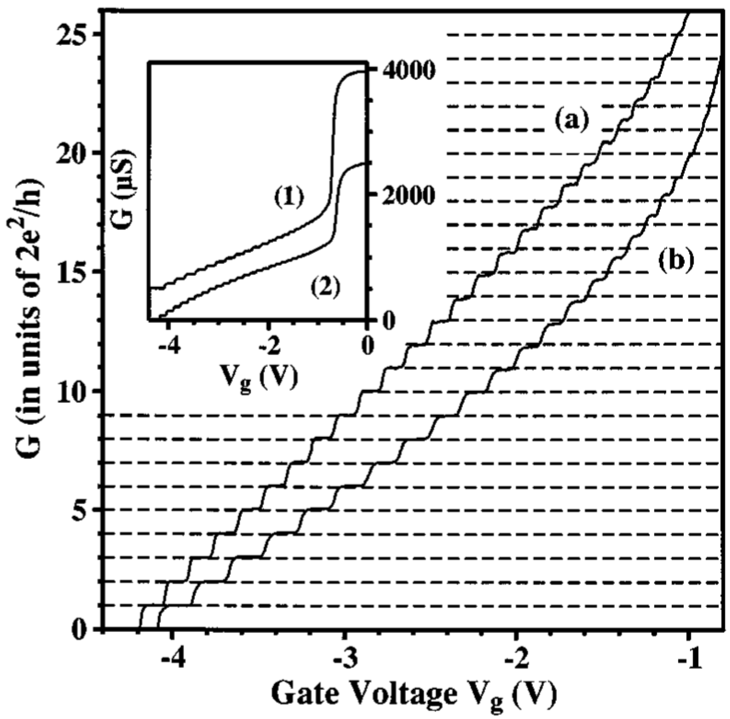
Advanced Quantum Physics

Lecture 2



David Ritchie

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Section 1 - Review of Quantum Physics

Infinite one-dimensional square well

- 1D time independent Schrodinger eqn.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2}+V(x)\psi_n=E_n\psi_n$$

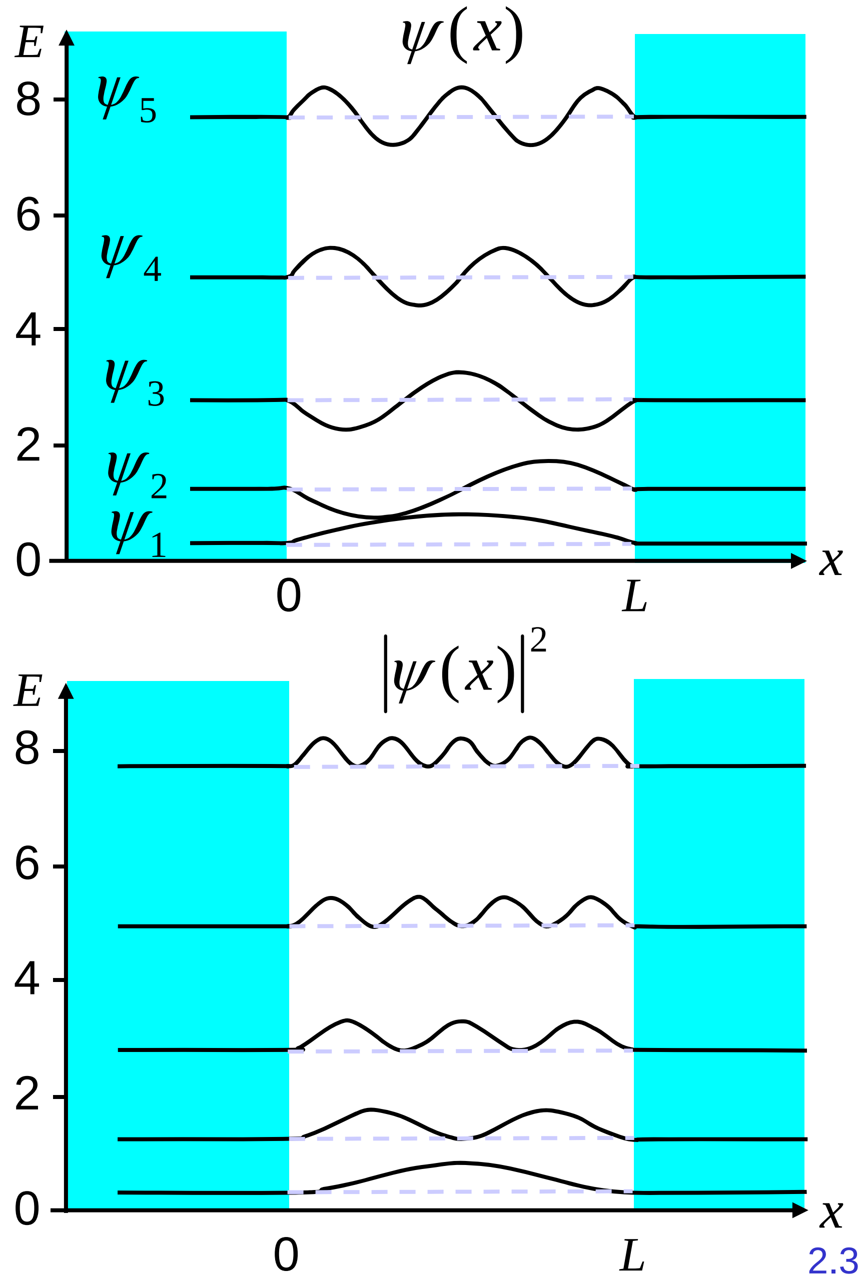
- Wavefunctions are of a form:

$$\psi_n=A\sin\left(\frac{n\pi x}{L}\right),\ E_n=\frac{\hbar^2}{2m}\cdot\frac{n^2\pi^2}{L^2}$$

- n=1,2,3… no. of maxima in $|\psi(x)|^2$
- A found by normalization $\int\psi^*\psi\,dx=1$.

Features:

- Quantized energy levels.
- Zero point energy.
- Symmetric or antisymmmetric ψ .
- If well is finite ψ penetrates barrier.



One-dimensional harmonic oscillator (1)

- Potential: $V\left(x\right)=\frac{1}{2}m\omega^2x^2$
- Energy levels:

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

$$n=0,1,2\ldots$$

- Wavefunctions: Gaussian x Hermite polynomial (H_n)

$$\psi_0=A_0e^{-q^2/2}$$

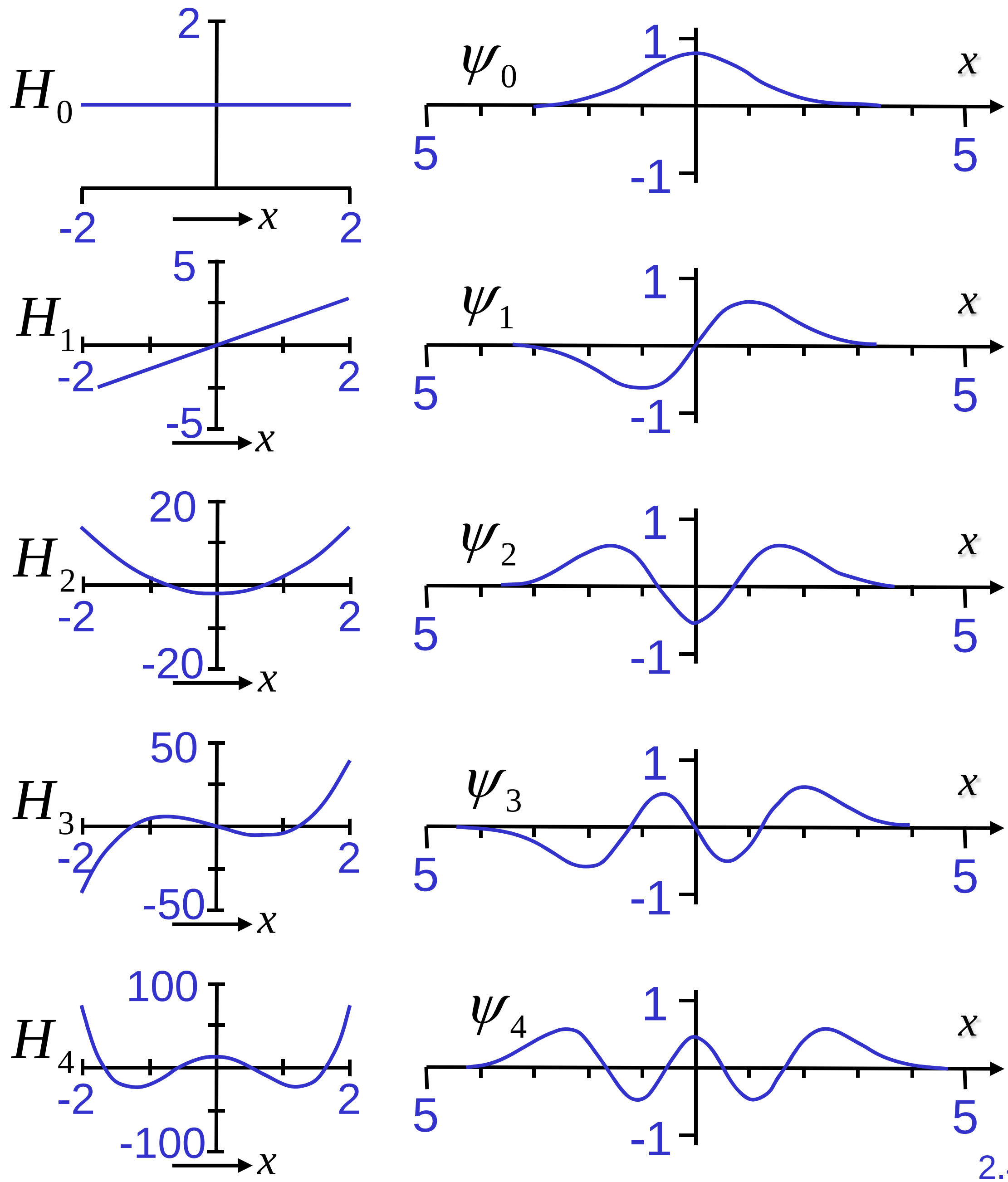
$$\psi_1=A_1qe^{-q^2/2}$$

$$\psi_2=A_2(2q^2-1)e^{-q^2/2}$$

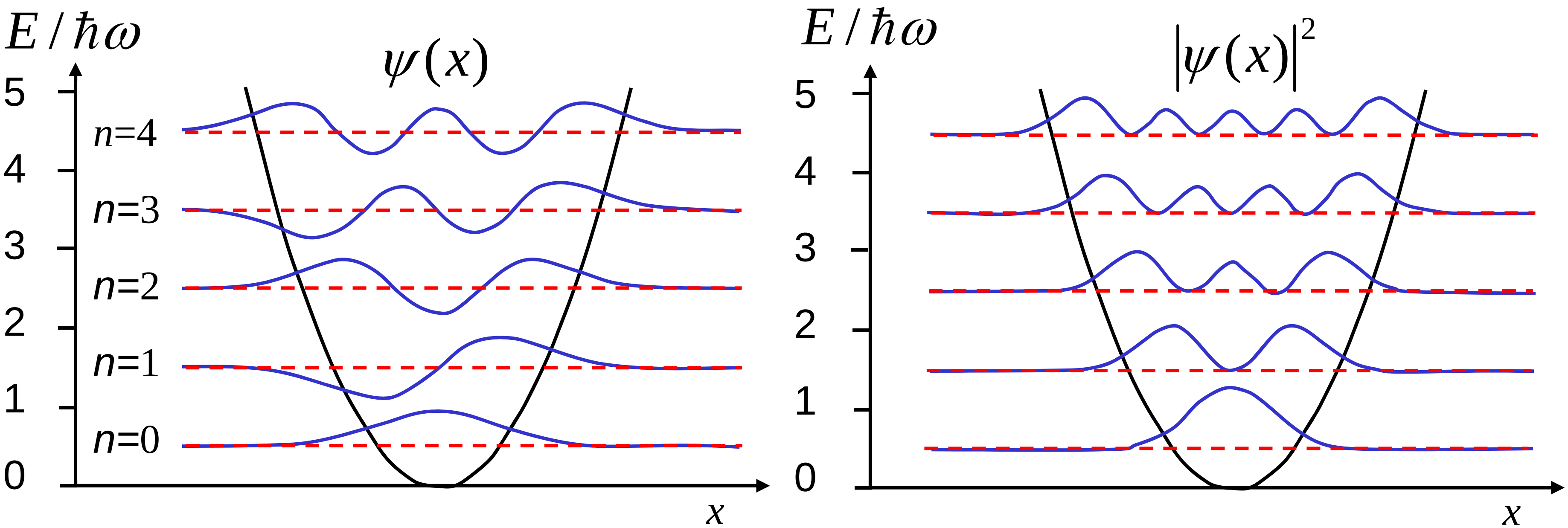
$$\psi_3=A_3(2q^3-3q)e^{-q^2/2}\ldots$$

where $\quad q^2=x^2m\omega/\hbar$

See section 5.3 QP Course



One-dimensional harmonic oscillator (2)

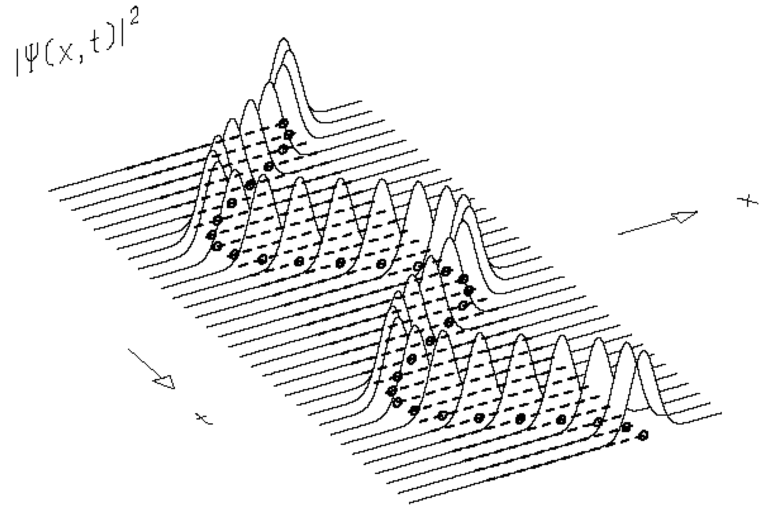


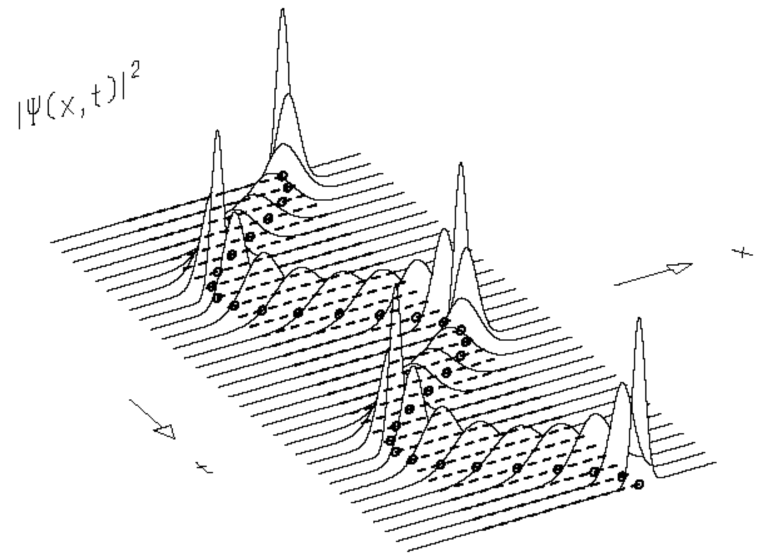
- Equally spaced energy levels $E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2 \ldots$
where n equals no. of zero crossing points in $\psi(x)$.
- Zero point energy $\frac{1}{2}\hbar\omega$ - uncertainty relation.
- Alternating symmetric/antisymmetric wavefunctions.
- Penetration of wavefunction into barrier.
- A good approximation to many physical systems.

Time development of wave-packet in Harmonic Oscillator

- The harmonic oscillator can be in a state which is a sum of many wavefunctions.
- Combination of stationary states can produce a moving wave-packet.
- Here we show probability density vs distance and time for 1D SHO.
- If the initial wave-packet width is the same as the width of the ground state then it remains fixed over time corresponding to a minimum uncertainty ‘coherent’ state.
- If the initial width of wave-packet is different from that of the ground state the width will vary with time.

See section 7.4 QP course





‘The picture book of quantum mechanics’, Brant and Dahmen

3D Harmonic Oscillator – Cartesian coordinates (1)

- 3D Hamiltonian; $$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \tfrac{1}{2}mr^2\omega^2 = \hat{H}_x + \hat{H}_y + \hat{H}_z$$

where $\hat{H}_x = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \tfrac{1}{2}mx^2\omega^2$ etc.

- Substitute $\psi^c_{n_x,n_y,n_z} = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$ into 3D Schrodinger eqn.:

$$\left(\hat{H}_x + \hat{H}_y + \hat{H}_z\right)\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z) = E\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$$

- Separate equation into three 1D Schrodinger equations;

$\hat{H}_x\psi_{n_x}(x) = E_x\psi_{n_x}(x)$ etc. with $E = E_x + E_y + E_z$.

- So $E_x = (n_x + \tfrac{1}{2})\hbar\omega$ etc. and hence $E_{n_x,n_y,n_z} = (n_x + n_y + n_z + \tfrac{3}{2})\hbar\omega$.
- $\psi_{n_x}(x)$ etc are the 1D Harmonic Oscillator wavefunctions – A Gaussian x Hermite polynomial.
- Energy levels often degenerate – different combinations of n_x, n_y, n_z giving same total energy e.g. $E_{210}=E_{102}=E_{021}$.

3D Harmonic Oscillator – Cartesian coordinates (2)

- Figure shows a wavefunction ψ^c_{210} as a function of (x,y) at $z=0,1,2$
- From discussion of 1D harmonic oscillator:

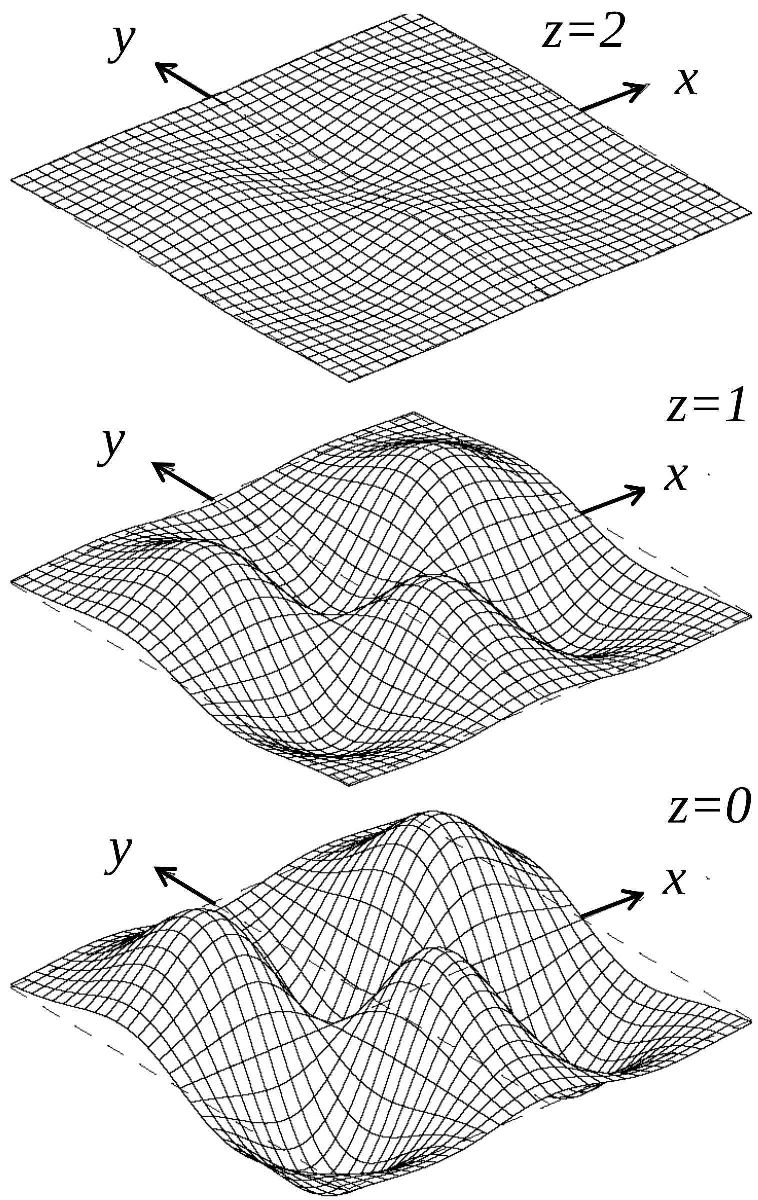
$$\psi^c_{210} = \psi_2(x)\psi_1(y)\psi_0(z)$$

$$= A\left[(\tfrac{2m\omega}{\hbar} x^2 - 1) e^{-x^2 m\omega/2\hbar} \right]$$

$$\times \left[y\sqrt{\tfrac{m\omega}{\hbar}} e^{-y^2 m\omega/2\hbar} \right] \left[e^{-z^2 m\omega/2\hbar} \right]$$

- Note steady reduction in amplitude as z increases (no zero-crossings).
- One zero-crossing in y-direction.
- Two zero-crossings in x-direction.

See section 8.5 QP course



'The picture book of quantum mechanics', Brant and Dahmen

3D Spherically Symmetric Potential

- Use spherical polars $\left(r,\theta,\phi\right)$ with a 3D symmetrical potential $V\left(r\right)$

$$\hat{H}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = -\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\hat{L}^2}{2mr^2}\psi + V(r)\psi$$

where $$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

- Since $\hat{H}$ commutes with $\hat{L}^2$ the solution is of the form:

$$\psi^p(r) = \frac{u(r)}{r}Y_{\ell m}(\theta,\phi)$$

$$\hat{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi)$$

$$\hat{L}_z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

radial part satisfies $$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + \left[\frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]u(r) = Eu(r)$$

- 1D Schrodinger equation for $u\left(r\right)$ with extra term $\dfrac{l\left(l+1\right)\hbar^2}{2mr^2}$

3D Harmonic Oscillator - polar coordinates (1)

- From previous slide, introducing the harmonic oscillator potential:

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2}+\left[\frac{l(l+1)\hbar^2}{2mr^2}+\tfrac{1}{2}mr^2\omega^2\right]u(r)=Eu(r)$$

- This has solutions: $\psi^p_{n_r lm}(r,\theta,\phi)=\dfrac{u(r)}{r}Y_{lm}(\theta,\phi)=R_{nl}(r)Y_{lm}(\theta,\phi)$

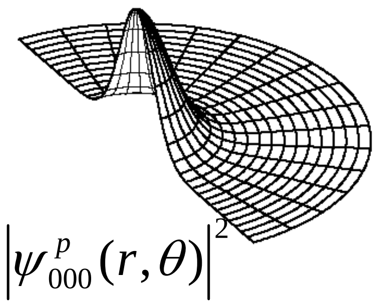
where $n_r=\left(n-l\right)/2$

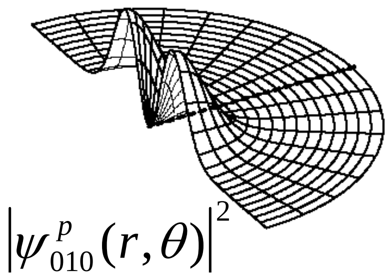
- In the case of $l=0$, for finite $\psi^p(0)$ then $u(0)=0$, so $u(r)$ must be one of the solutions with odd n_{1D} for the 1D simple harmonic oscillator
- The ground state energy for $l=0, n_{1D}=1$ is given by $E=\tfrac{3}{2}\hbar\omega$ - the same result as for the 3D Cartesian analysis.
- The ground state wavefunction is given by;

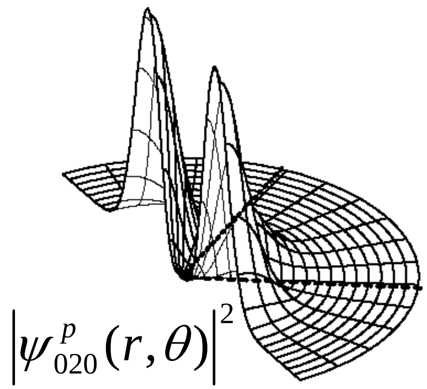
$$\psi^p_{000}(r)=Ae^{-r^2m\omega/2\hbar}=Ae^{-x^2m\omega/2\hbar}e^{-y^2m\omega/2\hbar}e^{-z^2m\omega/2\hbar}$$

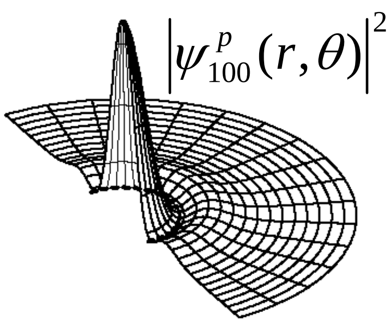
which is the same as that for 3D Cartesian coordinates.

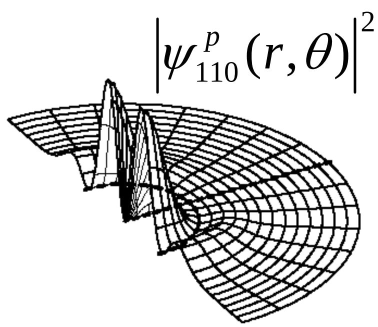
3D Harmonic Oscillator - polar coordinates (2)

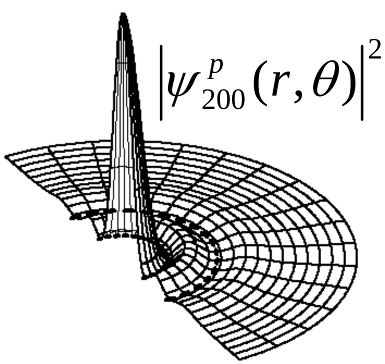


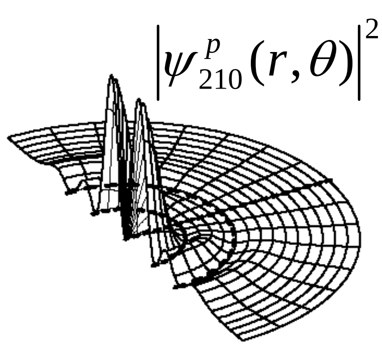












- For excited states the radial function $R_{nl}(r)$ may be calculated in terms of Laguerre polynomials.

- The squares of the wavefunctions

$$\psi^p_{n_r lm}(r,\theta,\phi) = R_{nl}(r)Y_{\ell m}(\theta,\phi)$$

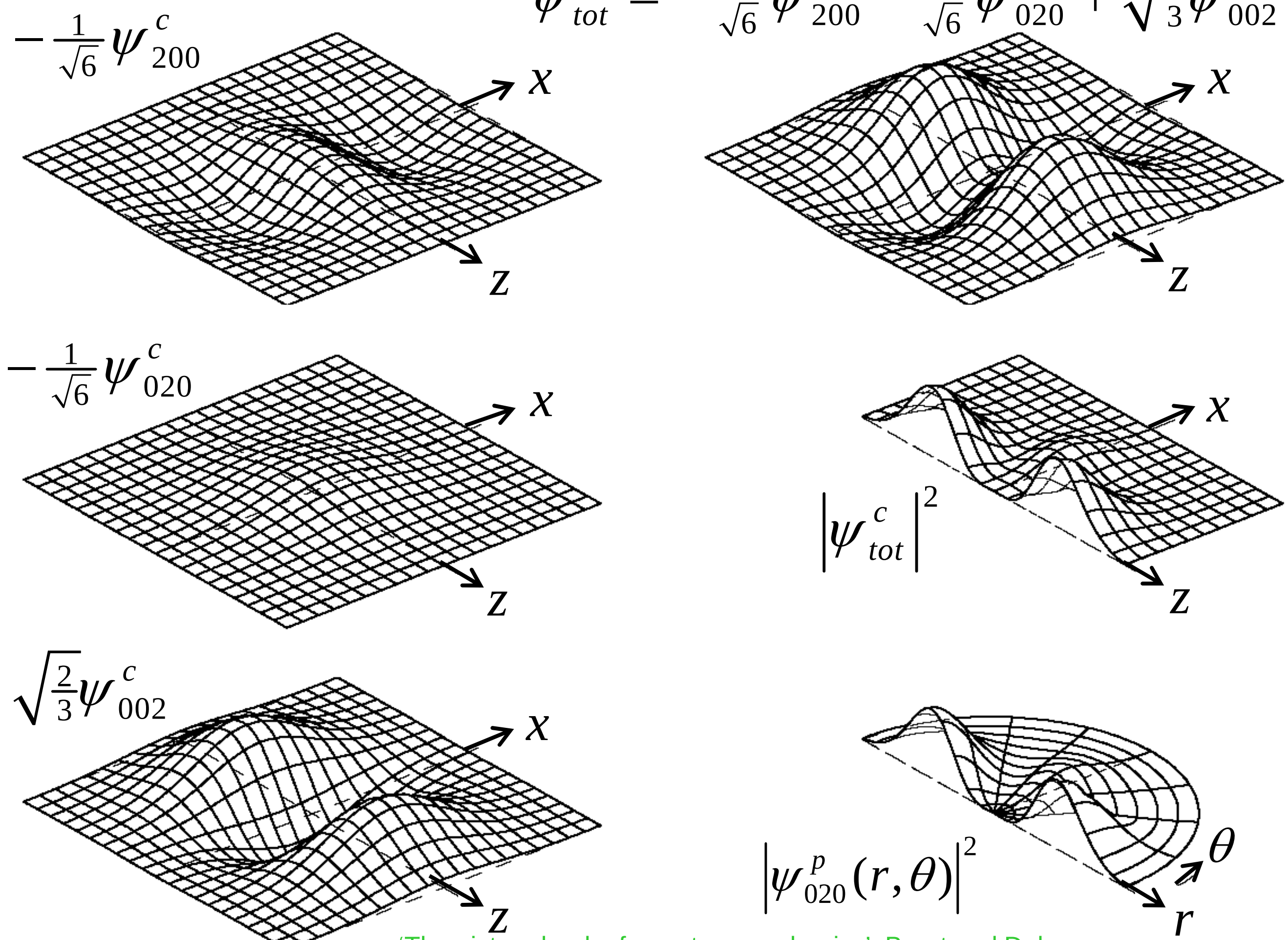
which are independent of ϕ are plotted to the left as a function of r and θ.

- There are n_r radial nodes and $l-|m|$ polar nodes.

3D Harmonic Oscillator Cartesian - Polar

•Add several degenerate eigenstates $(\psi^c_{200}, \psi^c_{020}, \psi^c_{002})$ from the Cartesian system to get the $\psi^p_{n_r lm} = \psi^p_{020}(r,\theta)$ eigenstate in the polar system (as it should...).

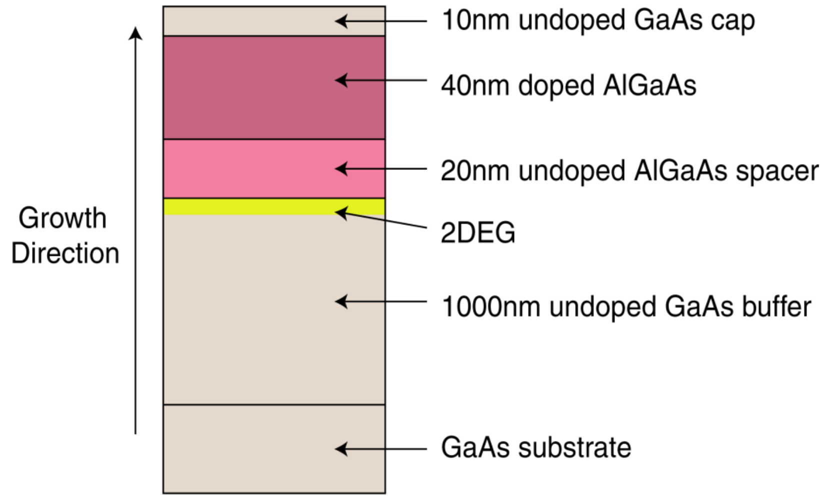
$$\psi^c_{tot} = -\tfrac{1}{\sqrt{6}}\psi^c_{200} - \tfrac{1}{\sqrt{6}}\psi^c_{020} + \sqrt{\tfrac{2}{3}}\psi^c_{002}$$

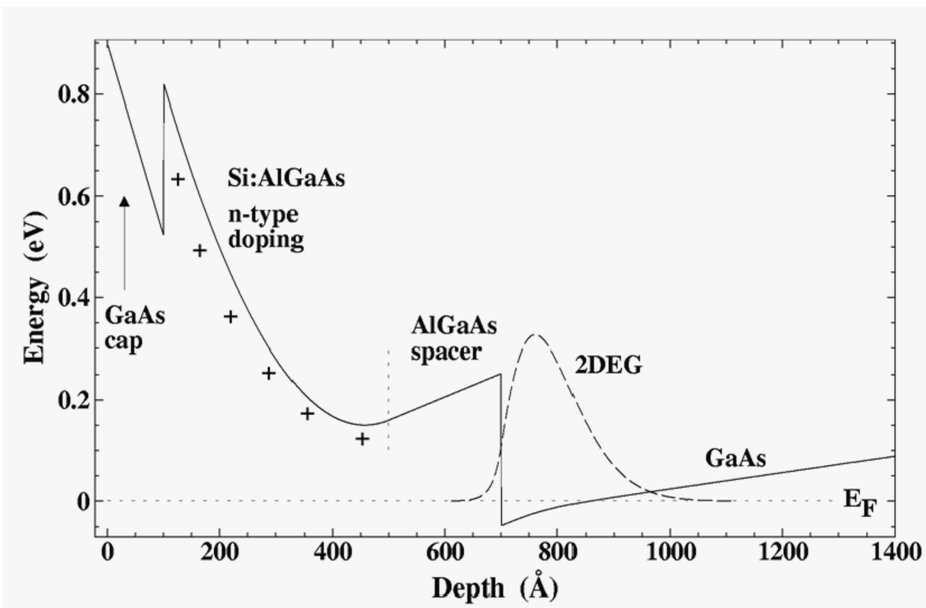


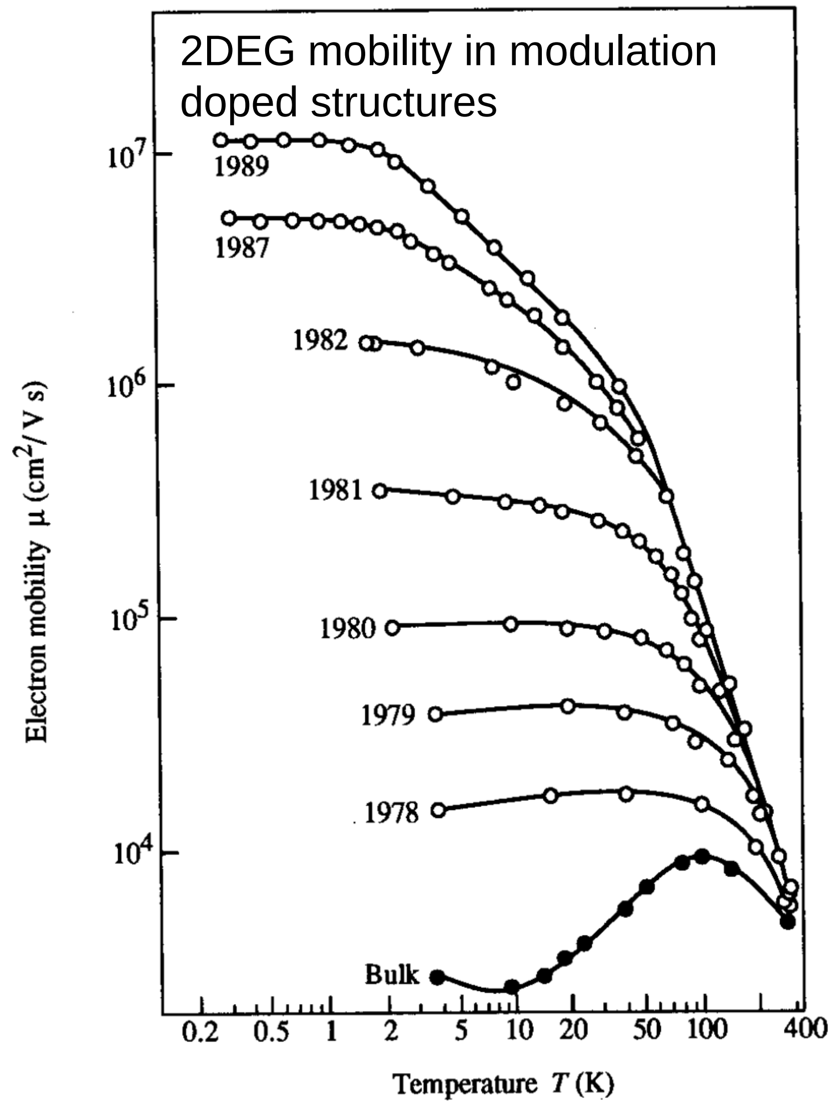
'The picture book of quantum mechanics', Brant and Dahmen

Two-dimensional electron gas (2DEG)

Dingle et al APL **33**, 665 (1978), Stormer et al SSC **29**, 705 (1979)







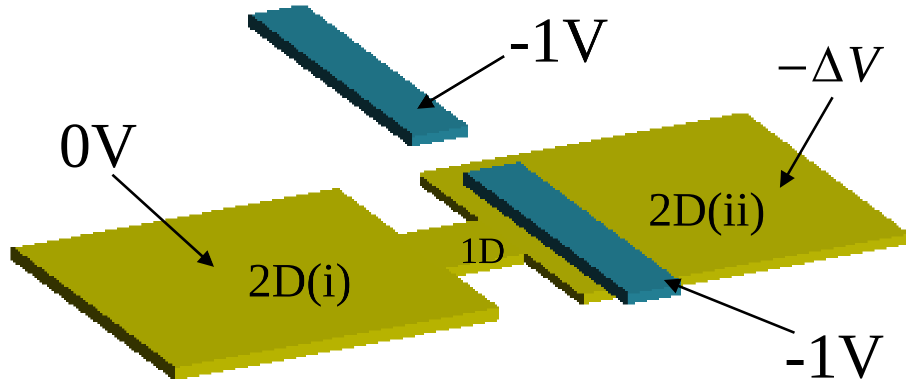
Pfeiffer et al APL **55**,1888 (1989)

Example – energy levels in 1D wire

•1D potential well defined in 2D gas by surface ‘gate’ fingers with negative (-1V) voltage w.r.t electron gas.

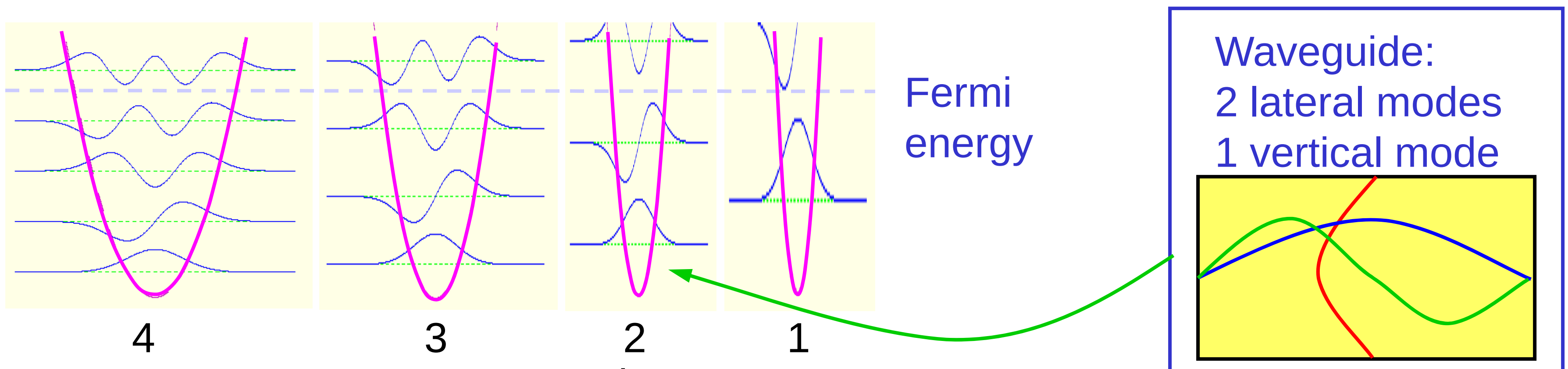
• $\Delta V \approx -100\mu V$ electrons travel from 2D(ii) to 1D to 2D(i) region.

•In 1D region electrons travel in different energy levels in parabolic potential well – no scattering occurs between levels at low temperatures (<1.5K).



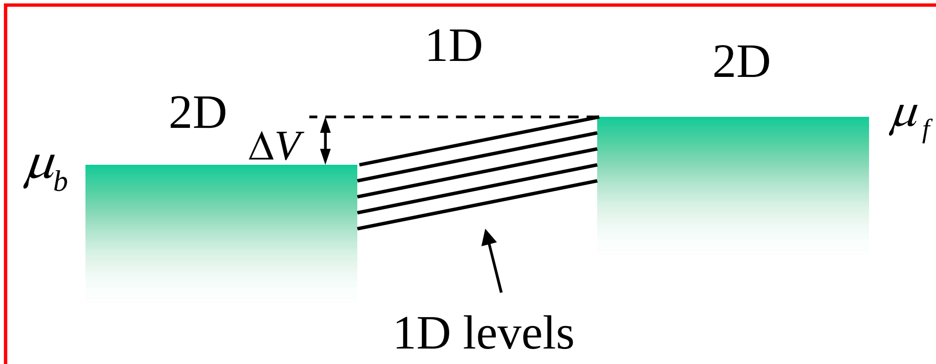
•Making gate voltage more negative decreases well width and increases level spacing – depopulating energy levels one by one.

Number of occupied subbands



V_g more negative→

Example – energy levels in 1D wire



- Each 1D level acts as a waveguide
- If a voltage of $\Delta V \approx 100\mu V$ is applied then a current starts to flow in each 1D channel.
- We assume $T \sim 0K$.

Spin degeneracy

$$I = \int_{\mu_b}^{\mu_f} e v_g \frac{dn}{dE} dE = \int_{\mu_b}^{\mu_f} e\left(\frac{1}{\hbar}\frac{dE}{dk}\right)\left(\frac{2}{2\pi}\frac{dk}{dE}\right) dE = \frac{2e}{2\pi\hbar}\left(\mu_f - \mu_b\right) = \frac{2e^2}{h}\Delta V$$

Factor of 2 for current direction

So for υ filled levels conductance:

$$g = \frac{I}{\Delta V} = \upsilon \frac{2e^2}{h}$$

Length in k-space

Density of states

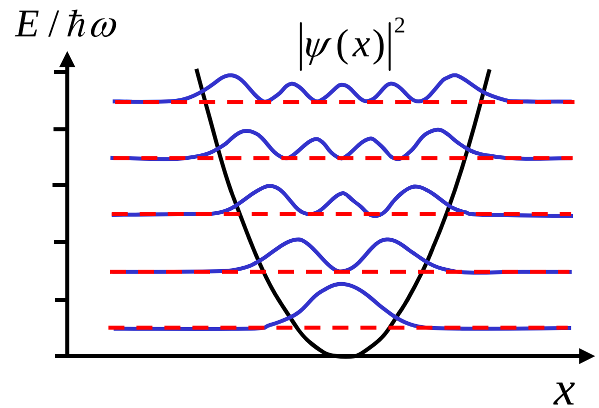
$$N = \frac{2k}{(2\pi / L)} = \frac{kL}{\pi} \Rightarrow n = \frac{k}{\pi} \Rightarrow \frac{dn}{dE} = \frac{1}{\pi}\frac{dk}{dE}$$

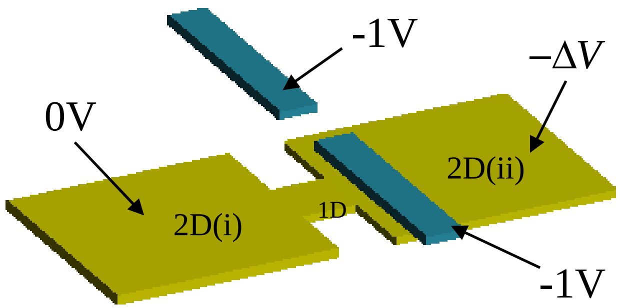
Spacing of states

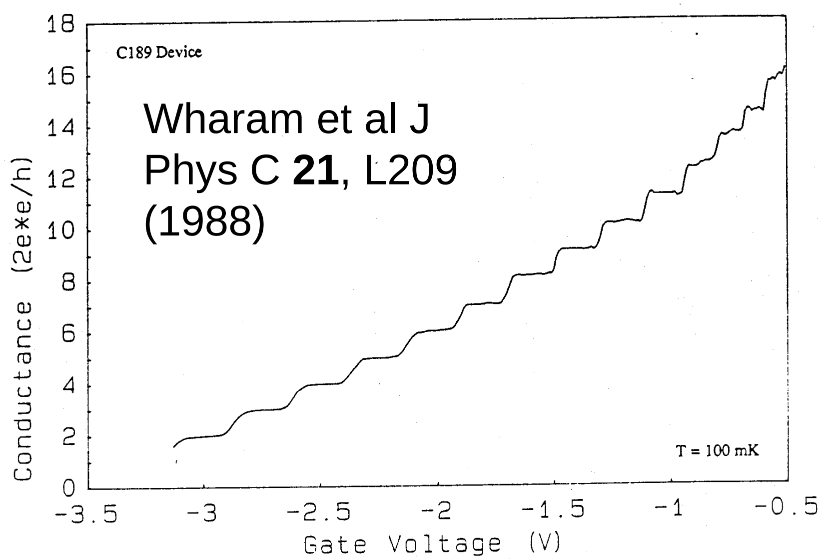
- Result only dependant on fundamental constants - effects of velocity and DoS cancel.

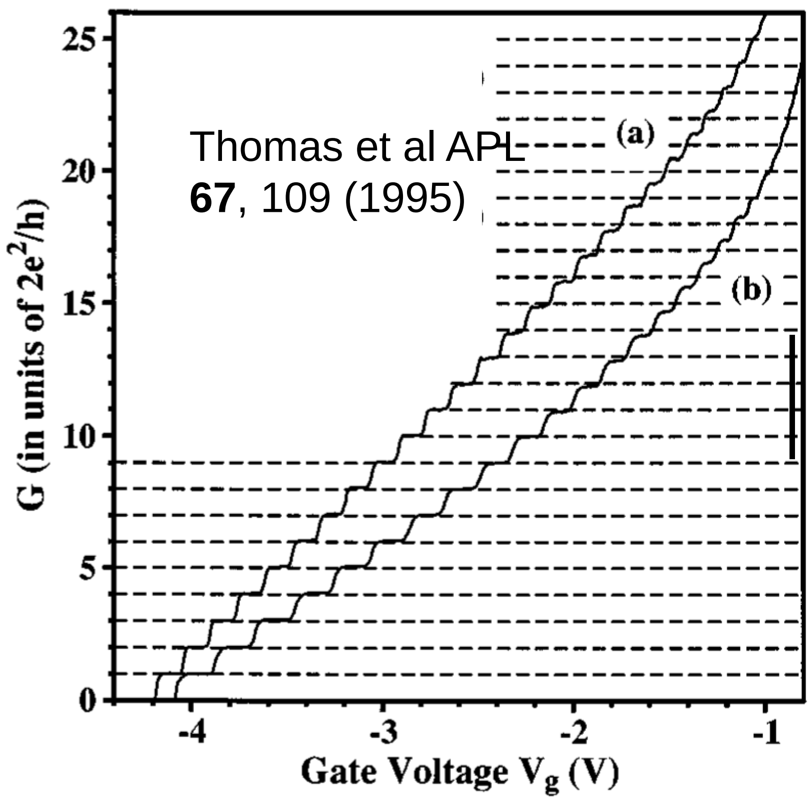
Quantized Conductance in 1D

- Making gate voltage more negative decreases well width and increases level spacing – depopulating energy levels one by one.









Lecture 2 - Summary

Solutions to Schrodinger's equation:

•One-dimensional square well.

•One-dimensional harmonic oscillator.

•Time development of wave-packet.

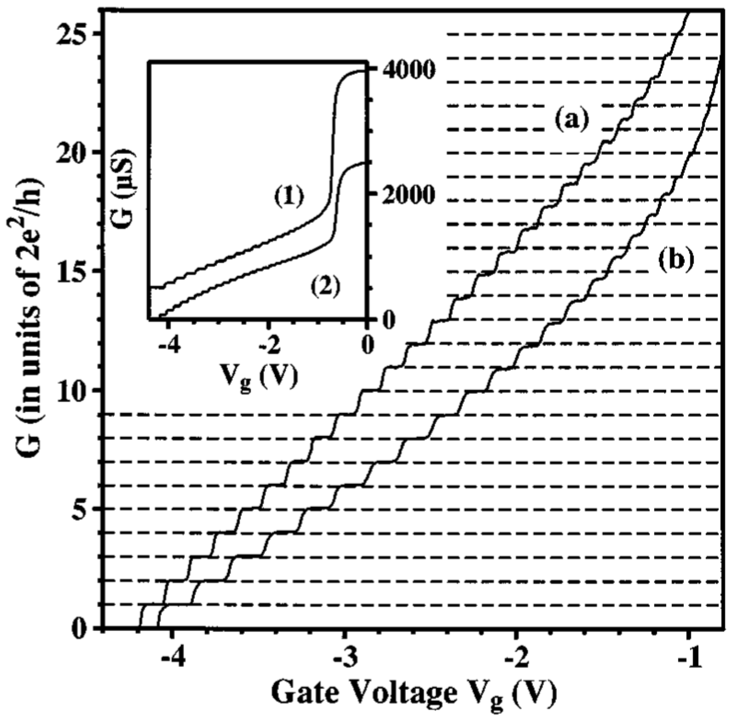
•3D harmonic oscillator in Cartesian and polar coordinates.

•Two-dimensional electron gas in a semiconductor.

•Energy levels in a one-dimensional wire.

•Quantised conductance through a one-dimensional wire.

Lecture 2



The End!!

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