

$$a_+ \psi_n = \sqrt{n+1} \psi_{n+1}$$

$$a_- \psi_n = \sqrt{n} \psi_{n-1}$$

$$a_+ = \frac{1}{\sqrt{2\hbar m \omega}} (-i\hat{p} + m\omega \hat{x})$$

$$a_- = \frac{1}{\sqrt{2\hbar m \omega}} (+i\hat{p} + m\omega \hat{x})$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-)$$

$$\hat{p} = i\sqrt{\frac{\hbar m \omega}{2}} (a_+ - a_-)$$

$$\Delta l = l' - l = \pm 1$$

$$\Delta m = m' - m = 0 \text{ in } x$$

$$\Delta m = m' - m = \pm 1 \text{ in } y, z$$

$$E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle$$

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0$$

$$i\hbar \frac{\partial \bar{\psi}}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \bar{\psi}}{\partial x^2} + V \bar{\psi}$$

$$E \bar{\psi} = M \bar{\psi}$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V \psi = E \psi$$

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$E_{\text{sh}} = \frac{E_1}{n^2}; E_1 = -13.6 \text{ eV}$$

$$\sigma_A^2 \sigma_B^2 \geq \left( \frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2$$

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

$$[\hat{x}, \hat{p}] = i\hbar$$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^0 | H^2 | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$

quantum dynamics

$$|\psi\rangle = \sum_{n=1}^{\infty} c_n e^{-iE_n t/\hbar} |\psi_n\rangle$$

1 take  $\bar{\psi}(t) = c_a(t) \psi_a e^{-iE_a t/\hbar} + c_b(t) \psi_b e^{-iE_b t/\hbar}$

2 solve Schr. eq.  $\hat{M} \bar{\psi} = i\hbar \frac{\partial \bar{\psi}}{\partial t}$  with  $\hat{H} = \hat{H}^0 + \hat{H}^1(t)$

3 find  $\frac{dc_a}{dt}$  as function of  $c_a$  and  $\frac{dc_b}{dt}$  as function of  $c_a$

4 in zeroth order, take  $c_a^{(0)}(t) = c_a(0)$  and  $c_b^{(0)}(t) = c_b(0)$

5 calculate higher order by substituting  $c_a^{(1)}(t)$  and  $c_b^{(1)}(t)$  into the both first order integrating

transition probability:  $P_{a \rightarrow b}(t) = |c_b(t)|^2$  if  $c_a(0) = 1$

stimulated emission  $\rightarrow$  one photon absorbed, two emitted

spontaneous emission rate:  $A = \frac{\omega^3 |\mu|^2}{30\pi \epsilon_0 \hbar c^3}$

$$\int_0^{\infty} x^n e^{-x/a} dx = n! a^{n+1}$$

$$\int_0^{\infty} x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi} \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1}$$

$$\int_0^{\infty} x^{2n+1} e^{-x^2/a^2} dx = \frac{n!}{2} a^{2n+2}$$

$$L_x = y p_z - z p_y$$

$$[L_x, L_y] = i\hbar L_z$$

$$L_+ = L_x + iL_y$$

$$[L^2, L_x] = 0$$

$$[L_x, L_+] = \pm \hbar L_+$$

$$[L^2, L_+] = 0$$

$$S^2 |s, m\rangle = \hbar^2 s(s+1) |s, m\rangle$$

$$S_x |s, m\rangle = \hbar m |s, m\rangle$$

$$[L_x, L_y] = i\hbar L_z$$

$$L_+ = L_x + iL_y$$

$$[L^2, L_x] = 0$$

$$[L_x, L_+] = \pm \hbar L_+$$

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$$S_x |s, m\rangle = \hbar m |s, m\rangle$$

Fermi energy:

$$E_F = \frac{\hbar^2}{2m} (3\rho)^{2/3}$$

Fermi surface separates occupied and unoccupied states

Fermi energy is difference in kinetic energy between highest occupied state and ground state

$$[A+B, C] = [A, C] + [B, C]$$

$$[A\hat{B}, C] = \hat{A}[B, C] + [A, C]\hat{B}$$

rooms are close together (interpenetrating) fermions are further apart

$L \rightarrow$  (has half-integer spin)

$S=1$ : triplet; symmetric

$S=0$ : singlet; antisymmetric

parahelium: antisymmetric spin

orthohelium: symmetric spin

electron configuration

|    |   |        |     |
|----|---|--------|-----|
| H  | (1s)                                    | $2s^1$ | 1/2 |
| He | (1s) <sup>2</sup>                       | $1s^2$ | 0   |
| Li | (He)(2s)                                | $2s^1$ | 1/2 |
| Be | (He)(2s) <sup>2</sup>                   | $2s^2$ | 0   |
| B  | (He)(2s) <sup>2</sup> (2p)              | $2p^1$ | 1/2 |
| C  | (He)(2s) <sup>2</sup> (2p) <sup>2</sup> | $2p^2$ | 0   |
| N  | (He)(2s) <sup>2</sup> (2p) <sup>3</sup> | $2p^3$ | 1/2 |

|    |   |        |     |
|----|---|--------|-----|
| Na | (Ne)(3s)                                | $3s^1$ | 1/2 |
| Mg | (Ne)(3s) <sup>2</sup>                   | $3s^2$ | 0   |
| Al | (Ne)(3s) <sup>2</sup> (3p)              | $3p^1$ | 1/2 |
| Si | (Ne)(3s) <sup>2</sup> (3p) <sup>2</sup> | $3p^2$ | 0   |
| P  | (Ne)(3s) <sup>2</sup> (3p) <sup>3</sup> | $3p^3$ | 1/2 |

good quantum numbers

fine structure / rel. correction  $\rightarrow n, l, m$

fine structure / spin-orbit coupling  $\rightarrow l, s, j, m_j$

and fine  $g^2 = L^2 + S^2 + 2L \cdot S$ , which gives  $L \cdot S = \frac{1}{2}(j^2 - L^2 - S^2)$

fine structure / total  $\rightarrow n, l, s, j, m_j$

weak field ZME:  $n, l, m, m_s$

strong field ZME:  $n, l, m_l, m_s$

$$W_{ij} = \langle \psi_i^0 | H^1 | \psi_j^0 \rangle$$

eigenvalues of matrix W give first-order energy corrections

$$S = \frac{\hbar}{2} \sigma$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

# WKB

amplitude phase  
 $\psi(x) = A(x) e^{i\phi(x)}$

integral over well  
 $p(x) = \sqrt{2m(E - V(x))}$

$\psi(x) = \frac{C}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x) dx} \quad (E > V)$

$\psi(x) = \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int |p(x)| dx} \quad (E < V)$

$T \sim e^{-2\gamma}$  with  $\gamma = \frac{1}{\hbar} \int_a^b |p(x)| dx$   
 ← integral over barrier

- use tunnel factor instead of phase for tunneling
- phase = integral over local wave number
- works good far from classical turning points
- determine bound state energies using:
  - practical walls

$= 0 \rightarrow \int_{\text{well}} p(x) dx = (n - \frac{1}{2})\pi \hbar$

$= 1 \rightarrow \int_{\text{well}} p(x) dx = (n + \frac{1}{4})\pi \hbar$

$= 2 \rightarrow \int_{\text{well}} p(x) dx = n\pi \hbar$

square well  
 $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$

for some operator  $\hat{Q}$ :

$\hat{Q}$ 's eigenfunctions are a complete set  $\rightarrow \hat{Q} |f_n\rangle = q_n |f_n\rangle \rightarrow |\psi\rangle$  can be thought the basis of  $\hat{Q}$ -eigenfunctions  $\rightarrow |\psi\rangle = \sum_n d_n |f_n\rangle$   
 then, probability of measuring  $q_n$  is given by  $|d_n|^2$   
 The coefficient  $\langle x | n \rangle = f_n(x)$  is a basis wavefunction; expansion of wavefunction  $\psi(x) = \langle x | \psi \rangle = \sum_n \langle x | n \rangle \langle n | \psi \rangle = \sum_n c_n f_n(x)$

## Variational principle

- finds upper bounds for GS energy
1. pick a trial wavefunction  $\psi$  with variational parameters  $b_1, \dots, b_n$
  2. normalize  $\psi$  (if not done yet)
  3. determine the expectation value of the Hamiltonian as function of  $b_i$ 's
  4. find the values of  $b_i$  that minimize  $E_{GS}$  using  $\frac{\partial E}{\partial b_i} = 0$
  5. fill in these values for  $b_i$  to obtain  $E_{GS}$

example variational principle:  $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$  an upper bound for

$\psi(x) = A e^{-bx^2} \rightarrow 1 = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$   
 $\langle H \rangle = \langle T \rangle + \langle V \rangle$   
 $\langle T \rangle = -\frac{\hbar^2}{2m} |A|^2 \int_{-\infty}^{\infty} e^{-bx^2} \frac{d^2}{dx^2} (e^{-bx^2}) dx = \frac{\hbar^2 b}{2m}$

## harmonic oscillator

$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$

$\psi_n(x) = \frac{1}{\sqrt{n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \psi_0(x)$

$E_n = \left(n + \frac{1}{2}\right) \hbar \omega$

## J-function, potential

(for a potential well):  $V(x) = -uJ(x)$

$E = -\frac{m a^2}{2\hbar^2}$

$\psi(x) = \frac{\sqrt{m a^2}}{\hbar} e^{-m a |x| / \hbar}$

$j$  goes from  $L + 5$  to  $L - 5$  in integer steps