrow k = \frac{n\pi}{L}$

H14

Blank for now (more details on H atom soln)

4/15

Blank for now (more details on H atom soln)

A weird (accidental?) thing happens.

The energy does not depend separately on l (orbital quantum #) and $K = q_{max}$ but only on $k+l$! Must do algebra to see this...

Call $n = k+l$ $\qquad E_n = \frac{-e^2}{2a_0} \, 1/n^2$

$\boxed{k \geq 1 \text{ to make } \Upsilon \text{ nontrivial so } l \leq n-1}$

Hydrogen atom spectrum

Additional degeneracy to $(2l+1)$ fold one from all m

Unique to $1/r$ potential

Classical analog of this special ness: closed orbits for $1/r$

BEGS Question: Some of you know $r^2 = V(r)$ also gives classically closed orbits. Does 3D Harmonic oscillator problem have special, more highly degenerate spectrum?

A1: Separates in real space E depends only on single quantum number $n_x + n_y + n_z$

A2: look back in terms of $Y_{lm}(\theta, \phi)$!

some more algebra to get normalization!

$$R_{10}(r) = 2(a_0)^{-3/2} e^{-r/a_0}$$

$$R_{20}(r) = 2(2a_0)^{-3/2}(1 - r/2a_0) e^{-r/2a_0}$$

$$R_{11}(r) = (2a_0)^{-3/2} \frac{1}{\sqrt{3}} r/a_0 \, e^{-r/2a_0}$$

Full wave functions (including $Y_{\ell m}(\theta, \phi)$)

$$\phi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$n \ell m$

$$\phi_{200} = \frac{1}{\sqrt{8\pi a_0^3}} (1 - r/2a_0) e^{-r/2a_0}$$

$$\phi_{21\pm1} = \mp 1/8\sqrt{\pi a_0^3} \; r/a_0 \; e^{-r/2a_0} \sin\theta \, e^{\pm i\phi}$$

$$\phi_{210} = 1/4 \; 1/\sqrt{2\pi a_0^3} \; r/a_0 \, e^{-r/2a_0} \cos\theta$$

all 4 have same $E_2 = -\frac{e^2}{2a_0}\frac{1}{2^2}$

etc.

Q:

Periodic table ← Is there just a single 100 state and 4 2ℓm states?

ϕ_{100}	H							He
ϕ_{200}	Li	Be	B	C	N	O	F	Ne

Old fashioned notation assigns letters to ℓ

$\ell = 0$ s
1 p
2 d
3 f

$n=1$ $\ell=0$ $m=0$ 1s
$n=2$ $\ell=1$ $m=0,\pm1$ 2p
$\ell=0$ $m=0$ 2s
$n=3$ $\ell=2$ $m=0,\pm1,\pm2$ 3d
$\ell=1$ $m=0,\pm1$ 3p
$\ell=0$ $m=0$ 3s

$$F = 1s^2 2s^2 2p^5$$