Multiparticle systems

~~(ARM ??)~~

In QM, we do not describe multiple particles by using individual wavefunctions; we describe the system of particles w/ a single wavefunction

eg. for 2 particles:

$\Psi(x_1, x_2, t)$

Then the probability density $P(x_1, x_2, t) = |\Psi(x_1, x_2, t)|^2$

$$\int_{x_1=a_1}^{b_1} dx_1 \int_{x_2=a_2}^{b_2} dx_2 \, |\Psi(x_1, x_2, t)|^2 = \text{probability of}$$

finding particle 1 between a_1 & b_1
and particle 2 between a_2 & b_2

$$\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \, |\Psi(x_1, x_2, t)|^2 = 1 \quad \text{(normalization condition)}$$

Energy of a system of two particles (nonrelativistic)

$$E = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V_{tot}(x_1, x_2)$$

where

$$V_{tot}(x_1, x_2) = V_{ext}(x_1) + V_{ext}(x_2) + V_{int}(x_1 - x_2)$$

$$\hat{H} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V_{tot}(x_1, x_2)$$

t.d.S.e. $\quad i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$

Stationary states $\quad \psi(x_1, x_2, t) = u(x_1, x_2)\, e^{-iEt/\hbar}$

states of well-defined total energy E (of the system)

then t.i.S.e

$$\hat{H}\, u(x_1, x_2) = E\, u(x_1, x_2)$$

Simplification:

assume 2 particles of equal masses m
that do not interact w/ one another,
but only with an external potential $V(x)$
[eg 2 particles in a box]

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x_1^2} + V(x_1)\,u - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x_2^2} + V(x_2)\,u = E\,u$$

- In this case, there exist eigenfunctions of $\hat{H}$ that are products of single-particle eigenfunctions

$$u(x_1, x_2) = u_n(x_1)\,u_m(x_2)$$

where $u_n(x)$ are solutions of the
"single particle t.i.S.e"

$$-\frac{\hbar^2}{2m}\frac{d^2 u_n(x)}{dx^2} + V(x)\,u_n(x) = E_n\,u_n(x)$$

- Furthermore, the linear combination

$$u(x_1, x_2) = \alpha\,u_n(x_1)\,u_m(x_2) + \beta\,u_m(x_1)\,u_n(x_2)$$

is also an eigenfunction of $\hat{H}$

[Exercise: prove these for 2 particles in a box] after ~~G2~~ G3

Exercise

Consider a system consisting of 2 particles confined to a box of width L. For simplicity let the mass m of the particles be equal. (This could describe a proton & a neutron in a nucleus.) The potential $V(x_1, x_2)$ vanishes provided both x_1 & x_2 are between 0 & L, otherwise it is infinite.

We are assuming that the particles do not interact with one another

Let $u_n(x)$ be the eigenfunction for a single particle of mass m in a box of width L (derived in class)

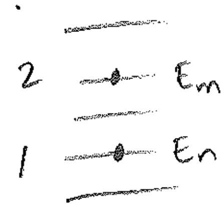
(a) Show that $u(x_1,x_2) = u_n(x_1)\,u_m(x_2)$ is a solution of the time-indep Sch eqn for the system of two particles.
What is the energy of this state? $[E_1(n^2+m^2)]$
What is the smallest possible energy? $[2E_1]$

(b) Repeat for $u(x_1,x_2) = u_n(x_1)\,u_m(x_2) + u_n(x_2)\,u_m(x_1)$ $[2E_1]$

(c) Repeat for $u(x_1,x_2) = u_n(x_1)\,u_m(x_2) - u_n(x_2)\,u_m(x_1)$ $[E_1 + E_2 = 5E_1]$

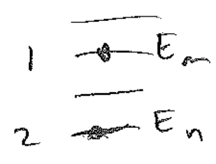
[After students have presented the preceding exercise
(otherwise, skip to J1)]

$u_A(x_1, x_2) = u_n(x_1)\, u_m(x_2)$ describes a state w/ $E = E_n + E_m$



we say "particle 1 is in energy level E_n
and " 2 " " " " E_m"

$u_B(x_1, x_2) = u_m(x_1)\, u_n(x_2)$ describes a state w/ $E = E_n + E_m$



we say "particle 1 ... E_m
2 ... E_n"

These states have well-defined individual energies and well defined total energy

Because these are degenerate, the linear combination

$\alpha u_A(x_1, x_2) + \beta u_B(x_1, x_2)$ ⇒ (normalize ⇒ $|\alpha|^2 + |\beta|^2 = 1$)

is also a state w/ ~~definite~~ total energy $E = E_n + E_m$, but not well defined individual energies

but not so simply described ⇒ ptl 1 has E_n
(+ ptl 2 has E_m) w/ prob $|\alpha|^2$

$\boxed{\text{"entangled state"}}$

ptl 1 has E_m
(+ ptl 1 has E_n) w/ prob $|\beta|^2$

and $|\alpha|^2 + |\beta|^2 = 1$
(normalize the state)

Consider 2 <u>identical</u> particles (ie mass, charge, etc. same)

Quantum mechanically, they are indistinguishable

[classically, one can distinguish a particle by its initial condition: electron emitted by cathode at $t=0$, and then follow the trajectory]

[prob of finding a particle at x_1 + a particle at x_2]

$$P(x_1, x_2) \stackrel{!}{=} P(x_2, x_1) \Rightarrow |u(x_1, x_2)|^2 = |u(x_2, x_1)|^2$$

There are two possibilities

$$\Rightarrow \begin{cases} u(x_1, x_2) = u(x_2, x_1) \\ \text{or} \\ u(x_1, x_2) = -u(x_2, x_1) \end{cases}$$

For $u(x_1, x_2) = u(x_2, x_1)$: Particles that satisfy this condition are called bosons (satisfy "Bose-Einstein statistics"). They have integer spin: $0, \hbar, 2\hbar, \ldots$ (Higgs, photon, graviton)

or

For $u(x_1, x_2) = -u(x_2, x_1)$: Particles that satisfy this condition are called fermions ("Fermi-Dirac statistics"). They have half-integer spin: $\frac{\hbar}{2}, \frac{3\hbar}{2}, \frac{5\hbar}{2}$ (electrons, protons, neutrons, quarks)

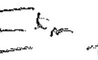
Note that, for identical fermions, $u(x, x) = 0$

because $u(x,x) = -u(x,x) \Rightarrow u(x,x) = 0 \Rightarrow P(x,x) = 0$

$\Rightarrow$ Probability of finding 2 identical fermions at <u>same</u> location x is zero (Pauli exclusion)

G6

An entangled state of 2 particles is

$$u(x_1,x_2) = \alpha\, u_n(x_1)\, u_m(x_2) + \beta\, u_m(x_1)\, u_n(x_2) = \alpha$$  $$+\ \beta$$ 

$|\alpha|^2 + |\beta|^2 = 1$

Identical particles must obey either

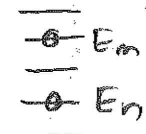
$u(x_1, x_2) = u(x_2, x_1)$ (bosons) $\Rightarrow \beta = \alpha$

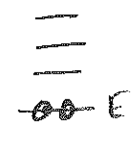
or $u(x_1, x_2) = -u(x_2, x_1)$ (fermions) $\Rightarrow \beta = -\alpha$

They are necessarily entangled

For bosons

$$u(x_1,x_2) = \begin{cases} \frac{1}{\sqrt{2}}\left[u_n(x_1)\, u_m(x_2) + u_n(x_2)\, u_m(x_1)\right], & n \neq m \\ u_n(x_1)\, u_n(x_2), & n = m \end{cases}$$

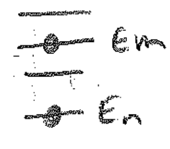




These obey $u(x_1, x_2) = u(x_2, x_1)$
(symmetric under exchange)

For fermions

$$u(x_1,x_2) = \begin{cases} \frac{1}{\sqrt{2}}\left[u_n(x_1)\, u_m(x_2) - u_n(x_2)\, u_m(x_1)\right], & n \neq m \\ 0, & n = m \end{cases}$$



(no two identical fermions in same state $\Rightarrow$ Pauli exclusion)

These obey $u(x_1, x_2) = -u(x_2, x_1)$
(antisymmetric under exchange)

Conclusion: we must use entangled states when describing identical particles in QM.

We can write fermion wave functions using determinants
(Slater determinant)

$$u(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} u_n(x_1) & u_n(x_2) \\ u_m(x_1) & u_m(x_2) \end{vmatrix} \quad \text{for } n \neq m$$

If $n = m$, then 2 rows are identical, determinant vanishes.
If $x_1 = x_2$, then 2 columns are identical, " "

~~after G4~~ after G7

Exercise

(a) Write down time-indep Schrodinger equation for 3 particles (of equal mass) ~~confined to a box~~ in a potential $V(x)$

(b) Write the solution of this eqn that describe 3 identical bosons
(The wavefunction must be sym'c under the exchange of any two of the particles.)
What is the minimum possible energy for such a state?

(c) Ditto for 3 identical fermions.
(The wavefunction ... antisymmetric ...)

Ans:

(a)
$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx_1^2}+\frac{d^2}{dx_2^2}+\frac{d^2}{dx_3^2}\right)u(x_1,x_2,x_3) + V(x_1,x_2,x_3)\,u = E\,u$$

(b)
$$u(x_1 x_2 x_3) = u_n(x_1)\,u_m(x_2)\,u_\ell(x_3) + (5 \text{ permutations})$$

$$E_{min} = 3E_1$$

(c)
$$u(x_1 x_2 x_3) = \begin{vmatrix} u_n(x_1) & u_n(x_2) & u_n(x_3) \\ u_m(x_1) & u_m(x_2) & u_m(x_3) \\ u_\ell(x_1) & u_\ell(x_2) & u_\ell(x_3) \end{vmatrix}$$

$$E_{min} = E_1 + E_2 + E_3 = (1+4+9)E_1 = 14E_1$$

for pcl in box

[after 3 fermion exercise is presented]

N fermion wave function

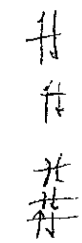
$$u(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{n_1}(x_1) & u_{n_1}(x_2) & \cdots & u_{n_1}(x_N) \\ u_{n_2}(x_1) & u_{n_2}(x_2) & \cdot & u_{n_2}(x_N) \\ \vdots & & & \\ u_{n_N}(x_1) & \cdots & & u_{n_N}(x_N) \end{vmatrix}$$

(Slater determinant)

ground state of N fermions $\Rightarrow$ fill up lowest N levels.

$$E_{gnd} = \sum_{n=1}^{N} E_n$$

Actually, if account for spin, can put 2 spin-$\frac{1}{2}$ fermions in each level



$$E_{gnd} = 2 \sum_{n=1}^{N/2} E_n \qquad \text{(assume N even)}$$

$$= 2 E_1 \sum_{1}^{N/2} n^2 \qquad \text{(for particle in a box)}$$

[• Now $\sum_1^p n = \frac{1}{2} p(p+1)$ [gauss]

• Also $\sum_1^p n^2 = \frac{1}{6} p(p+1)(2p+1)$]

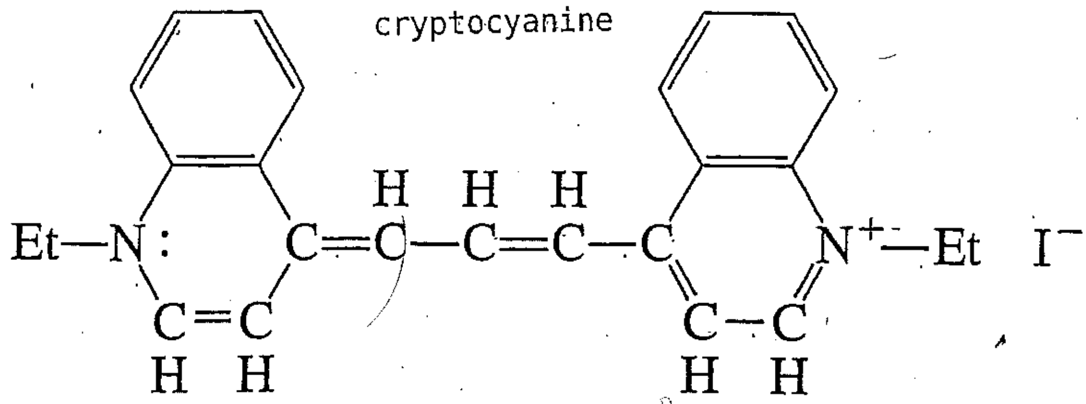
$$= \frac{1}{12} N(N+1)(N+2)\, E_1$$

[proof: $f(p) = f(p-1) + p^2$

$\underbrace{p(p+1)(2p+1)}_{2p^3 + 3p^2 + p} = \underbrace{(p-1)p(2p-1)}_{2p^3 - 3p^2 + p} + 6p^2$]

[

cryptocyanine

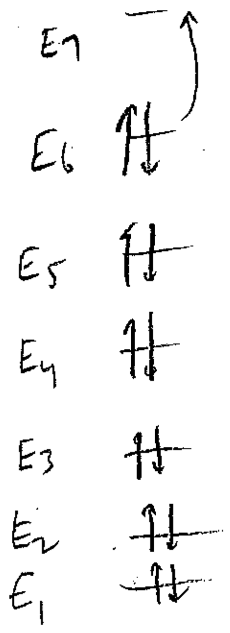


example of particle in a box:

- cryptocyanine: organic dye w/ conjugated bonds
- some of the electrons are delocalized
- and free to travel along the chain ($L = 1.67\,nm$)
- $\exists$ 12 "free" electrons (9 from C, 3 from N)

just talk about this, don't write

$$E_n = E_1 n^2, \quad E_1 = \frac{\hbar^2 \pi^2}{2mL^2}, \quad L = 1.67\,nm, \quad m = \text{mass of electron}$$



Electrons are spin-$\frac{1}{2}$ particles
w/ 2 distinct spin states ($\uparrow$ and $\downarrow$)
∴ its are not identical
$\Rightarrow$ 2 electrons in each spatial state ("orbital") w/ opposite spins

ground state energy $\Rightarrow 2\sum_{i=1}^{6} E_i =$

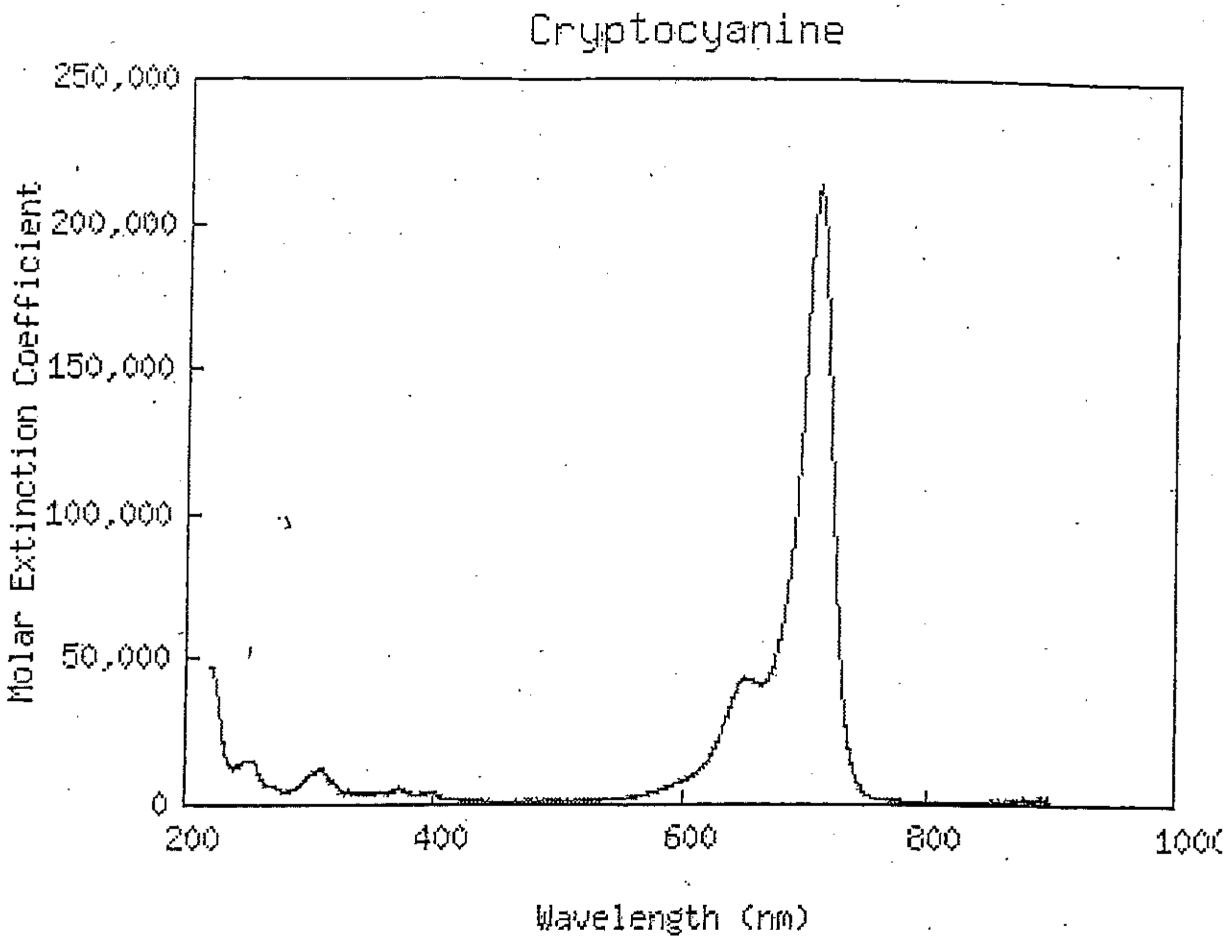
first excited state $\Rightarrow 2\sum_{i=1}^{5} E_i + E_6 + E_7$

$$\Delta E = E_7 - E_6 = (49 - 36)E_1 =$$

molecule can absorb a photon w/ this energy

$$E_{photon} = \frac{hc}{\lambda}$$

$$\lambda = \frac{2\pi\hbar c}{13 E_1} = 7 \times 10^{-7}\,m = 700\,nm \quad \text{(dark green)}$$



Cryptocyanine
Molar Extinction Coefficient
250,000
200,000
150,000
100,000
50,000
0
200
400
600
800
1000
Wavelength (nm)

necessary? → only if asks Slater same why determinant has $\sqrt{n!}$

option

Revisit waveform for 2 identical particles

$$P(x_1, x_2) = u^*(x_1, x_2)\, u(x_1, x_2)$$

Normalization condition

$$\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, P(x_1, x_2) = 1$$

For 2 fermions: $u(x_1, x_2) = A\left(u_m(x_1)\, u_n(x_2) - u_n(x_1)\, u_m(x_2)\right)$

$$1 = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, |A|^2 \left(u_m^*(x_1)\, u_n^*(x_2) - u_n^*(x_1)\, u_m^*(x_2)\right)\left(u_m(x_1)\, u_n(x_2) - u_n(x_1)\, u_m(x_2)\right)$$

$$= |A|^2 \int_{-\infty}^{\infty} dx_1\, u_m^*(x_1)\, u_m(x_1) \int_{-\infty}^{\infty} dx_2\, u_n^*(x_2)\, u_n(x_2)$$

$$- |A|^2 \int_{-\infty}^{\infty} dx_1\, u_m^*(x_1)\, u_n(x_1) \int_{-\infty}^{\infty} dx_2\, u_n^*(x_2)\, u_m(x_2)$$

+ other cross term + other diagonal term

$$= |A|^2\, 1 \cdot 1 - |A|^2\, 0 \cdot 0 - |A|^2\, 0 \cdot 0 + |A|^2\, 1 \cdot 1 = 1$$

$$1 = 2|A|^2 \quad \text{so} \quad A = \frac{1}{\sqrt{2}}$$

```
one[x_1] := Sin[Pi x]; Plot[one[x1]^2, {x1, 0, 1}]

two[x1_] := Sin[2 Pi x1] ; Plot[ two[x1]^2, {x1, 0, 1}]

u[x1_, x2_] := Sin[2 Pi x1] Sin[Pi x2];
DensityPlot[ u[x1, x2]^2, {x1, 0, 1}, {x2, 0, 1}]

DensityPlot[ (1 / 2) u[x1, x2]^2 + (1 / 2) u[x2, x1]^2, {x1, 0, 1}, {x2, 0, 1}]

anti[x1_, x2_] := u[x1, x2] - u[x2, x1];
DensityPlot[(1 / 2) anti[x1, x2]^2, {x1, 0, 1}, {x2, 0, 1}]

sym[x1_, x2_] := u[x1, x2] + u[x2, x1];
DensityPlot[(1 / 2) sym[x1, x2]^2, {x1, 0, 1}, {x2, 0, 1}]
```

Wolfgang Pauli stories

very smart: treatise on SR + GR at age 21

very critical: during seminars would nod until he disagreed w/ speaker, then would shake his
[Freund] head, at last "that is utterly false"

[Peierls] someone showed Pauli a paper by a young physicist which he suspected was not of great value:
Pauli: "It's not right. It's not even wrong"

[Close] about Yang: "So young. And already so unknown"

unsuccessful at expts
when he walked into a lab, expts wd inexplicably fail. Stern banned him from his lab

inexplicable explosion in lab
Pauli on train passing thru town

banquet w/ large chandelier rigged to crash when Pauli entered the room to demonstrate the Pauli effect.
Malfunctioned!

after he died, granted an audience w/ God
Asked god to explain the ratio of proton mass to electron.
why 1837. God → blackboard
Pauli shook his head + said "It is utterly false"