⑤ Trapped Particles

20 yrs ago QM taught initially using idealised potentials (sq wells, harmonic oscillators) as warm up exercises to "real" potentials in atomic and molecular physics.

Using nanotechnology can construct real objects where electrons are trapped in potentials which are excellent approx to simple cases and where the sizes are small enough for quantum phenomena (typically tens of nanometers)

eg. in chips building nanoscale circuits
precipitate nanocrystals out of solutions.
genetically engineered viral assembly!

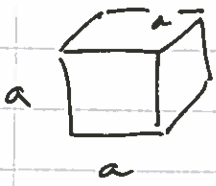
quantum dot : trapping potential in 3D
small enough for quantum behaviour.

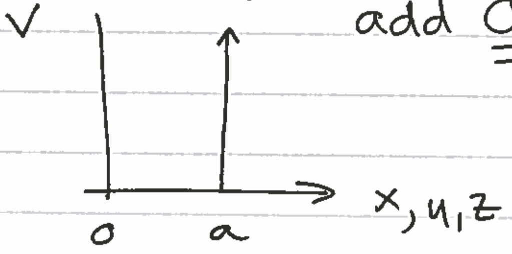
quantum wire : trapping in 2D, free in 3rd

quantum well : trapping in 1D, free in 2D.

Typical dimensions : 5 - 100 nm
ie. 25 - 500 atoms (atomic radii ~0.1 nm)

Example: Metallic nanocubes of silver ~ 50-100 nm
electrons free to move throughout until reach the wall.
Treat as 3D infinite sq well.





add ONE electron into well.

Inside: $-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$ or $\nabla^2\psi = -k^2\psi$

$$k^2 = \frac{2mE}{\hbar^2}$$

Boundary conditions : wave function zero along 6 walls

$$\left.\begin{aligned}\psi(0,y,z)&=0\\ \psi(a,y,z)&=0\end{aligned}\right\}$$ for faces $\perp$ to x axis.

and similar for other faces.

Cubic problem → Cartesian coordinates

TISE: $$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=-k^2\psi$$

Try a separable sol$^{\underline{n}}$ $\psi(x,y,z)=X(x)Y(y)Z(z)$

substitute into TISE and divide by $X.Y.Z$ gives

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2}=-k^2$$

func$^{\underline{n}}$ of x only + y only + z only = constant

each term must be equal to a constant

$$-k_x^2 \quad -k_y^2 \quad - \quad k_z^2 = -k^2$$

3D partial diff eq$^{\underline{n}}$ ⇒ 3 ordinary diff eq$^{\underline{n}}$s

boundary conditions also separate

eg. $\psi(0,y,z)=X(0)Y(y)Z(z)=0$

implies $X(0)=0$

Three similar problems to solve:

eg. $\dfrac{d^2X}{dx^2}=-k_x^2X$ subject to $X(0)=0$, $X(a)=0$

Guitar string with clamped ends.

Solutions : $X=A\cos k_xx+B\sin k_xx$

but $A=0$ otherwise $X(0)\neq0$

and $B\sin k_xa=0 \longrightarrow k_x=\dfrac{n_x\pi}{a}$ $n_x=1,2,3\ldots$

Normalise $\int|X(x)|^2dx=1 \rightarrow B=\sqrt{\dfrac{2}{a}}$

similar sol$^{\underline{n}}$s for $Y(y)$ and $Z(z)$

Full wavefunction

$$\psi(x,y,z) = \left(\frac{2}{a}\right)^{3/2} \sin\frac{n_x \pi x}{a} \sin\frac{n_y \pi y}{a} \sin\frac{n_z \pi z}{a}$$

Eigenvalue: $k^2 = k_x^2 + k_y^2 + k_z^2$

$$= \left(\frac{\pi}{a}\right)^2 (n_x^2 + n_y^2 + n_z^2) \qquad (n_x, n_y, n_z = 1, 2 \ldots)$$

with Energy $E = \frac{\hbar^2 k^2}{2m} = \frac{1}{2m}\left(\frac{\hbar\pi}{a}\right)^2 (n_x^2 + n_y^2 + n_z^2)$

one Comb ~~state~~ → two [illegible] when consider spin up/down.

Ground state: $n_x = n_y = n_z = 1 \qquad E_{111} = \frac{3}{2m}\left(\frac{\hbar\pi}{a}\right)^2$

First excited Level ~~states~~:

$n_x = 2 \quad n_y = n_z = 1 \qquad E_{211} = \frac{3}{m}\left(\frac{\hbar\pi}{a}\right)^2$ ~~states~~

or $n_x = 1 \; n_y = 2 \; n_z = 1$ have same energy

or $n_x = 1 \; n_y = 1 \; n_z = 1$

i.e. ~~level is degenerate, with a degeneracy of 3~~ states

3 with same energy combinations. actually equ. 6 (if you consider electrons can be spin up or spindown)

For a = 50nm

$$E_{111} = \frac{3}{2mc^2}\left(\frac{\hbar c \pi}{a}\right)^2 = \frac{3}{2 \times 0.511 \times 10^6}\left(\frac{197\pi}{50}\right)^2 =$$

$\hbar c = 197$ eV.nm

$= 0.45 \times 10^{-3}$ eV

$E_{211} = 0.9 \times 10^{-3}$ eV.

} first two levels for single electron.

For each Ag atom, one conduction electron.

radius of Ag atom $\doteq .145$ ~~p~~nm

so cube contains $\left(\frac{50}{2 \times .145}\right)^3$ atoms $\equiv$ ~~[illegible]~~ 5×10^6 atoms

CAREFUL TO TALK ABOUT COMBINATIONS, LEVELS, STATES

So 5×10^6 electrons in a Ag nanocube
single-electron energies aren't that relevant: a mess of many electrons in levels but all interacting with one another via Coulomb.

Optoelectronic properties determined more as an electron gas filling the metallic box.
Light scattering via sloshing of this plasma around the cube.
Oscillations of the electron gas are quantised and called plasmons. Surface plasmons often dictate the colour of materials. – energies depend on size of electron gas ie. cube size.

Eg. medieval nanotechnology
addition of different amounts of silver or gold chloride into molten glass produces different sizes of nanoparticles that reflect different colours.

→ need to be cleverer / or have more control to be able to access single particle states in a nanosystem.

⑥ Semiconductor Quantum Dots.

with semiconductor material can control number of electrons by doping and/or connecting to external potentials.

Two varieties:

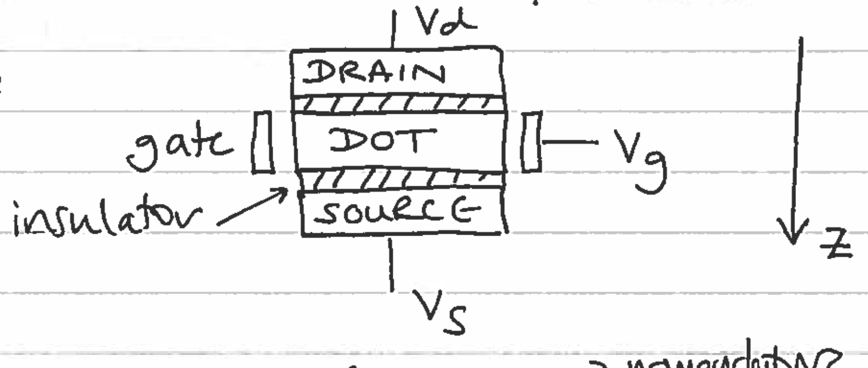
colloidal systems (suspended in liquid) 2-10nm or 10-50 atoms in diameter (PbS, InAs, InP etc) size determines properties fluoresce in visible, make brackets, can be attached to biomolecules for tracking.

constructed on surfaces of Si chip using lithography epitaxy like miniature transistors but with quantum behaviour. (we'll consider this one as "controllable").

Nanoscale lump of undoped semiconductor with three electrical contacts:

undoped – conduction levels are initially empty
contacts – used to control number of electrons

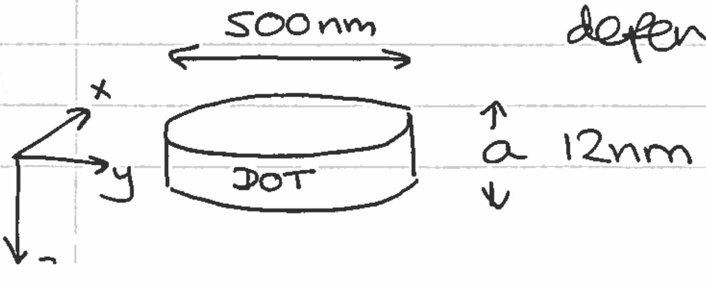
Cylindrical dot:
vertical section



"drain" – source of electrons if $V_d < V_s$
"source" – drains out electrons
"gate" – changes average potential in dot

} nomenclature based on conventional +ve charge

names irrelevant: drain and source swap roles depending on V_d relative to V_s

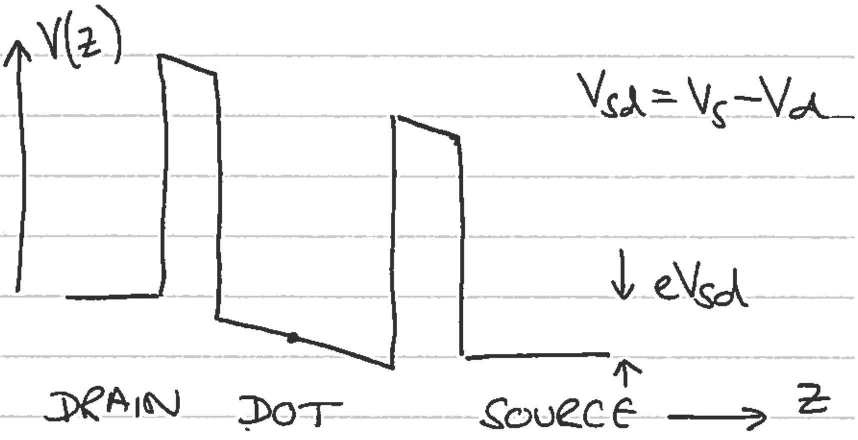


Built with painstaking ~~&~~ stacking of layers and electron beam lithography

DOT is made of undoped InGaAs
Electrons moving in InGaAs have an effective mass. This effectively accounts for the results of many interactions with the surrounding material: $m^* = 0.06 m_e$

To a reasonable approximation: $V(x,y) = \frac{1}{2}k(x^2+y^2)$
where $k = m^* \omega^2$
$\hbar\omega = 5\,\text{meV}$ i.e. a 2D harmonic oscillator

In the z-direction:



potential in centre →
$\propto V_g$
gate voltage controls the level of the floor

[hmm – double barrier?]

If insulating walls are high and effect of tilting floor low } infinite sq well in z direction.

$$\text{Hamiltonian: } \hat{H} = \frac{-\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}k(x^2+y^2)$$

Separate bits are functions of one coordinate alone
Use separable solⁿ for TISE:
$$\psi(x,y,z) = X(x)Y(y)Z(z)$$
⇒ three separate eigenvalue problems:

two 1D Harmonic oscillators (x and y) $\quad -\frac{\hbar^2}{2m^*}\frac{d^2X}{dx^2} + \frac{1}{2}kx^2X = E_xX$

one infinite square well in z $\quad -\frac{\hbar^2}{2m^*}\frac{d^2Z}{dz^2} = E_zZ$

Eigenvalues are: $E_x = (n_x + \frac{1}{2})\hbar\omega \quad n_x = 0, 1, 2 \ldots$

$E_y = (n_y + \frac{1}{2})\hbar\omega \quad n_y = 0, 1, 2 \ldots$

$E_z = \frac{\hbar^2}{2m^*}\left(\frac{n_z \pi}{a}\right)^2 \quad n_z = 1, 2, 3 \ldots$

Energy $E = E_x + E_y + E_z$

ie. $E_{n_x n_y n_z} = (n_x + n_y + 1)\hbar\omega + \frac{\hbar^2}{2m^*}\left(\frac{n_z \pi}{a}\right)^2$

Typical energy for z excit^n:

$$E_z(n_z=1) = \frac{1}{2m^* c^2}\left(\frac{\hbar c \pi}{a}\right)^2 = \frac{1}{2 \times 0.06 \times 0.511 \times 10^6}\left(\frac{197\pi}{12}\right)^2$$

$= 0.043$ eV

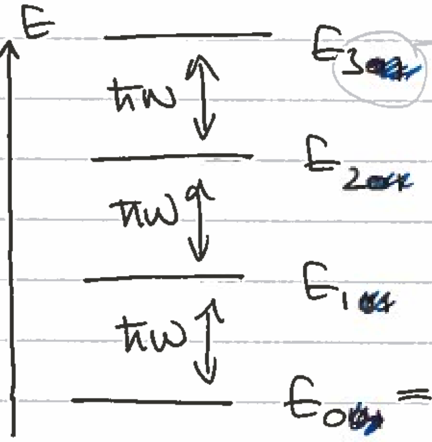
This is much larger than $\hbar\omega = 0.005$ eV

low-lying states have $n_z = 1$ plus excitations in xy

Energy levels:

Ground state (0,0,1)

GS



$E_0 = \hbar\omega + \frac{\hbar^2}{2m^*}\left(\frac{\pi}{a}\right)^2$

not^n confusing.

turning on x phonons one by one.

But: x and y ~~phonons~~ excit^n s are equivalent

1st ES

$n_x = 1 \; n_y = 0$
$n_x = 0 \; n_y = 1$ } same energy E_{101} ~~doubly degenerate~~ 2 combs of (n_x, n_y)

2nd ES EL

The ~~two-phonon state~~ second excited level is ~~triply degenerate~~:

(n_x, n_y): (2,0) (1,1) (0,2) 3 combs (n_x, n_y)

And the ~~three~~ third ~~phonon~~ state

(3,0) (2,1) (1,2) (0,3) fourfold

But with electron spin (up/down) can put two electrons in each (n_x, n_y) ~~state~~ level

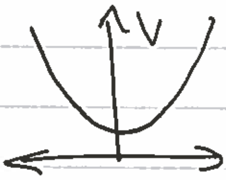
Pauli exclusion principle: Fermions can't share same

Level	# electrons in Level	# electrons in dot
Ground	$2 \times 1 = 2$	2
1st	$2 \times 2 = 4$	$2+4=6$
2nd	$2 \times 3 = 6$	$6+6=12$
3rd	$2 \times 4 = 8$	$12+8=20$

↑ magic numbers!

levels are all full (closed shells) at a magic number
adding one more electron beyond a magic number "costs" $\hbar\omega$
so similar to:
Noble gas atoms ($Z = 2, 10, 18 \ldots$) electrons
magic nuclei ($N, Z = 2, 8, 20, \ldots$) protons or neutrons

Ideal oscillator extends from $-\infty$ to $+\infty$ without physical edge.



But gs wavefunction extends over a distance known as the oscillator length parameter

$$b = \sqrt{\frac{\hbar}{m^x \omega}}$$

$$= \sqrt{\frac{(\hbar c)^2}{m^x c^2 \hbar\omega}} = 197 \Big/ \sqrt{0.06 \times 0.511 \times 10^6 \times 5 \times 10^{-3}}$$

$$= 16\,\text{nm}$$

This is much less than the physical diameter of the dot (500nm) so for low lying states the edges should not effect things.

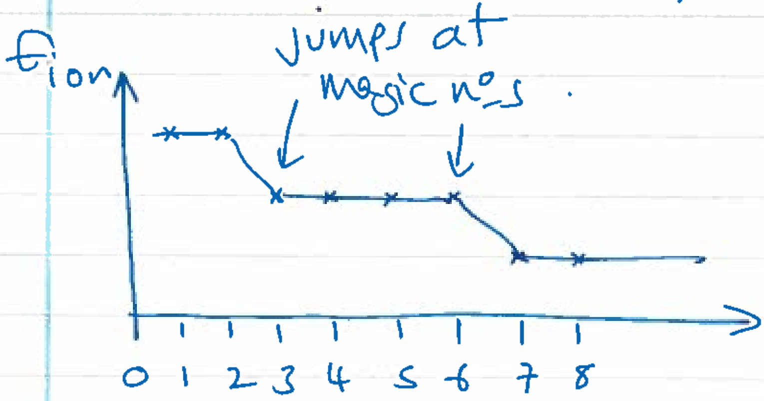
stripped
2014.

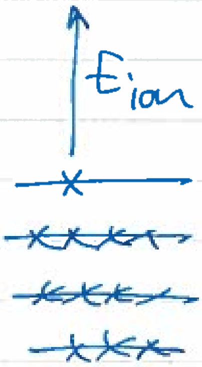
Summary:

- filling levels in a quantum system with ~~elect~~ fermions
- combination of spin and level degeneracy mean that at certain electron numbers start to fill next level up (magic numbers).

- related to physical properties as a function of electron number.

eg. first ionisation energy

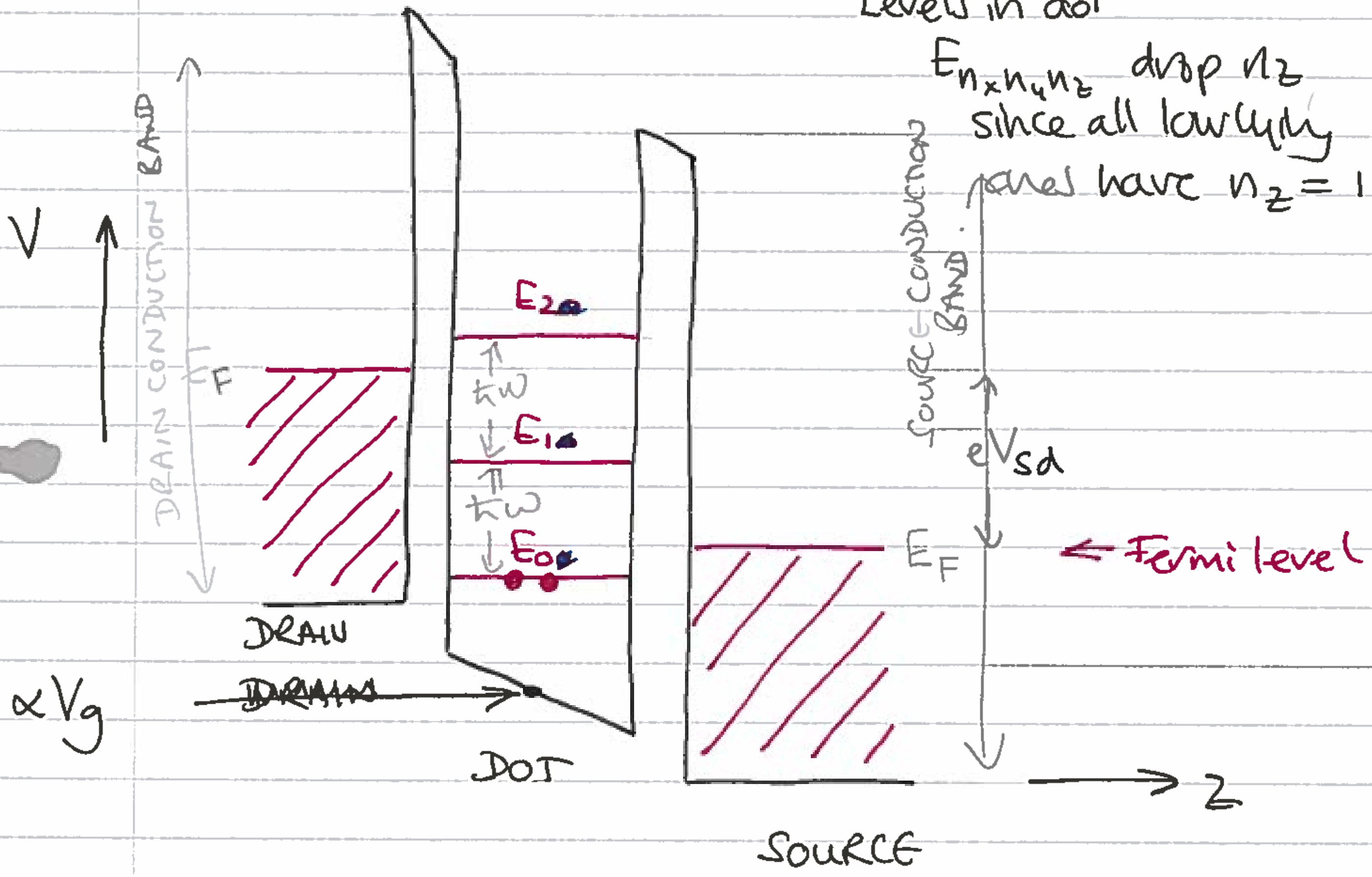




measure physical properties
look for magic numbers } check on our understanding.

↳ measuring current flow through our quantum dot will do this!

⑦ Conduction in a Semi Conductor Quantum Dot



Levels in dot
$E_{n_x n_y n_z}$ drop n_z since all low lying ones have $n_z = 1$

Electrons fill conduction bands up to "Fermi energy" in a conductor (drain and source) according to Pauli principle

Imagine tuning V_g so that the second level E_{1o} lies between Fermi levels of source and drain

Electrons from the drain (source of e^-) can tunnel into dot to occupy E_{0o}, but can't get out because levels of same energy are occupied in source.
(blocked) → levels in dot below E_F^{source} full.

Electrons from drain can't jump up into E_{2o} without extra energy (so keep the dot cold!)
(unreachable)
→ levels in dot above E_F^{drain} empty

E_1 is the interesting level, as electrons can tunnel in from drain and out into an empty state in the source

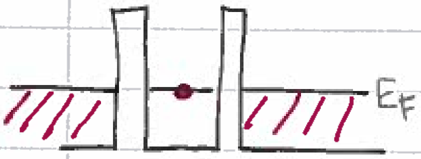
In fact, between states of the same energy, resonant tunnelling occurs

→ transmission prob large and current flows through two insulators!

in this situation large probability for finding an electron in the dot in E_1.

This conduction only happens when V_g is tuned so that an electron state lies in the window eV_{sd} between Fermi levels.

If $V_{sd} = 0$, V_g needs tuning to exactly line up the state with the Fermi levels.



otherwise no current flows. as required states are either unreachable or blocked.

Expt: make a dot (ha, ha!) Need to remind as V_g changes levels below fill up.

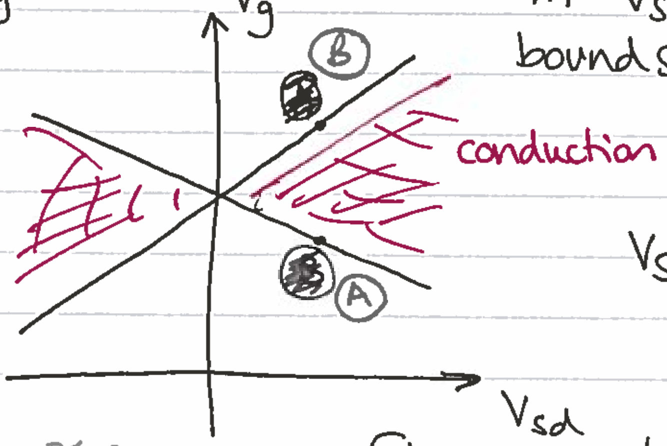
measure conductance as a function of V_{sd} and V_g

"diamonds" appear within which there is no current flow

Increasing V_g lowers the floor by $\propto -eV_g$

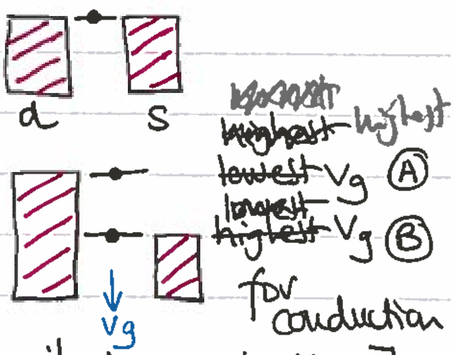
↓

ut higher and upper levels in conduction zone



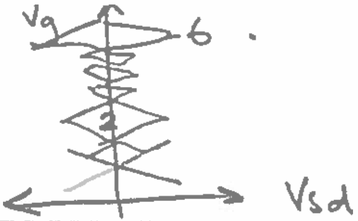
At $V_{sd} = 0$ need alignment of bound state and Fermi levels.

$V_{sd} > 0$



[ignore complex pattern within conduction]

Somehow not doing a good job of making this connection.



Different zones of conduction formed when different bound states are in the window eV_{sd}.
ie. when V_g has shifted the floor by two amounts.

Indeed, largest diamonds are at our calculated magic numbers.
But, the first two electrons should go into a level at the <u>same</u> energy – appear to do so at different V_g!

What physics has been missed?
only considered the electron in PE of well.
not the Coulomb repulsion between electrons.

Eg. one electron in E_{00} $E = E_{00}$

two electrons in E_{00} $E = 2E_{00} + \underset{\substack{\uparrow \\ \text{Coulomb energy}}}{\Delta E_e}$

More electrons → less attraction → ~~[illegible]~~ system at higher energy

This effect is known as "Coulomb blockade" for a quantum dot.

It "lifts" the degeneracy of multi-electron states.

"Physics" uses of quantum dots:

artificial atoms : study individual atom, controlling how
many electrons are in it
can excite with external e/m fields
then watch it decay

use them as basic elements of a quantum computer
"Qbits" or "qubits" — information storage

electron traps : single electron transistors
manipulate spins with magnetic fields

electron pair traps : entangle their spins
then transport to different parts of
the circuit whilst maintaining their
quantum connection.

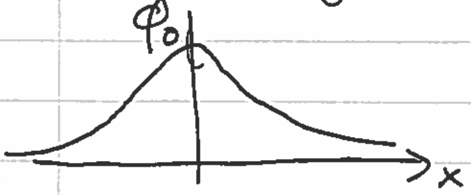
Technological uses :	
photography catalysis biological labelling	} mainly colloidal
photonics optoelectronics	} both.

⋮

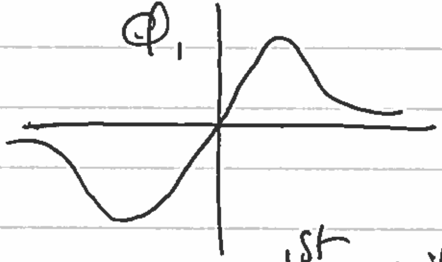
(8) Orthogonality, Basis States and Dirac Notation.

[Review important property that drives to the heart of the wave function, discuss a powerful analogy with mathematics of vectors and introduce a space saving notation].

The lowest eigenfunctions of a particle in a well tend to look like:



ground state

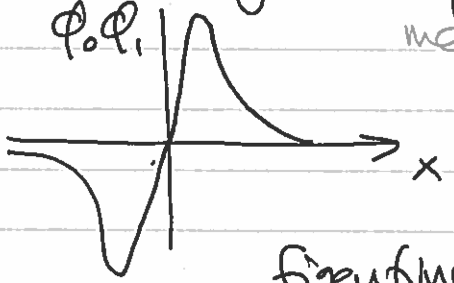


1st excited state

n^{th} excited state has a wave function with n nodes (ie. places where $\varphi = 0$ without being forced to by boundary conditions).

If you multiply two eigenfunctions together, product has positive and negative regions - symmetry around $x=0$ means ~~which~~ when integrating over all space lead to cancellations and a zero result.

eg.



Eigenfunctions are said to be orthogonal.

Along with having real eigenfunctions, this is a general property of Hermitian operators:

eigenfunction

$$\hat{A}\varphi_n = a_n\varphi_n$$

Hermitian operator

real eigenvalue

when $\int \varphi_m^*(\underline{r})\,\varphi_n(\underline{r})\,d^3\underline{r} = 0$ orthogonal

or $a_m = a_n$ degenerate

You proved this in PHMS20101: make sure you still can.
NB// Turns out that for states that are degenerate you can $\overset{\uparrow}{\text{choose to}}$ construct eigenfunctions that are orthogonal.
(see Rae Chpt 4)

Orthogonality is extremely useful; it helps deconstruct functions.
Example: the general sol$^{\underline{n}}$ of TDSE $\Psi(\underline{r},t) = \sum_n c_n e^{\frac{-iE_nt}{\hbar}} \phi_n(\underline{r})$
ie. a linear superposition of separable sol$^{\underline{n}}$s (energy eigenfunctions)

$$\Psi(\underline{r},0) = \sum_n c_n \phi_n(\underline{r})$$

[looks like a Fourier series]

To find a coefficient c_m:
(i) multiply $\Psi(\underline{r},0)$ by ϕ_m^*
(ii) integrate over all space
All terms where $n \neq m$ vanish by orthogonality leaving:

$$\int \phi_m^*(\underline{r}) \Psi(\underline{r},0) d^3\underline{r} = c_m \int |\phi_m(\underline{r})|^2 d^3\underline{r}$$

$$\downarrow$$

called an "overlap" integral.

$= c_m$ if eigenfunctions are normalised.

These coefficients c_n are probability amplitudes with $|c_n|^2$ being the prob. of ~~getting~~ measuring the energy to be the corresponding eigenvalue E_n.
(think about how you could prove this via $\langle \hat{H} \rangle$)
If $\Psi(\underline{r},0)$ is also properly normalised:

$$\int |\Psi(\underline{r},0)|^2 d^3\underline{r} = \sum_n |c_n|^2 = 1$$

ie. probs sum to unity.

since terms like $c_1^* c_2 \int \phi_1^*(\underline{r}) \phi_2(\underline{r}) d^3 r$ vanish by orthogonality

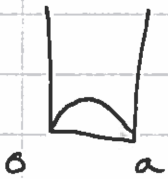
For the special case when $\Psi = \phi_n$ we know that the energy must be E_n.

$$c_m = \int \varphi_m^* \Psi \, d^3\underline{r} = \int \varphi_m^* \varphi_n \, d^3\underline{r} = 0$$

i.e. prob of measuring a different energy is zero.

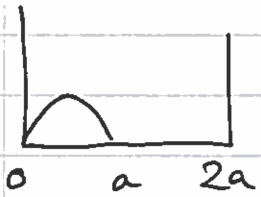
So Eigenfunctions must be orthogonal otherwise these probs would not make any sense!

Example: particle in infinite sq well is in the groundstate



$$\varphi(x) = \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a}$$

Suddenly the right wall moves to 2a. (the SUDDEN approximation)



$\varphi(x)$ is no longer an eigenfunction. What is probability of measuring the particle to have an energy corresponding to the 1st excited state of the new system.

Eigenfunction of new system

$$\varphi_n = \sqrt{\frac{2}{2a}} \sin\frac{n\pi x}{2a} \quad n = 1, 2 \ldots \text{ etc.}$$

$$\varphi_2 = \sqrt{\frac{1}{a}} \sin\frac{\pi x}{a}$$

$$c_2 = \int \varphi_2^* \phi_1 \, dx = \frac{\sqrt{2}}{a} \int_0^a \sin\frac{\pi x}{a} . \sin\frac{\pi x}{a} \, dx$$

NB $\phi_1 = 0$ for $x > a$

$$= \frac{\sqrt{2}}{a} \frac{1}{2} a = \frac{1}{\sqrt{2}}$$

Prob of measuring E_2 $= |c_2|^2 = \frac{1}{2}$

Hermitian operators have a further property called completeness. any well behaved function can be expanded in terms of their eigenfunctions, you can

proof is "nasty and laborious, I'm afraid most physicists simply assume completen and hope for the best.

Expand a wavefunction:

$$\Psi(\underline{r}) = \sum_n c_n \phi_n(\underline{r})$$

can use any set of eigenfunctions, not just those of $\hat{H}$. This ~~[illegible]~~ set of eigenfunctions is known as the basis set.

cf $\underline{b} = b_x \hat{i} + b_y \hat{j} + b_z \hat{k}$

basis set ⟷ unit vectors (many coord systems - choices for unit vectors, similarly many bases) so choose carefully!

c_n ⟷ ~~[illegible]~~
prob amps ⟷ components

If a particle is described by $\Psi(\underline{r})$, what's the prob of finding it in state $\chi(\underline{r}) = \sum d_n \phi_n(\underline{r})$?
Given by the square of the overlap:

$$\int \chi^*(\underline{r}) \Psi(\underline{r}) d^3\underline{r} = \sum_n d_n^* c_n$$

cross terms vanish by orthogonality!

Looks like scalar product: $\underline{d}.\underline{b} = d_x b_x + d_y b_y + d_z b_z$.

Dirac notation:
denote a state by $|\psi>$ a bit like writing $\underline{b}$ for a vector.
instead of list of components

The overlap is then written as -

$$\underbrace{<\chi|}_{\text{bra}}\underbrace{\psi>}_{\text{ket}} = \int \chi^* \psi \, d^3 r$$

simple notation: avoids writing out integrals -
powerful: use for states that can't be described by mathematical functions (e.g. intrinsic spin!)

[Practise using this next time]