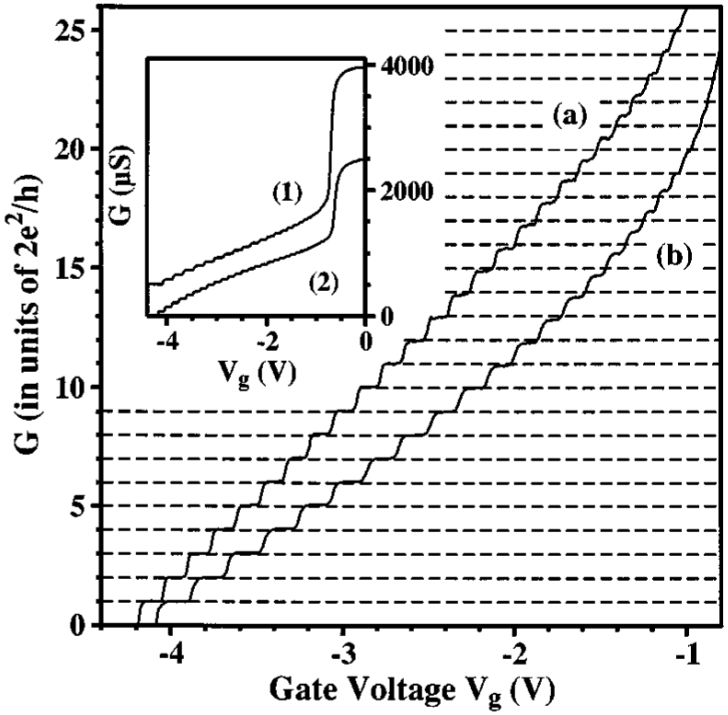
Quantum Condensed Matter Physics

Lecture 17



David Ritchie

Quantum Condensed Matter Physics

1. Classical and Semi-classical models for electrons in solids (3L)
2. Electrons and phonons in periodic solids (6L)
3. Experimental probes of band structure (4L)
4. Semiconductors and semiconductor devices (5L)

….Photovoltaic solar cell; Shockley-Queisser limit, efficiencies, commercialisation. Field effect transistor; JFET, MOSFET. Microelectronics and the integrated circuit.

Band structure engineering; electron beam lithography, molecular beam epitaxy. Two-dimensional electron gas, Shubnikov-de Haas oscillations, quantum Hall effect, conductance quantisation in 1D. Single electron pumping and current quantisation, single and entangled-photon emission, quantum cascade laser.

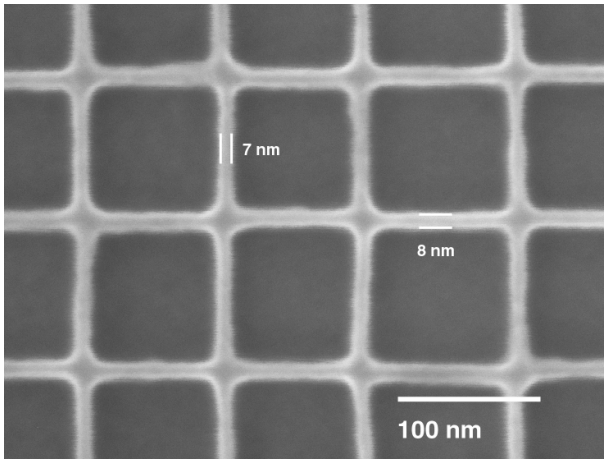
5. Electronic instabilities (2L)
6. Fermi Liquids (2L)

Band structure engineering

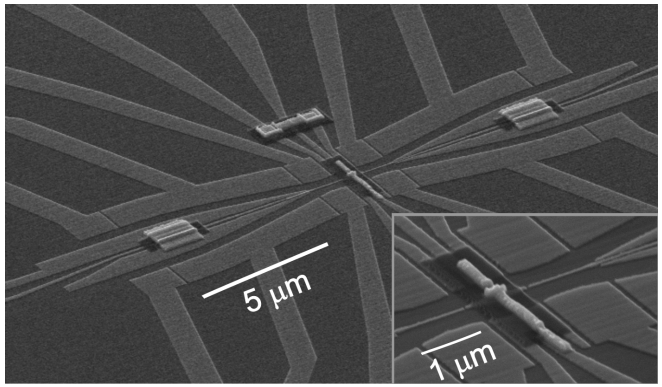
- The spatial control of band structure using different materials, can result in the confinement of electrons and/or holes to 2D,1D or 0D
- Relies on the development of advanced crystal growth techniques such as molecular beam epitaxy (MBE) and metal organic chemical vapour deposition (MOCVD) to grow near perfect crystals on single crystal substrates at growth rates around 1 monolayer/s
- Epitaxial *heterostructures* of different materials can be grown with near monolayer control over semiconductor composition and doping
- Heated substrate creates large lateral motion of atoms before incorporation into the growing crystal and leads to very smooth layers
- Ultra-high purity materials can be grown with impurity levels as low as 1 part in 10^{10} leading to electron transport mean free paths as high as 0.1mm
- Both growth techniques used for routine production of lasers for CD, DVD players (mainly MOCVD) and high frequency transistors (mainly MBE)
- Electron beam lithography is used to produce laterally patterned structures on 100nm scale
- A very wide range of semiconductors can be used to produce many device structures – several examples to follow

Electron beam lithography

- Technique used to form very high resolution patterns (down to a few nm) in thin layer of polymer resist
- Patterns are transferred to sample by etching or deposition of metals or insulators followed by lift-off
- Widely used technique with many applications in research as well as the real world.



A micrograph of a grid formed in ZnO demonstrating a sub-10nm resolution

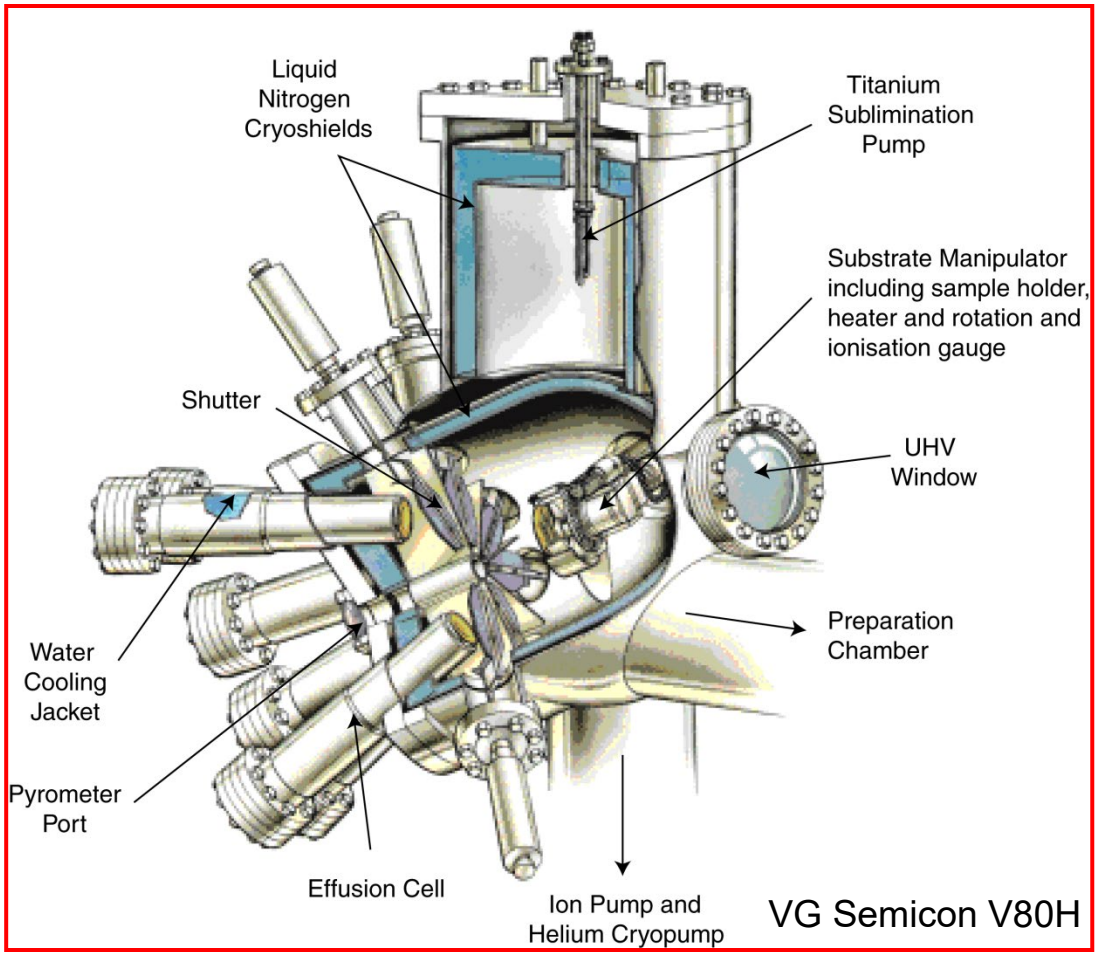


A SAW driven electron interferometer

Images from GAC Jones and J Griffiths

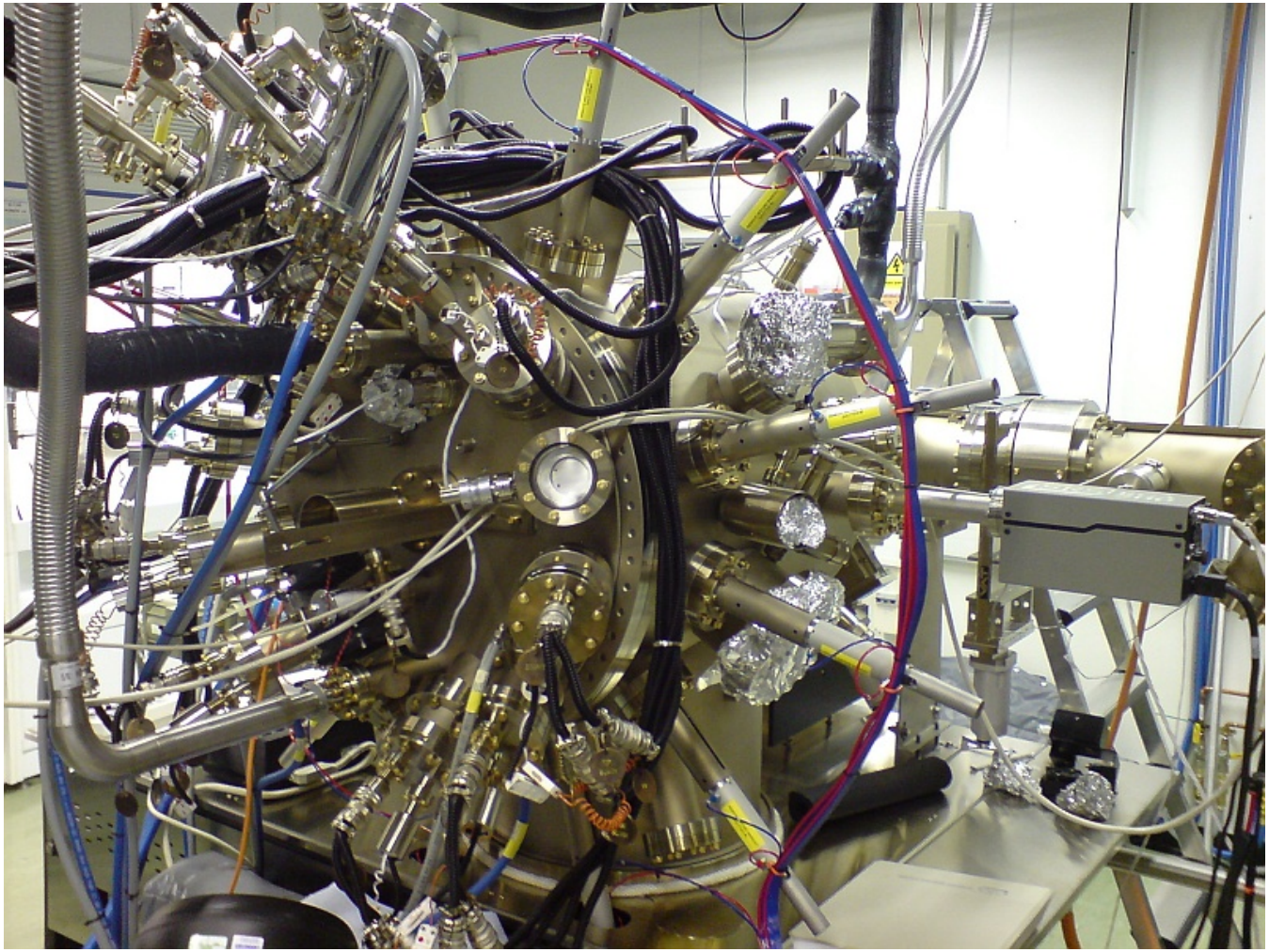
Molecular beam epitaxy (MBE) Growth Chamber

- MBE system capable of sub-monolayer precision growth of ultra-high purity III-V semiconductors
- System comprises ultra-high vacuum growth, preparation and loadlock chambers made from stainless steel and using copper gasket seals
- Ion, turbo and cryo-pumps
- LN_2 cryoshield (400L/day)
- System baked at 200^{o}C to remove impurities
- Ga, Al, As, In, Si, C sources
- Shutters control desposition



- Ultra-high vacuum: 10^{-11} mbar total – mostly hydrogen
- Pressure of impurities:10^{-15} mbar – around 1 part in 10^{10} in crystal
- Growth of thick layers to bury contamination – up to 6 months to reach highest purity.

VEECO GEN III MBE growth chamber

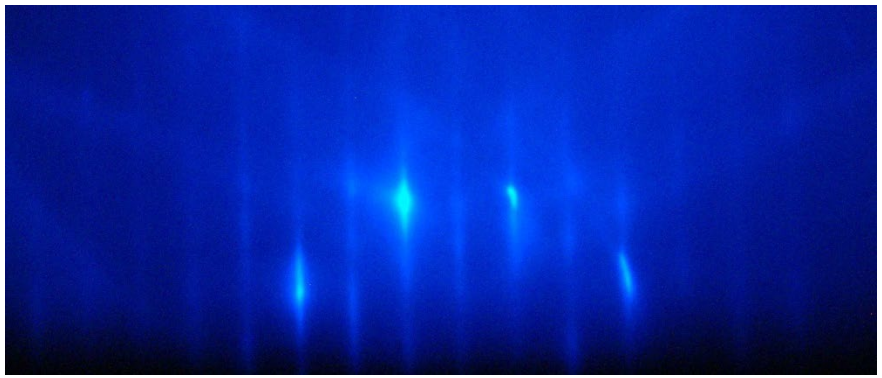


- MBE growth system used in Semiconductor Physics research group for production of ultra-high purity low-dimensional structures including, high mobility 2D electron and hole gases as well as self-assembled quantum dots

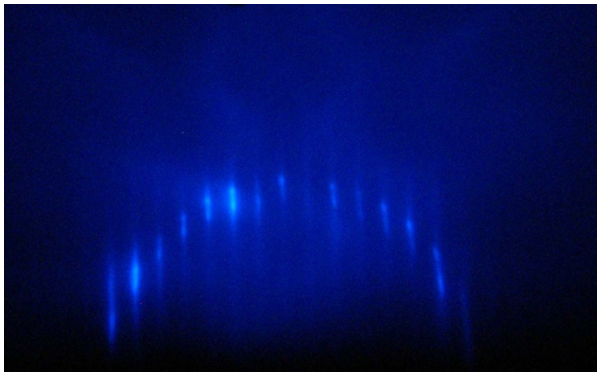
Reflection high energy electron diffraction (RHEED)

- RHEED technique used to measure surface structure of growing crystal

[ll0] Azimuth (2x)



[$\bar{1}$l0] Azimuth (x4)



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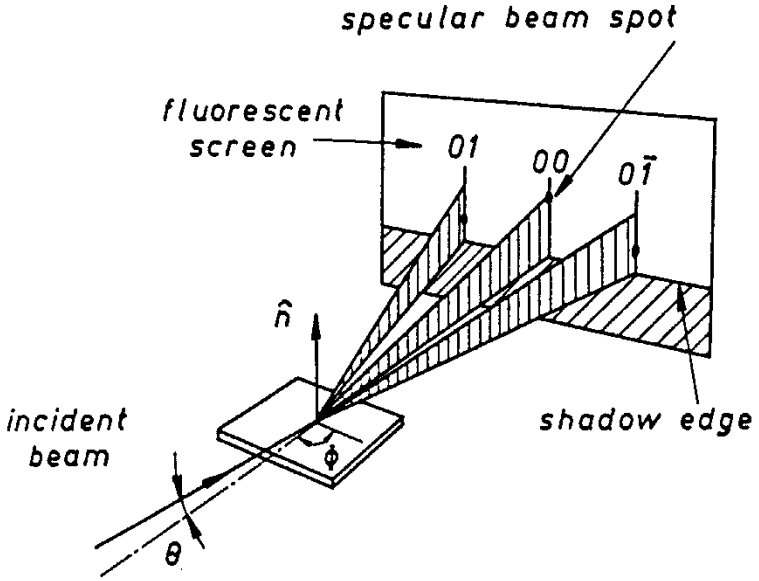
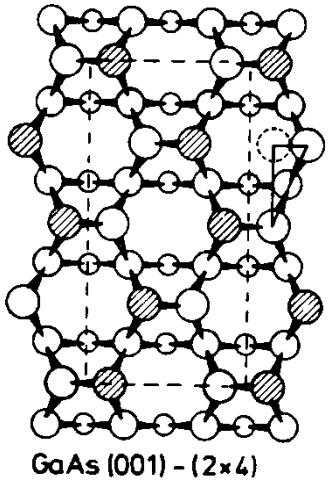
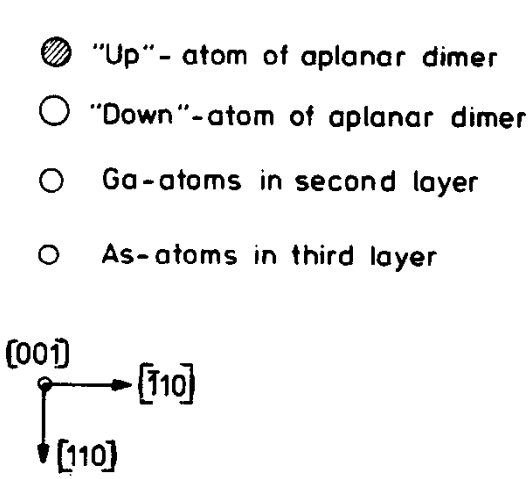
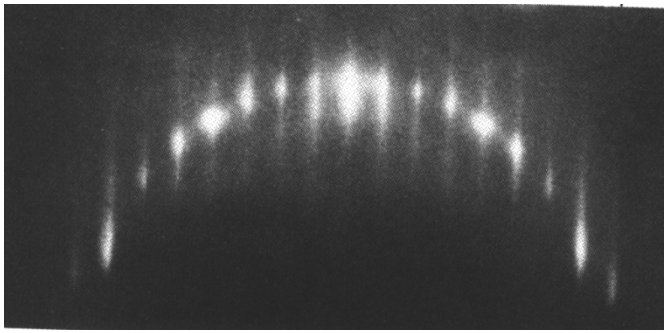




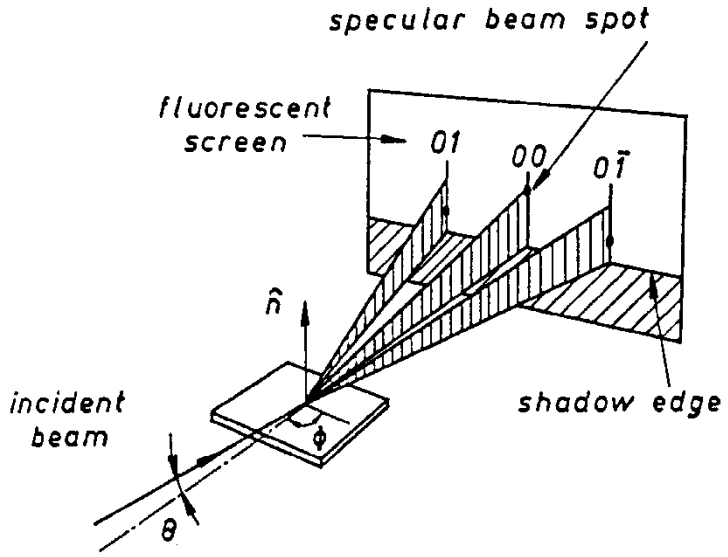


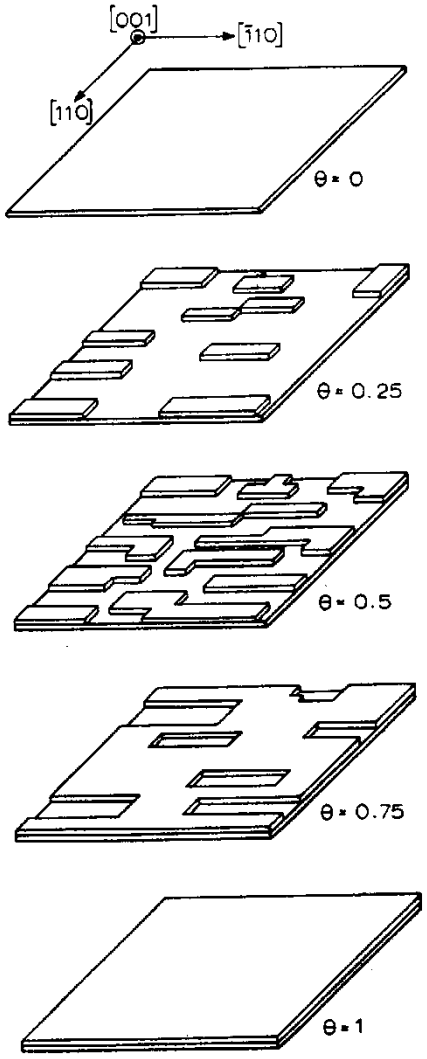
RHEED Oscillations

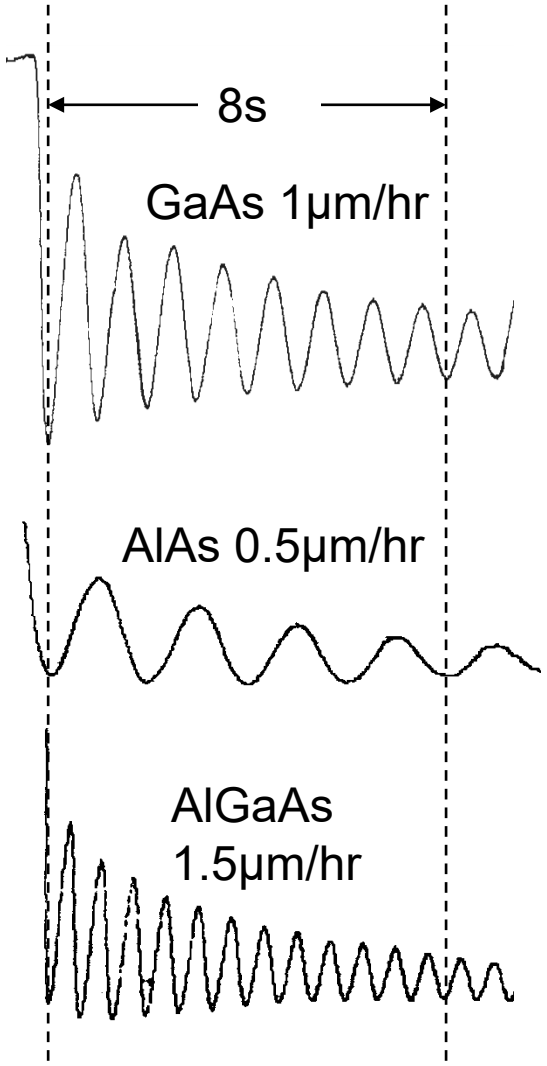
- Observation of semiconductor growth monolayer by monolayer using measurement of intensity of specularly reflected electrons



2x4 pattern $(\bar{1}10)$ direction

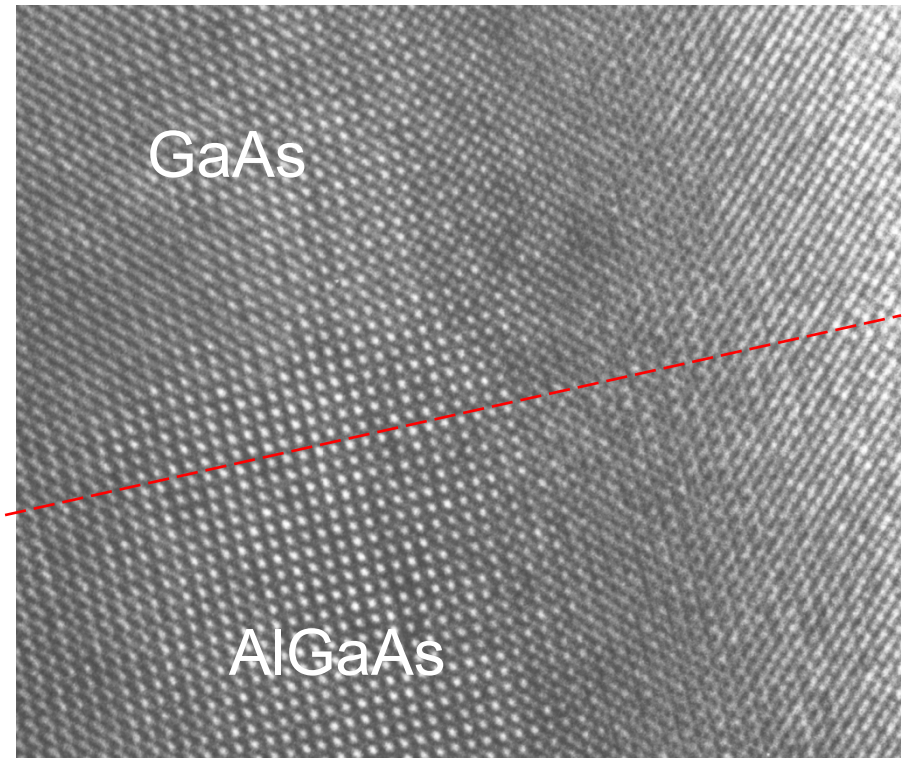




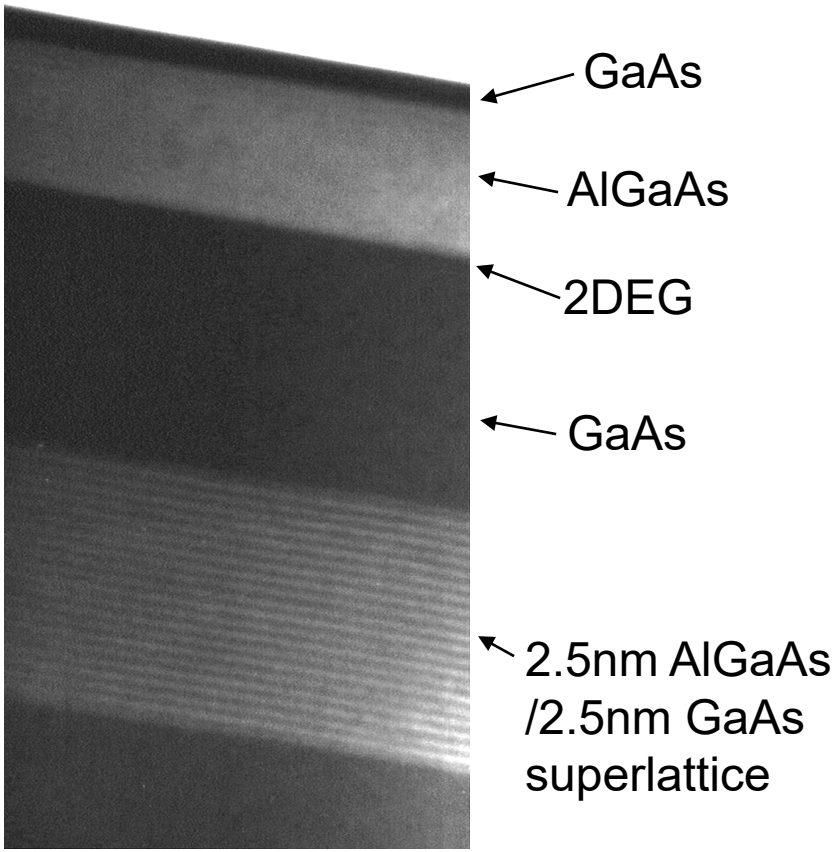


Transmission electron microscopy (TEM) of GaAs/AlGaAs Epilayers

- Provides very high resolution images of epitaxially grown structures



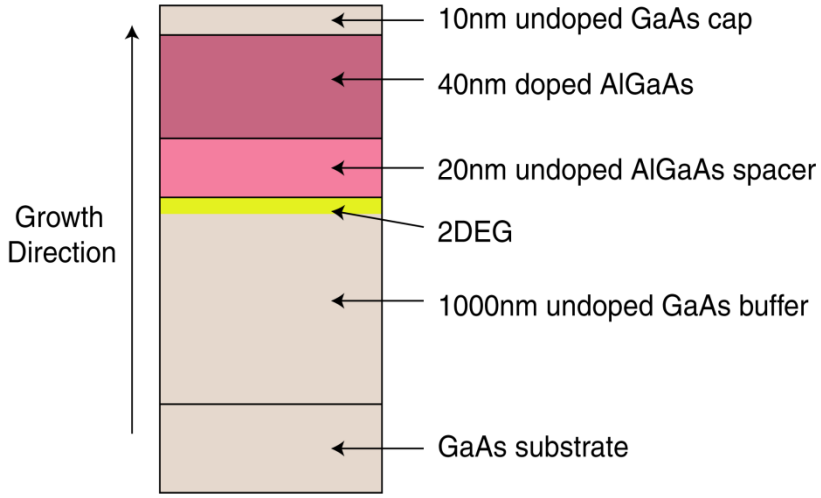
High Resolution TEM GaAs/AlGaAs interface (T Walther, Materials Science)

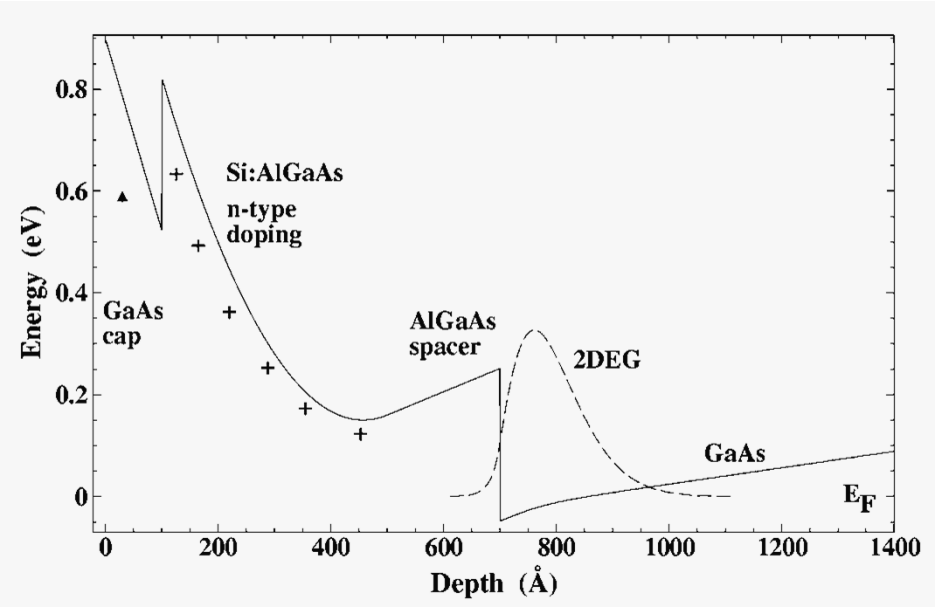


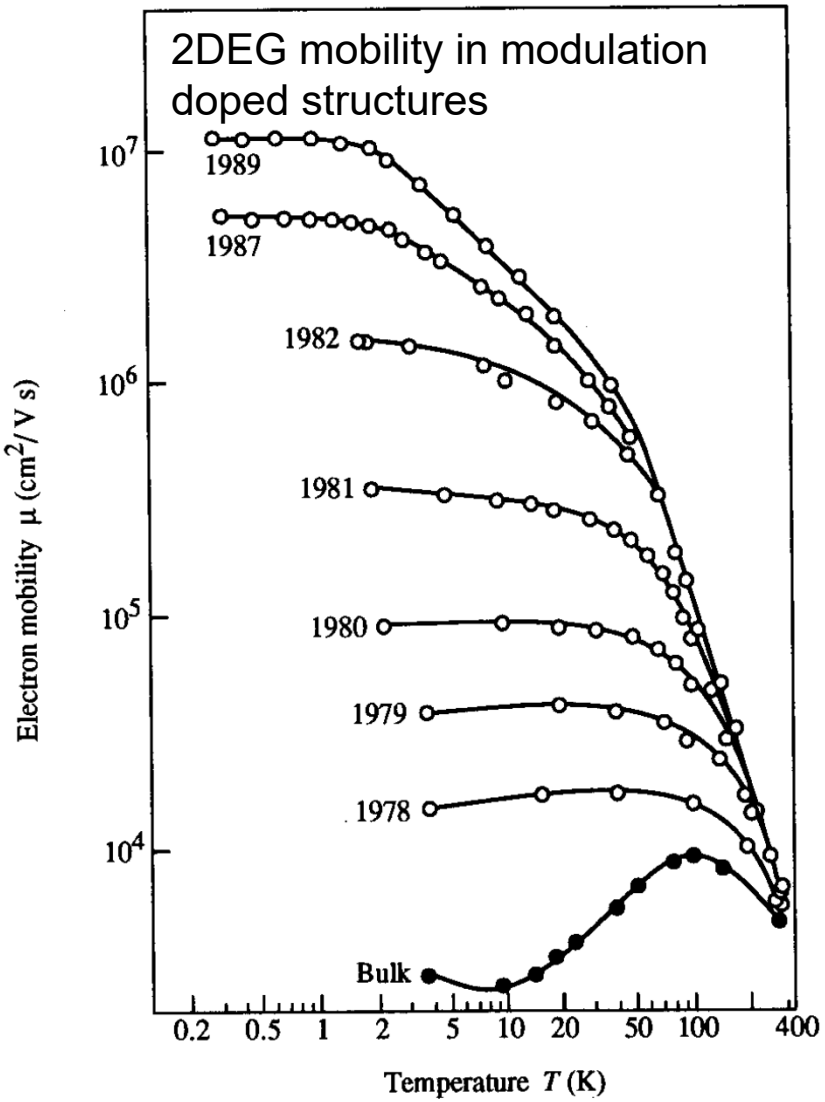
TEM of GaAs/AlGaAs 2DEG structure with superlattice buffer (W M Stobbs, Materials Science)

Two-dimensional electron gas (2DEG)

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



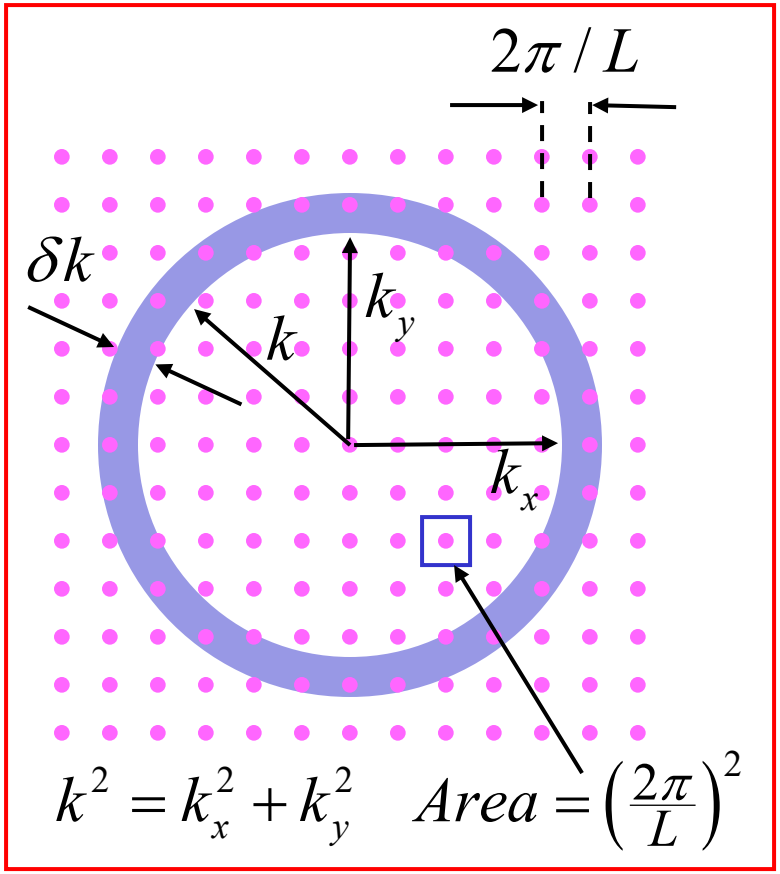




Pfeiffer et al APL **55**,1888 (1989)

Two-dimensional electron gas (1)

- Density of states in two dimensions
- Electrons fill states up to the Fermi energy.
- In 2D the density of states is calculated:
- Consider a lattice of points in k-space,
- 2D gas $L \times L$ in size.
- Spacing between points is $2\pi / L$, area in k-space occupied by each mode: $(2\pi / L)^2$
- If states filled to $k^2 = k_x^2 + k_y^2$, area in k-space of occupied states between k and $k + \delta k$ is $2\pi k \delta k$.
- No. of occupied states
- in this region:



$$\delta n = \frac{2\pi k \delta k}{(2\pi / L)^2} = \frac{k \delta k L^2}{2\pi}$$

Two-dimensional electron gas (2)

$$\omega_L = \frac{eB}{2m}$$

- From the last slide no. of states between k and $k+\delta k$

$$\delta n = \frac{2\pi k \delta k}{(2\pi/L)^2} = \frac{k\delta k L^2}{2\pi} \quad \text{hence} \quad \frac{dn}{dE} = \frac{kL^2}{2\pi}\frac{\delta k}{\delta E}$$

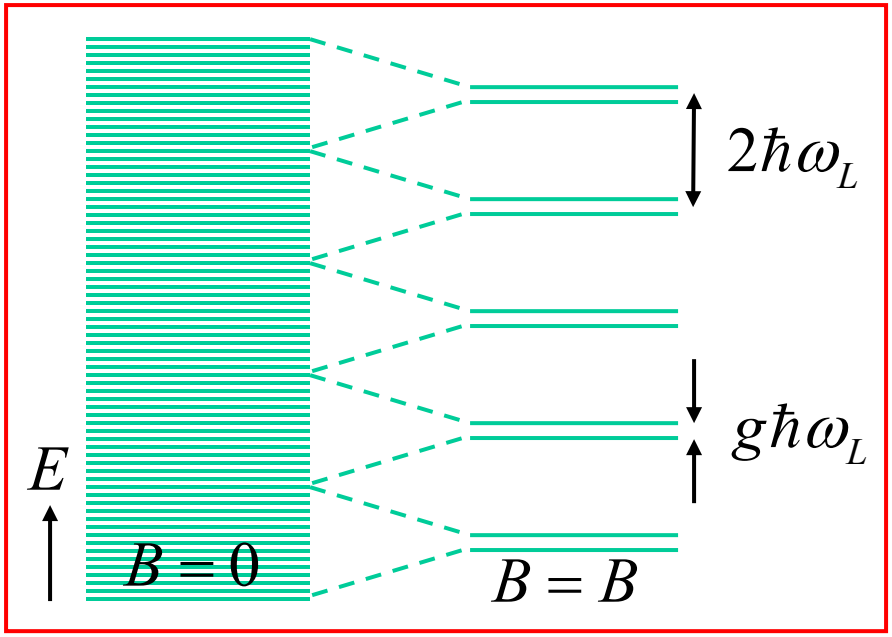
- For a free electron: $E = \hbar^2 k^2 / 2m$ so $\dfrac{\partial k}{\partial E} = \dfrac{m}{\hbar^2 k} \Rightarrow \dfrac{dn}{dE} = \dfrac{L^2}{2\pi}\dfrac{m}{\hbar^2}$

- Hence per unit area, with a factor of 2 for spin, the density of states is:

$$g(E) = \frac{2}{L^2}\frac{\partial n}{\partial E} = \frac{m}{\pi\hbar^2}$$

(independent of E)

- Application of a magnetic field in the z-direction.
- Constant density of states splits into pairs of Landau levels.
- Difference in average energy of adjacent pairs: $\Delta E = 2\hbar\omega_L$
- Pair splitting due to spin- $\Delta E_s = g\hbar\omega_L$ determined by electron g-factor:



Two-dimensional electron gas (3)

- As magnetic field increases , energy splitting between Landau levels increases:

$$\Delta E = 2\hbar\omega_L = \frac{\hbar eB}{m} \qquad \left(\omega_L = eB/2m\right)$$

- As field increases highest Landau levels become depopulated one-by-one and the electrons distributed to other levels.
- If occupation of a Landau level per unit area is: n_L
- Taking into account spin degeneracy the average density of states in presence of a field is $2n_L / 2\hbar\omega_L = n_L / \hbar\omega_L$
- Equating this to density of states at $B = 0$: $g(E) = m/\pi\hbar^2$

$$n_L = \frac{m\omega_L}{\pi\hbar} = \frac{eB}{2\pi\hbar}$$

- If there are υ filled Landau levels at a field B_1 the total density of electrons per unit area is given by:

$$n_e = \frac{\upsilon eB_1}{2\pi\hbar}$$

Two-dimensional electron gas (4)

- Suppose there are υ occupied Landau levels: $n_e = \upsilon e B_1 / 2\pi\hbar$
- If the field is increased from B_1 to B_2 and the highest Landau level is depopulated.
- The electrons are re-distributed among $\upsilon - 1$ levels.
- Hence: $$n_e = \upsilon \frac{eB_1}{2\pi\hbar} = (\upsilon - 1)\frac{eB_2}{2\pi\hbar}$$
- On eliminating υ: $$n_e = \frac{e}{2\pi\hbar}\left(\frac{1}{B_1} - \frac{1}{B_2}\right)^{-1}$$
- This means that the depopulation of the Landau levels is periodic in $\frac{1}{B}$
- At low temperatures where $KT \ll \hbar\omega$ the depopulation of the Landau levels is seen in the resistance of a high mobility 2D electron gas.
- Fermi level between Landau levels - behaves like an insulator
- Fermi level in a Landau level – behaves like a conductor.
- Resistance oscillates with $\frac{1}{B}$ - Shubnikov-de-Haas effect.

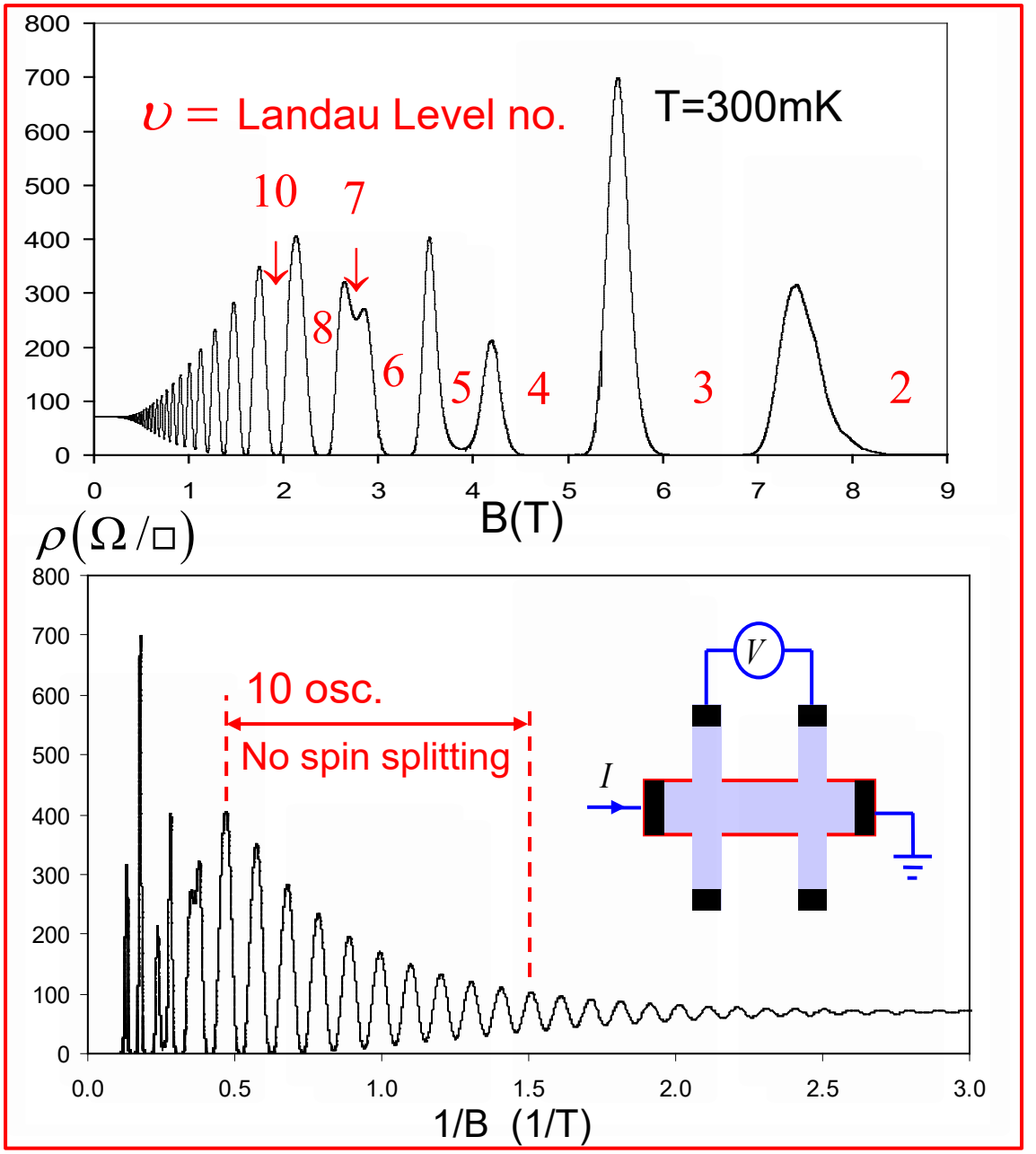
Shubnikov-de-Haas effect

- Oscillations in resistance
- of a high mobility 2D
- electron gas.
- Periodic in 1/B
- We can calculate electron density
- 10 oscillations in $1.05T^{-1}$
- Each oscillation is two levels - no spin splitting (yet)

$$\frac{1}{B_1}-\frac{1}{B_2}=\frac{0.105}{2}T^{-1}$$

$$n_e=\frac{e}{2\pi\hbar}\left(\frac{1}{B_1}-\frac{1}{B_2}\right)^{-1}$$

$$\Rightarrow n_e=4.60\times10^{15}\,m^{-2}$$

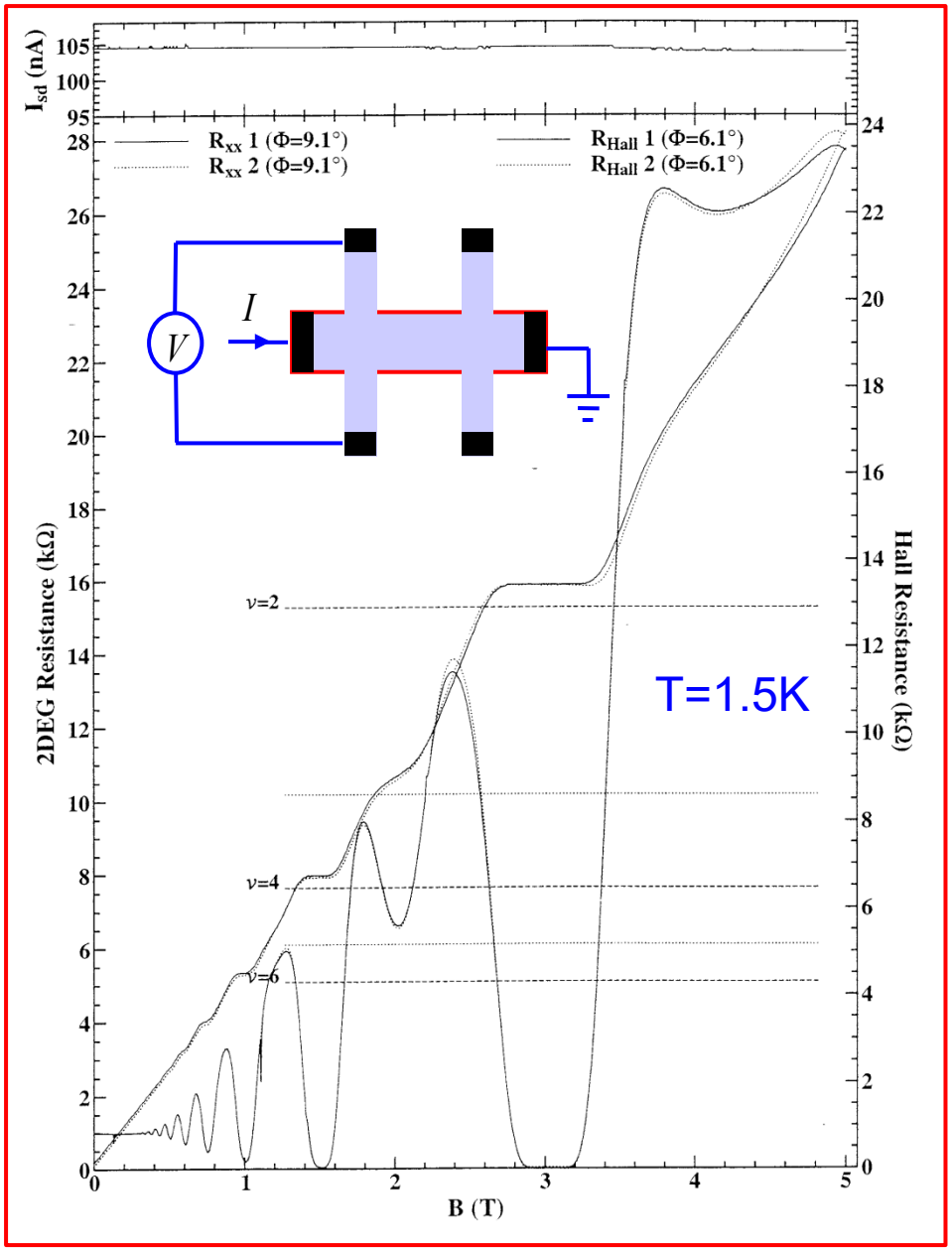


Quantum Hall effect

- Measure voltage perpendicular to current - Hall effect : $R_h = \frac{V}{IB} = \frac{1}{n_e e}$
- n_e density/unit area
- In high mobility 2D electron gas Hall voltage deviates from straight line forming plateaux when there are full Landau levels - where:

$$\frac{V}{I} = \frac{2\pi\hbar}{\upsilon e^2} = \frac{25812.807}{\upsilon}\Omega$$

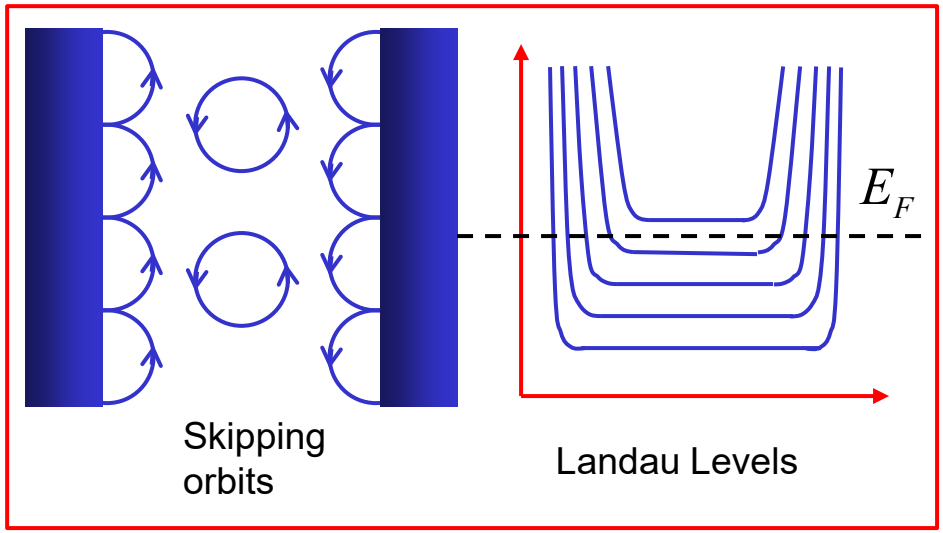
- with υ being the no. of filled Landau levels at the plateaux
- When R_h on plateau resistance $\rightarrow 0$
- Since 1990 used as standard of resistance (5 parts in 10^8)
- Effect very insensitive to sample disorder, astonishing accuracy for solid state experiment, Nobel prize 1985 awarded to von Klitzing



von Klitzing, Dorda and Pepper Phys Rev Lett. **45**, 494 (1980)

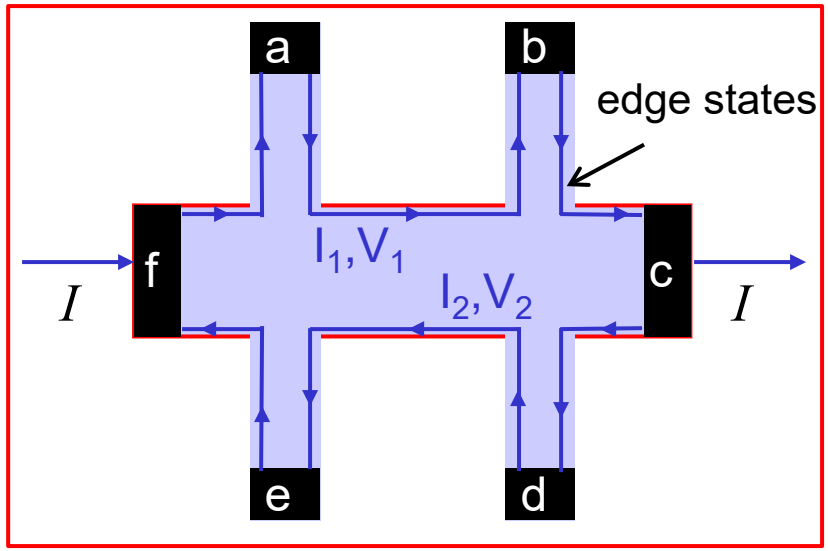
Quantum Hall effect (2)

- Best explanation uses *edge states*
- In a high magnetic field classically electrons will move in circles and 'skip' along the edge of the sample.
- Landau Level picture – levels rise at edges of sample forming *edge states*
- With υ full Landau levels only υ edge states contribute to conduction.



- Regard edge states as 1D conductors

$$g = \frac{\partial I}{\partial V} = \upsilon \frac{e^2}{2\pi\hbar} \Rightarrow I_1 = \upsilon \frac{e^2}{2\pi\hbar} V_1, \quad I_2 = \upsilon \frac{e^2}{2\pi\hbar} V_2$$



- With net current flowing into sample:

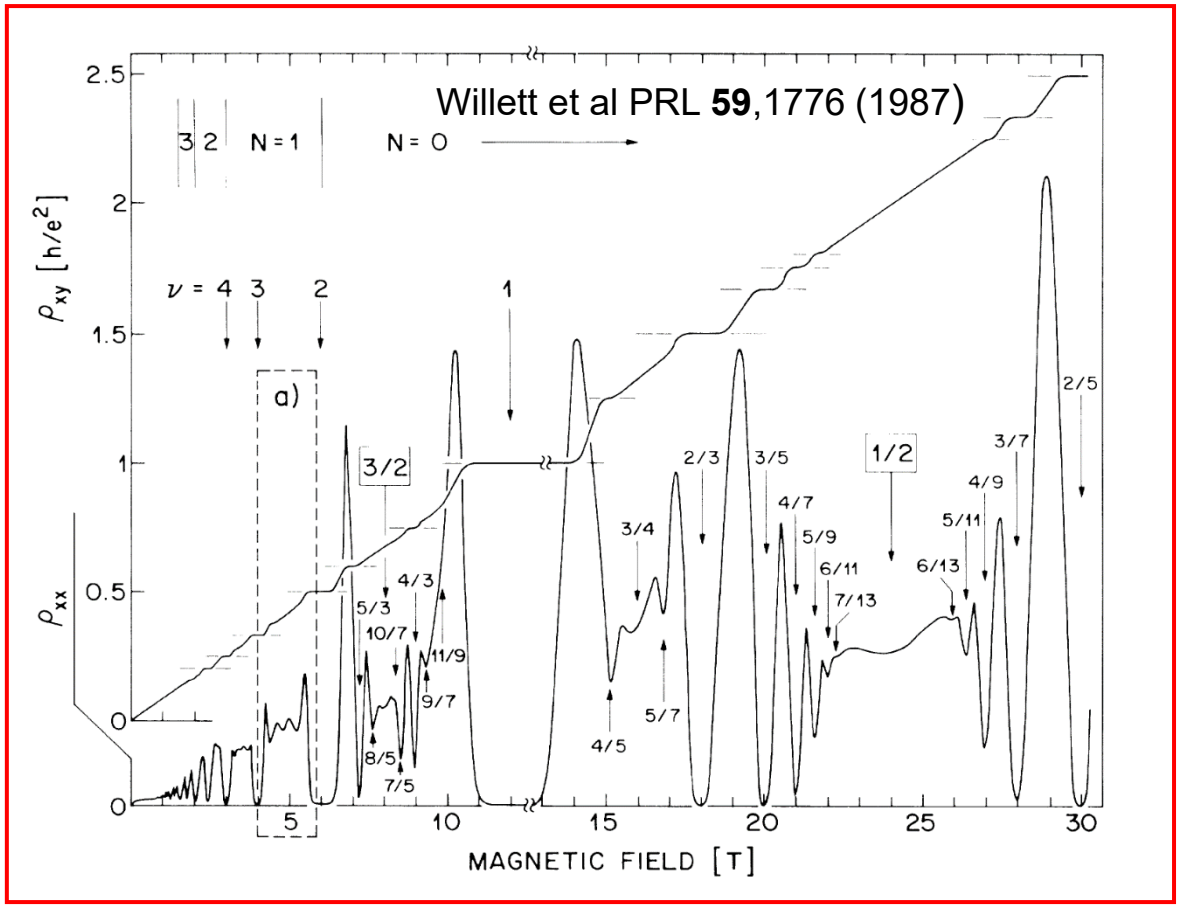
$$\Rightarrow I = I_1 - I_2 = \upsilon \frac{e^2}{2\pi\hbar}(V_1 - V_2)$$

$$\Rightarrow \frac{V_1 - V_2}{I_1 - I_2} = \frac{V_a - V_e}{I} = \frac{2\pi\hbar}{\upsilon e^2} = \frac{25812.807}{\upsilon}\Omega$$

- With this picture quantum Hall plateaux very narrow - to observe them we must introduce disorder and localize some electrons!

Fractional Quantum Hall Effect

- Observed in very high mobility 2D electron and hole gases
- Collective behaviour with electron gas condensing into a liquid state
- Most useful explanation: *composite fermion* theory
- Vortices (flux quanta) captured by each electron forming quasi-particles
- Renormalises magnetic field with SdH oscillations developing at higher and lower magnetic fields
- Fractional states develop in Hall Voltage

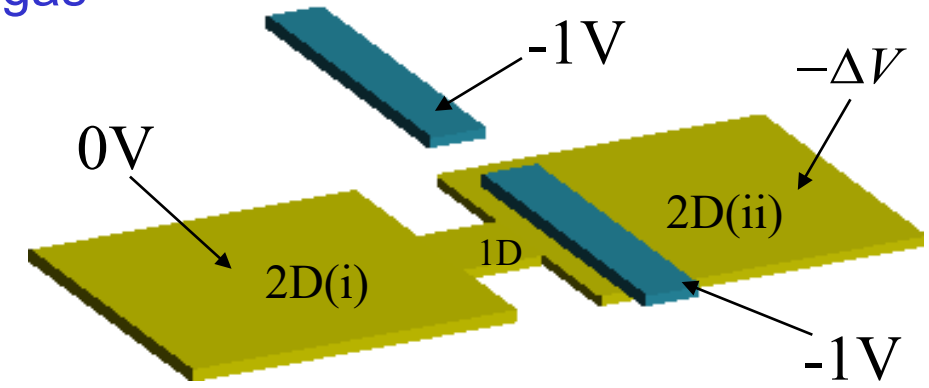


$\mu = 1.6 \times 10^6 cm^2 V^{-1} s^{-1}$
$n = 3.0 \times 10^{11} cm^{-2}$
T=150mK

1998 Nobel Prize: Laughlin Stormer and Tsui

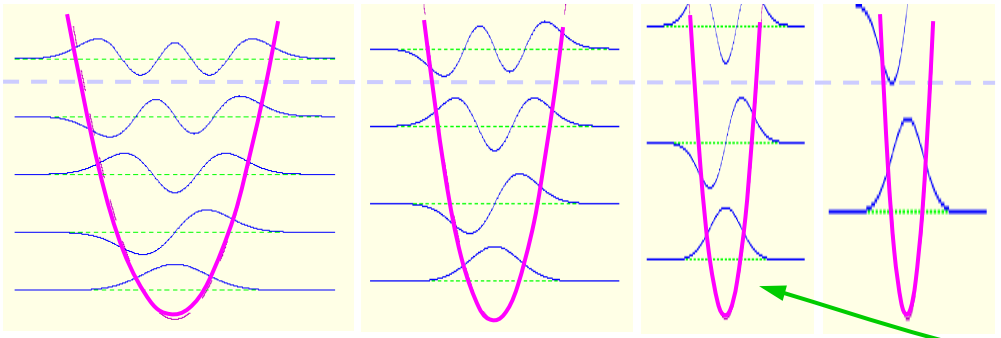
Quantized Conductance in 1D

- 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)

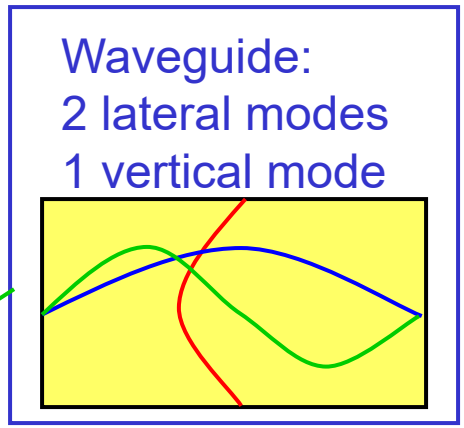


- Making gate voltage more negative decreases well width and increases level spacing – depopulating energy levels one by one.

Number of occupied subbands



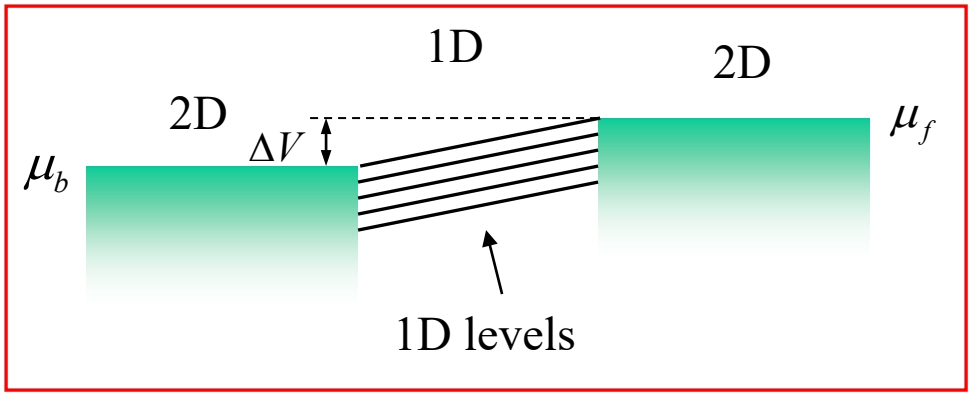
Fermi energy



V_g more negative→

Quantized Conductance in 1D (2)

- 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:

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

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

Length in k-space

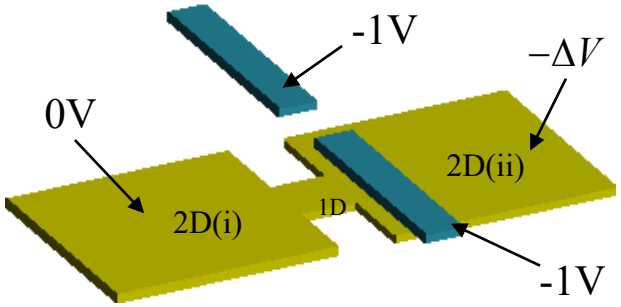
Density of states

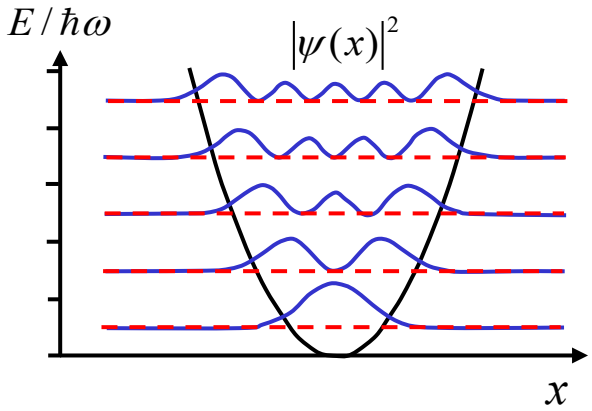
$$N = \frac{2k}{(2\pi / L)} = \frac{kL}{\pi} \Rightarrow n = \frac{k}{\pi} \Rightarrow \frac{dn}{dE} = \frac{1}{\pi}\frac{dk}{dE}$$

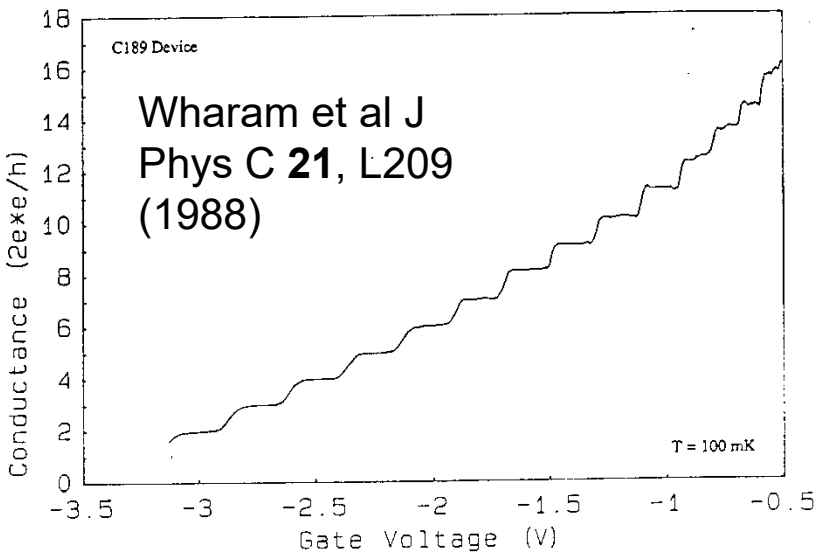
Spacing of states

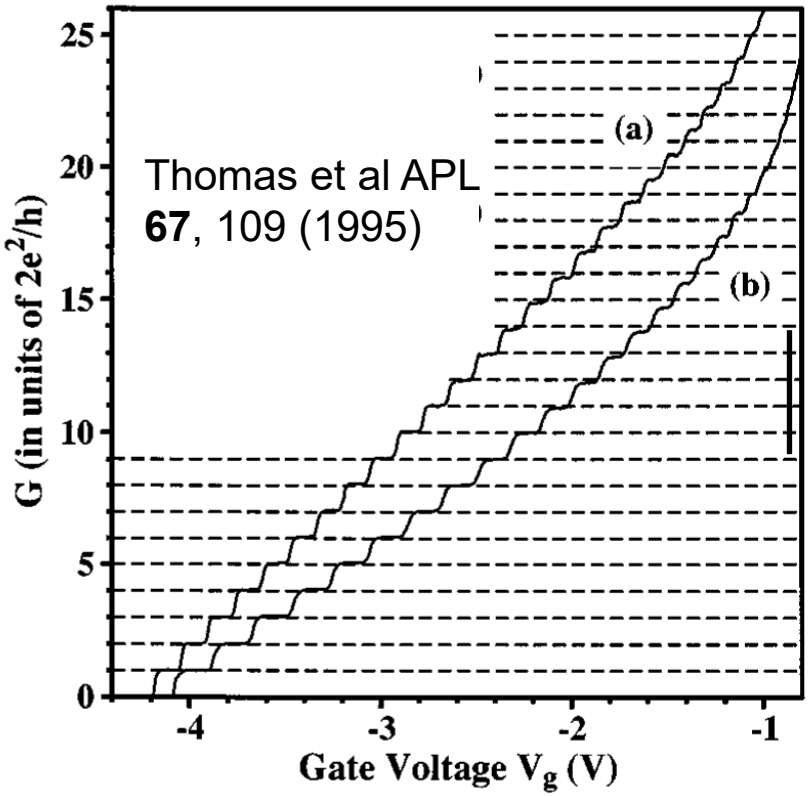
Quantized Conductance in 1D (3)

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







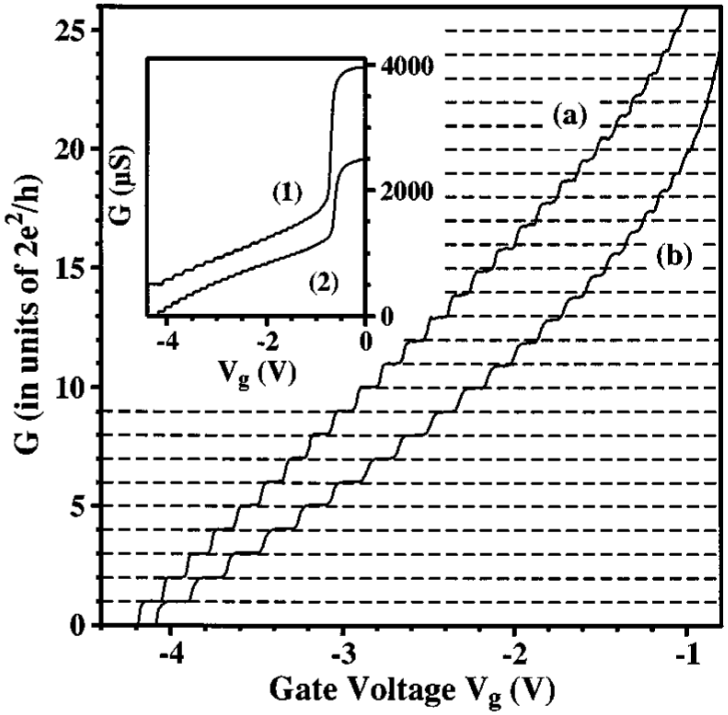


Summary of Lecture 17

- Band structure engineering, use of electron beam lithography and molecular beam epitaxy
- Two-dimensional (2D) electron gas – density of states splitting into Landau levels with increasing magnetic field.
- Depopulation of Landau levels with increasing magnetic field, oscillations in resistance of electron gas – Shubnikov-de Haas effect. Measurement of 2D electron density.
- The quantum Hall effect – observed in 2D electron gas, plateau in Hall voltage when Landau level is full, provides resistance standard accurate to 5 parts in 10^8.
- Fractional quantum Hall effect
- Energy levels in a one-dimensional wire
- Quantised conductance through a one-dimensional wire

Quantum Condensed Matter Physics

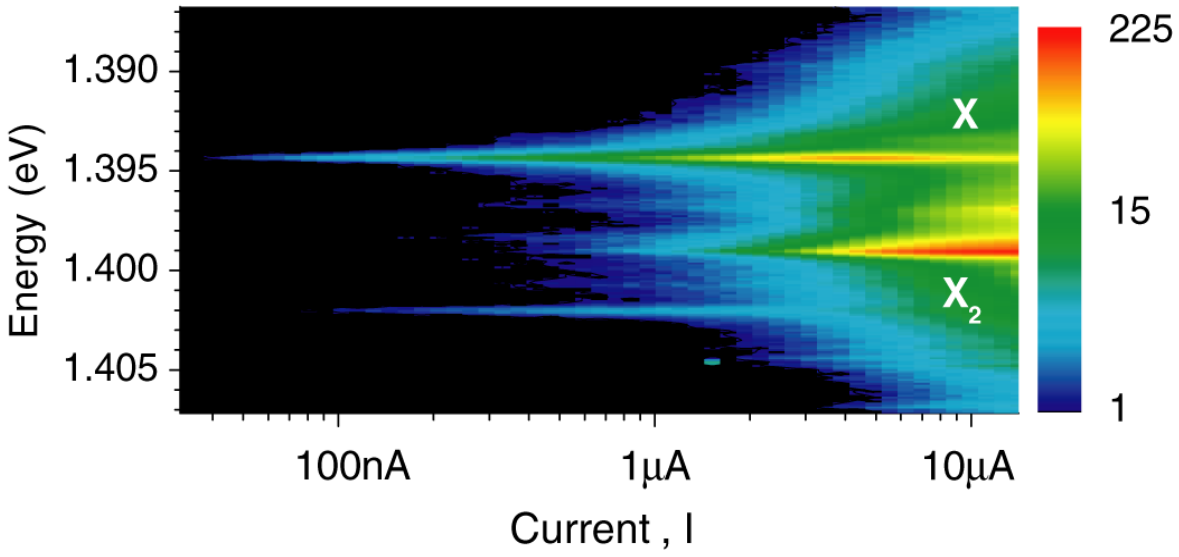
Lecture 17



The End

Quantum Condensed Matter Physics

Lecture 18



David Ritchie

Quantum Condensed Matter Physics

1. Classical and Semi-classical models for electrons in solids (3L)
2. Electrons and phonons in periodic solids (6L)
3. Experimental probes of band structure (4L)
4. Semiconductors and semiconductor devices (5L)

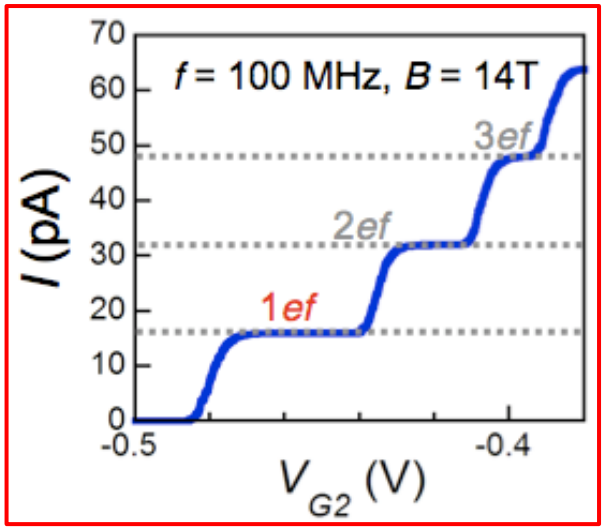
….Photovoltaic solar cell; Shockley-Queisser limit, efficiencies, commercialisation. Field effect transistor; JFET, MOSFET. Microelectronics and the integrated circuit.

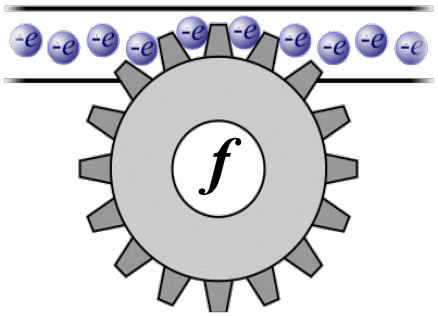
Band structure engineering; electron beam lithography, molecular beam epitaxy. Two-dimensional electron gas, Shubnikov-de Haas oscillations, quantum Hall effect, conductance quantisation in 1D. *Single electron pumping and current quantisation, single and entangled-photon emission, quantum cascade laser.*

5. Electronic instabilities (2L)
6. Fermi Liquids (2L)

The Single-Electron Pump

- Single-electron pump - device that transfers one electron per cycle at a well known frequency
- Can be used to generate a quantized current
- First realised using arrays of Al/Al-oxide tunnel junctions between metallic islands Geerligs et al, PRL **64**, 2691 (1990)
- Frequency can be measured very accurately – traceable back to caesium atomic clock
- Fundamental electron charge is well known $e = 1.602176565\text{x}10^{-19}$ C ± 0.022 ppm
- Can potentially be used for a new quantum current standard for the Ampère





$$I = \frac{\mathrm{d}Q}{\mathrm{d}t} \Rightarrow I_{pump} = e \times f$$

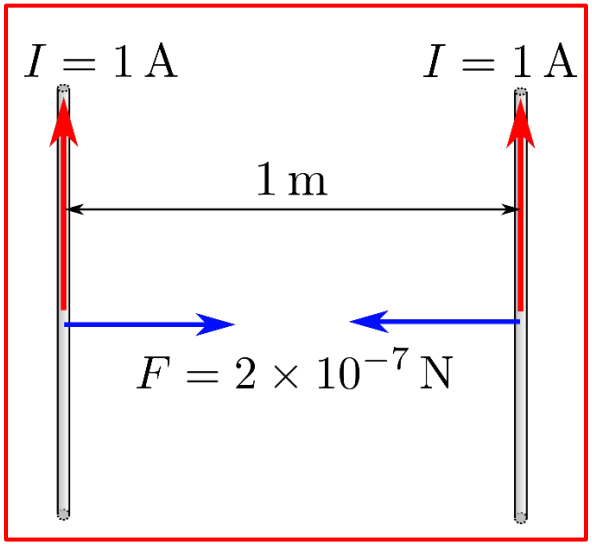
Can also pump n electrons: $I_p = nef$

Single-electron pump slides – Dr Joanna Waldie

Why Do We Need a New Ampère?

- S.I. definition of the Ampère:
- *The constant current which, if maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed 1 m apart in vacuum, would produce between these conductors a force equal to 2×10^{-7} newtons per metre of length.*

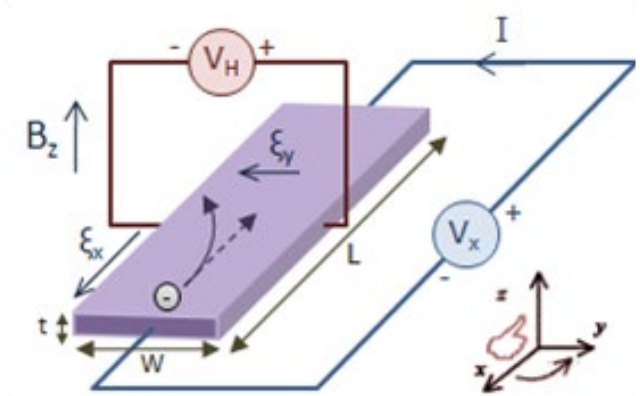
Best accuracy: a few parts in 10^7



- In practise we realise the Ampère using quantum resistance and voltage standards combined by Ohm's law

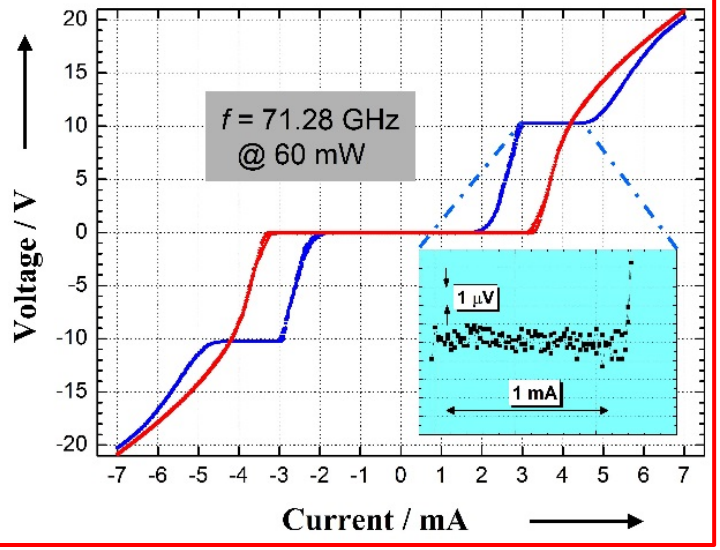
Quantum Hall resistance

$$R_H = \frac{h}{e^2}\times\frac{1}{n}$$



Josephson Voltage

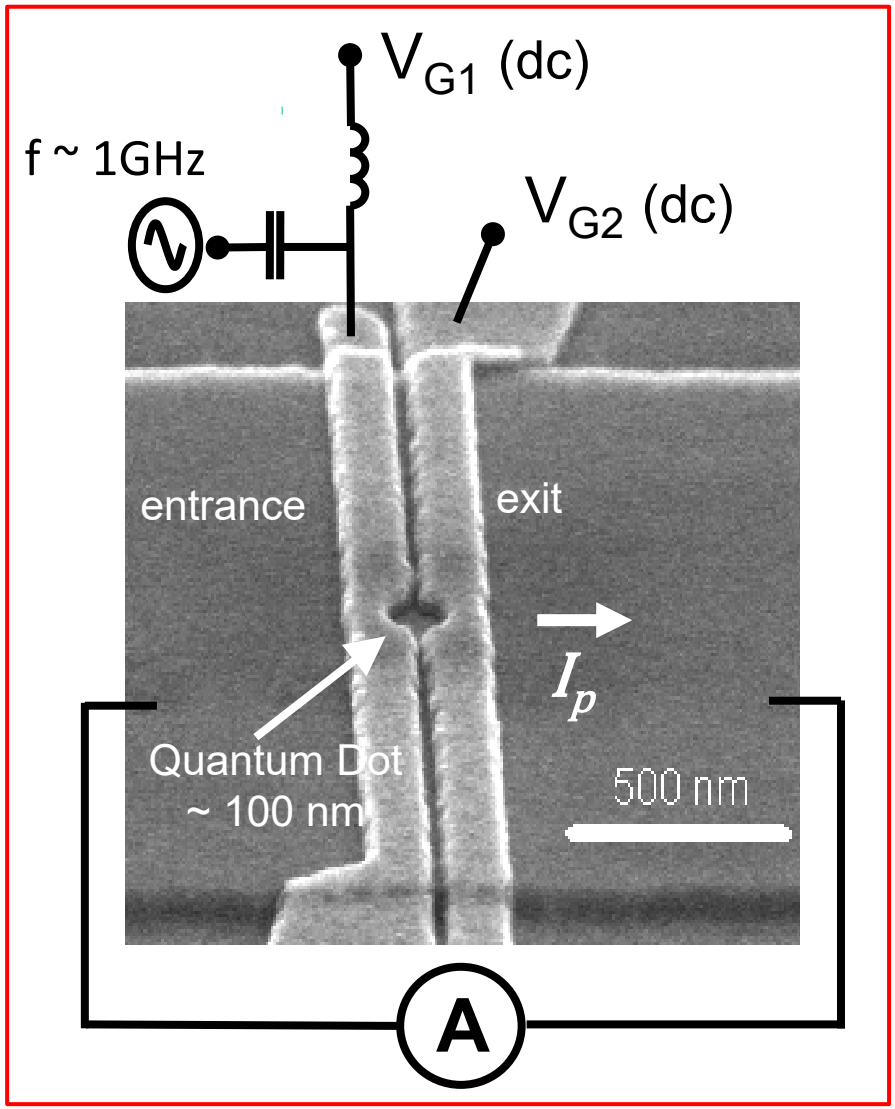
$$V_j = \frac{h}{2e}\times nf$$



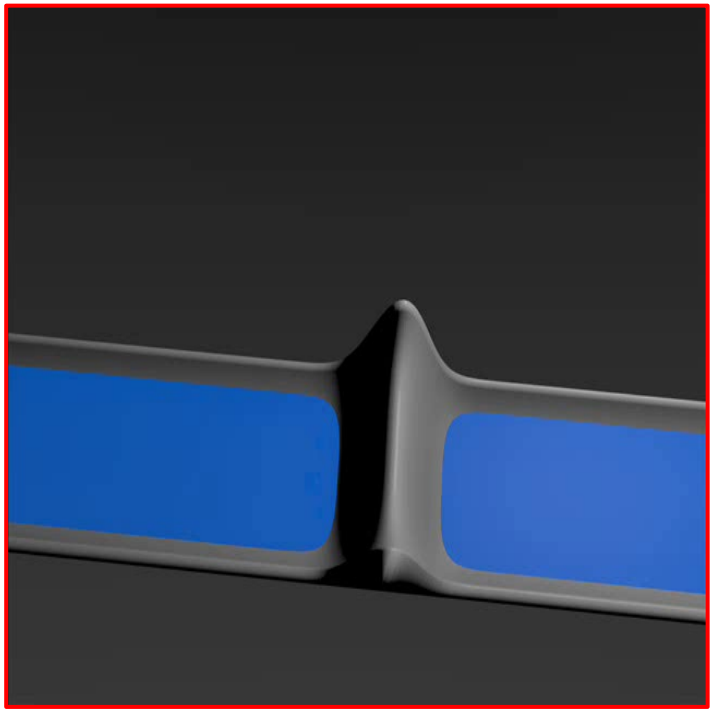
We need a new standard for the Ampère based on fundamental constants

Semiconductor Quantum Dot Electron Pump

- Uses a quantum dot defined by gates in a GaAs/AlGaAs 2DEG



- Electron Pumping Mechanism



Blumenthal et al, Nature Phys **3**, 343 (2007)
Kaestner et al, APL **92**, 192106 (2008)

Semiconductor Quantum Dot Electron Pump

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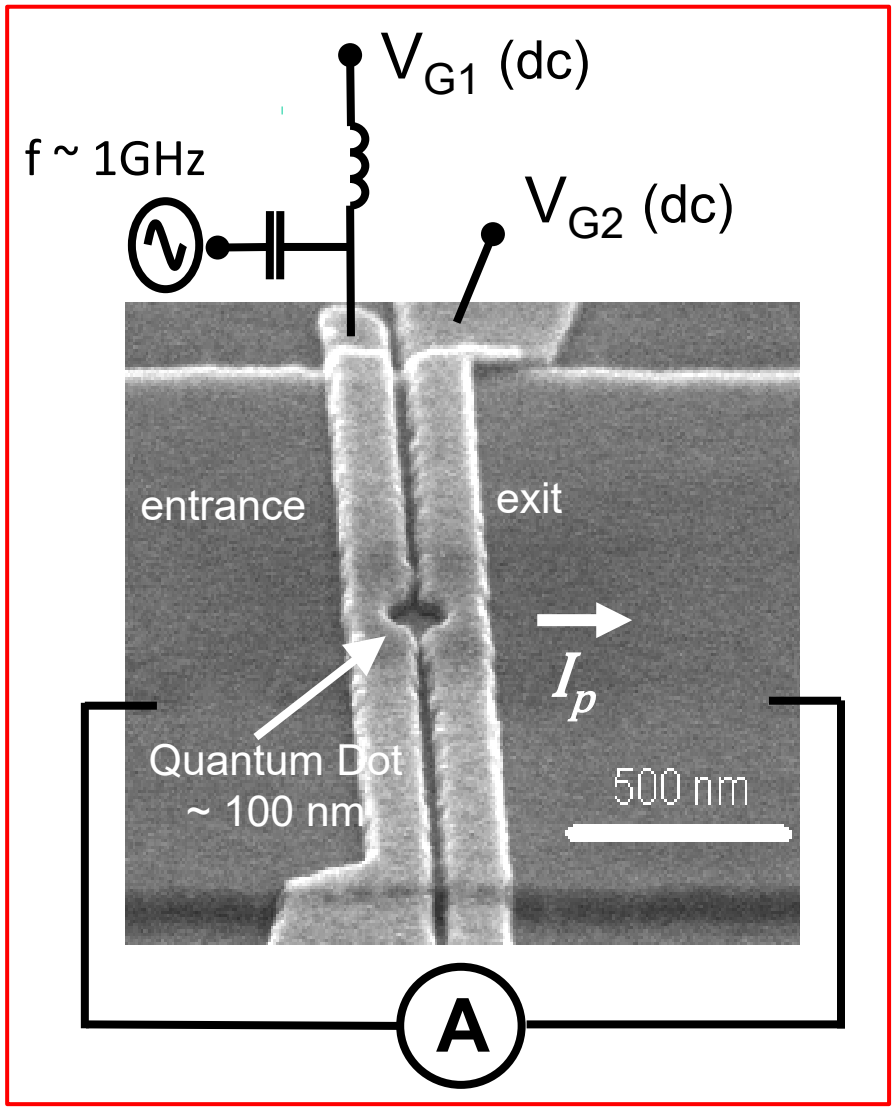

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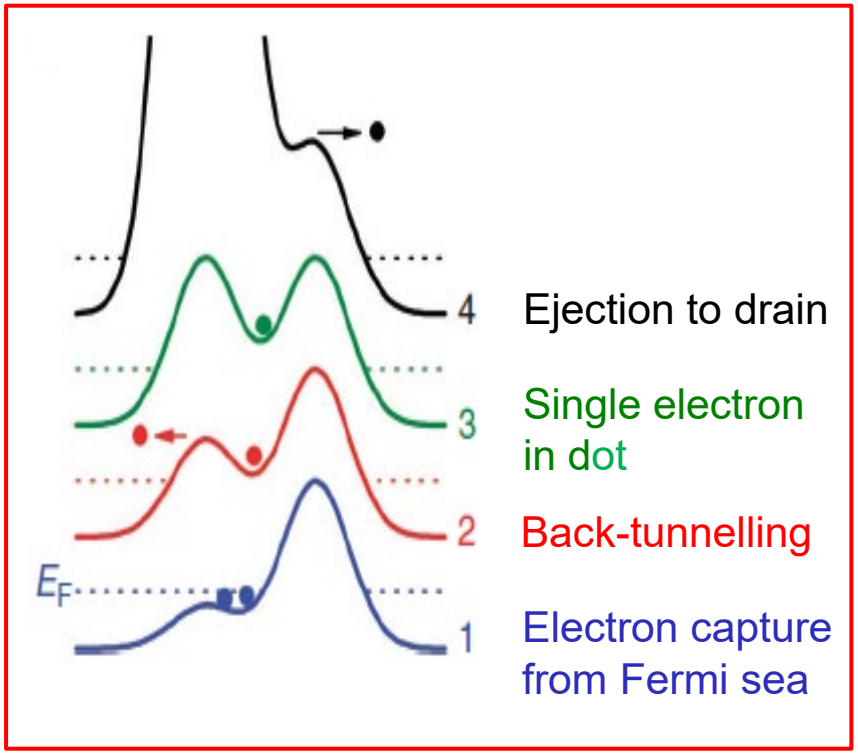
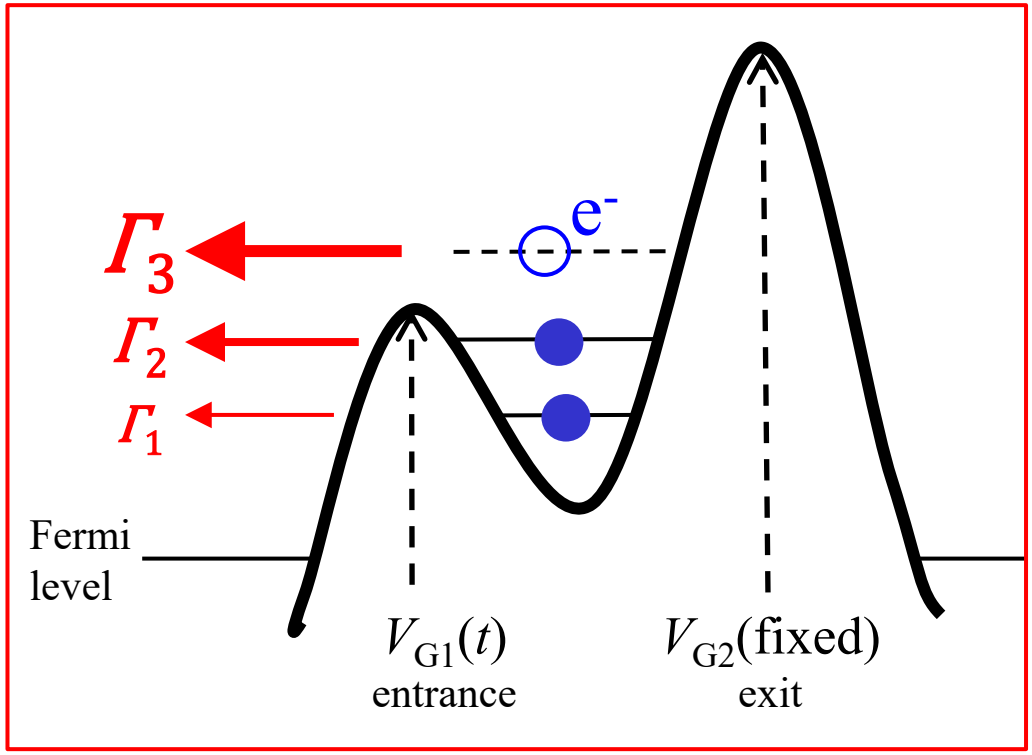


Blumenthal et al, Nature Phys **3**, 343 (2007)
Kaestner et al, APL **92**, 192106 (2008)

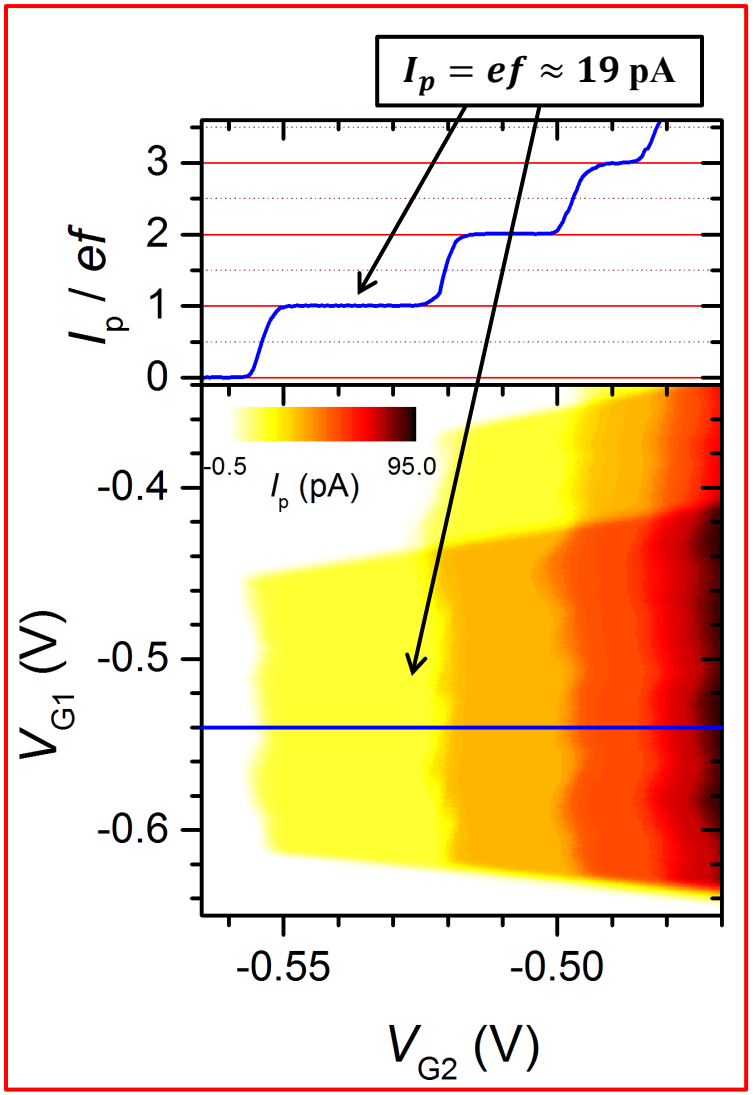
Current Quantization

- Origin of quantization accuracy
- Quantized energy levels in dot implies large separation of tunnelling rates back to source reservoir



Kashcheyevs + Kaestner PRL **104**, 186805 (2010)

- Pumped current at f = 120 MHz

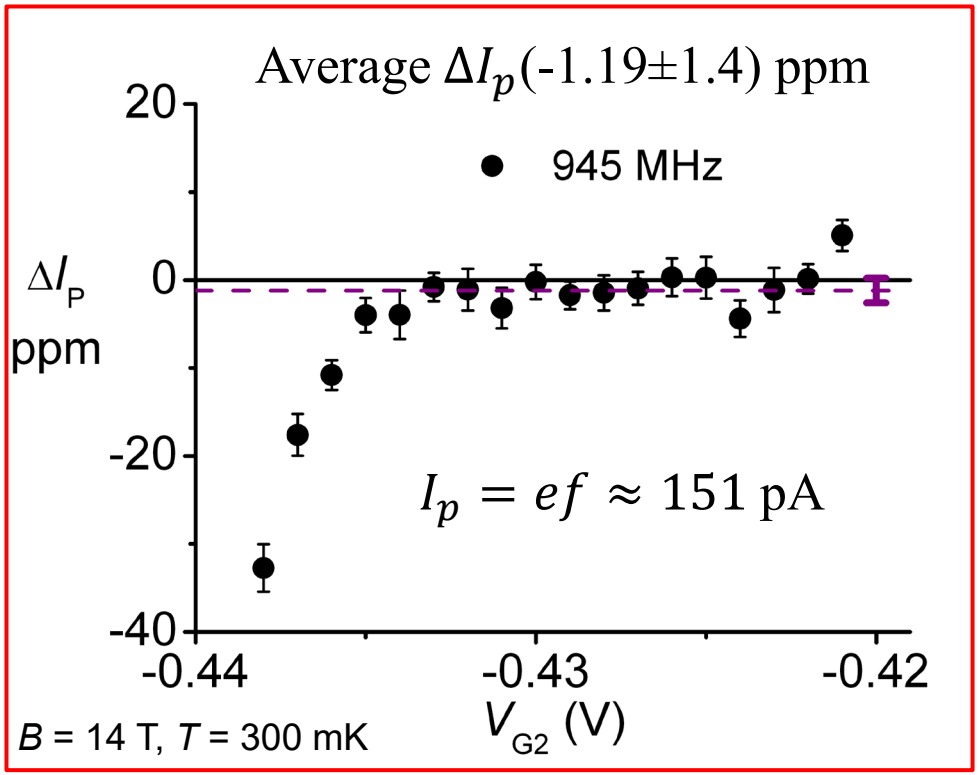


Current pump – accuracy

- To measure the error rate in ppm:

$$\Delta I_p = 10^6 \times \frac{(I_p - ef)}{ef}$$

- Gives a value of 1.2ppm
- Quantisation accuracy improved by:
  (a) Low temperature (< 1 K)
  (b) Small dot – large energy level spacing
  (c) Perpendicular magnetic field
  (d) Custom waveforms to drive pumping, designed to avoid excited states in dot
- UK National Physical Laboratory most accurate semiconductor pump so far: 150pA with error rate 1.2ppm



Giblin et al Nature Comms **3**, 930 (2012)

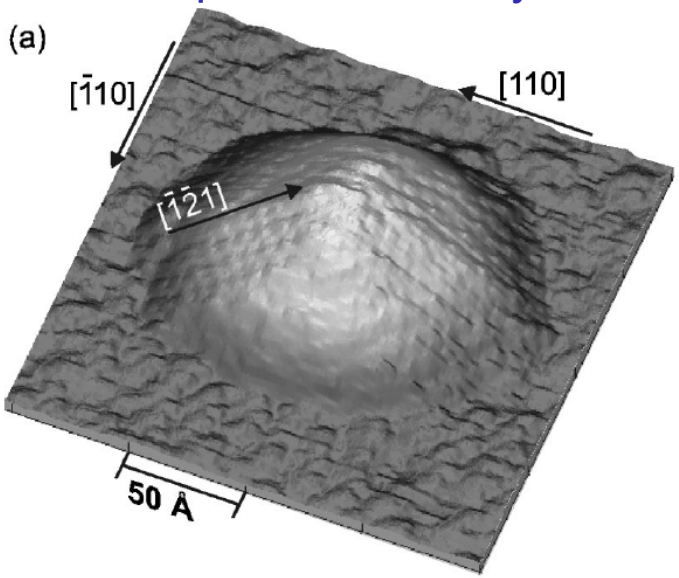
But to redefine the Ampère need < 0.1 ppm!!

NPL National Physical Laboratory

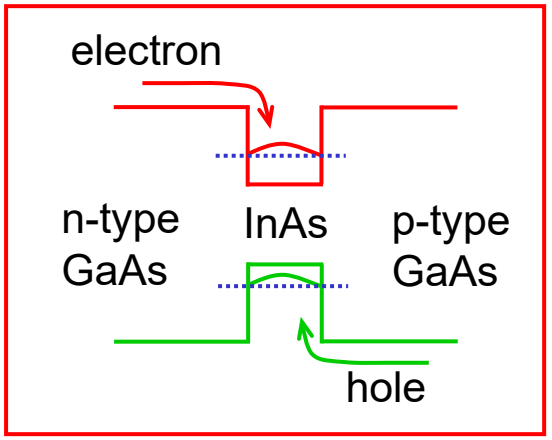
Single Photon Source

- Recent developments in semiconductor growth technology have enabled the production of single photon sources based on self-assembled InAs quantum dots.
- InAs has a lattice constant 7% greater than GaAs.
- InAs grown on GaAs wets surface and forms 3D islands.
- Burying islands in GaAs changes properties due to interdiffusion.
- Dot diameter 10-25nm, height 4-8nm, density 10^{9}-10^{11}cm^{-2}.
- Dots coherently strained – display good photoluminescence and electrical properties.
- Dots tend to store electrons and holes due to narrow InAs bandgap.

Atomically resolved structure of InAs quantum dots by STM



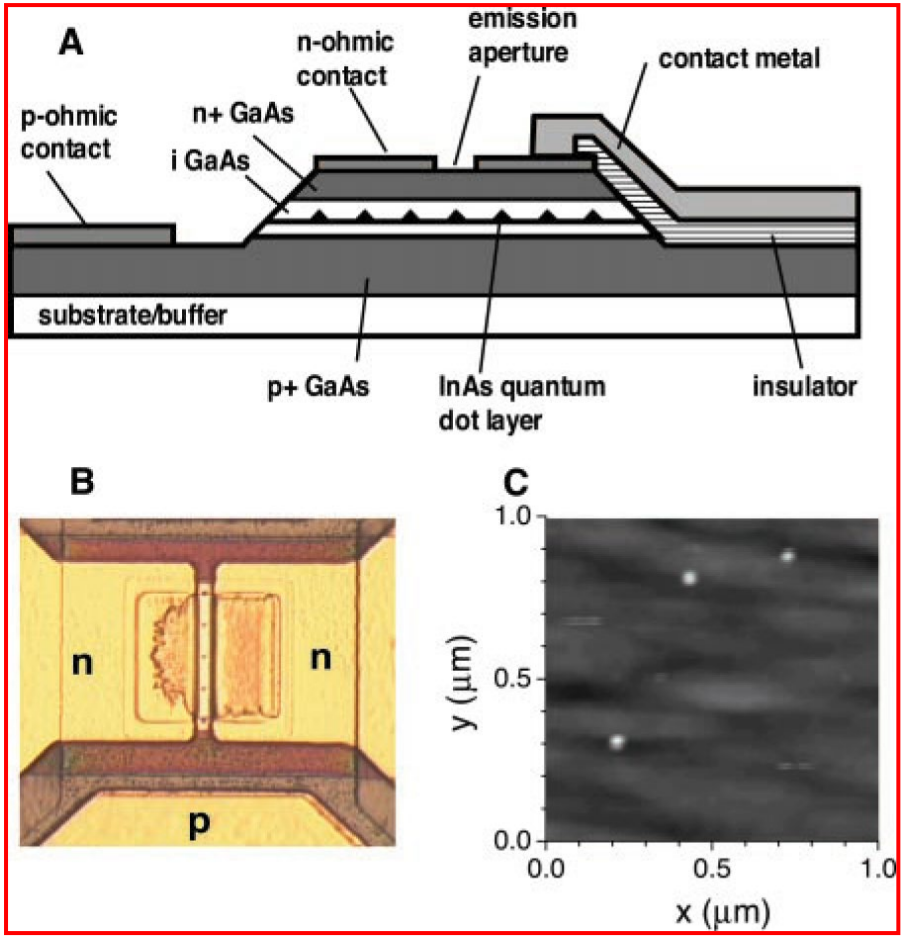
J. Márquez et al, Appl. Phys. Lett. **78,** 2309 (2001)

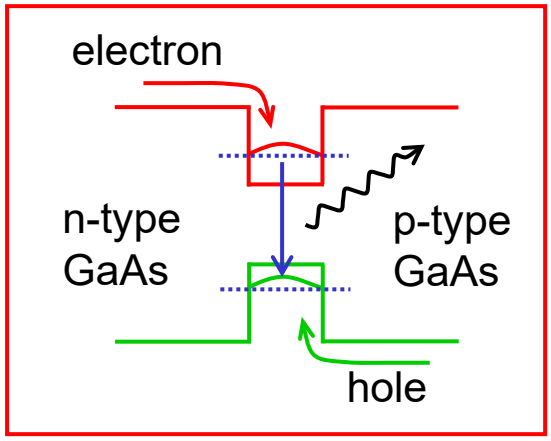


Single Photon Source (2)

Yuan et al Science **295**, 102 (2002)

- Layered structure made from GaAs, grown by molecular beam epitaxy (MBE).
- GaAs p-type/ undoped/n-type structure with InAs self assembled quantum dots in undoped region.
- Low dot density $5 \times 10^8 cm^{-2}$ and micron sized aperture ensures optical emission observed from only a few quantum dots.

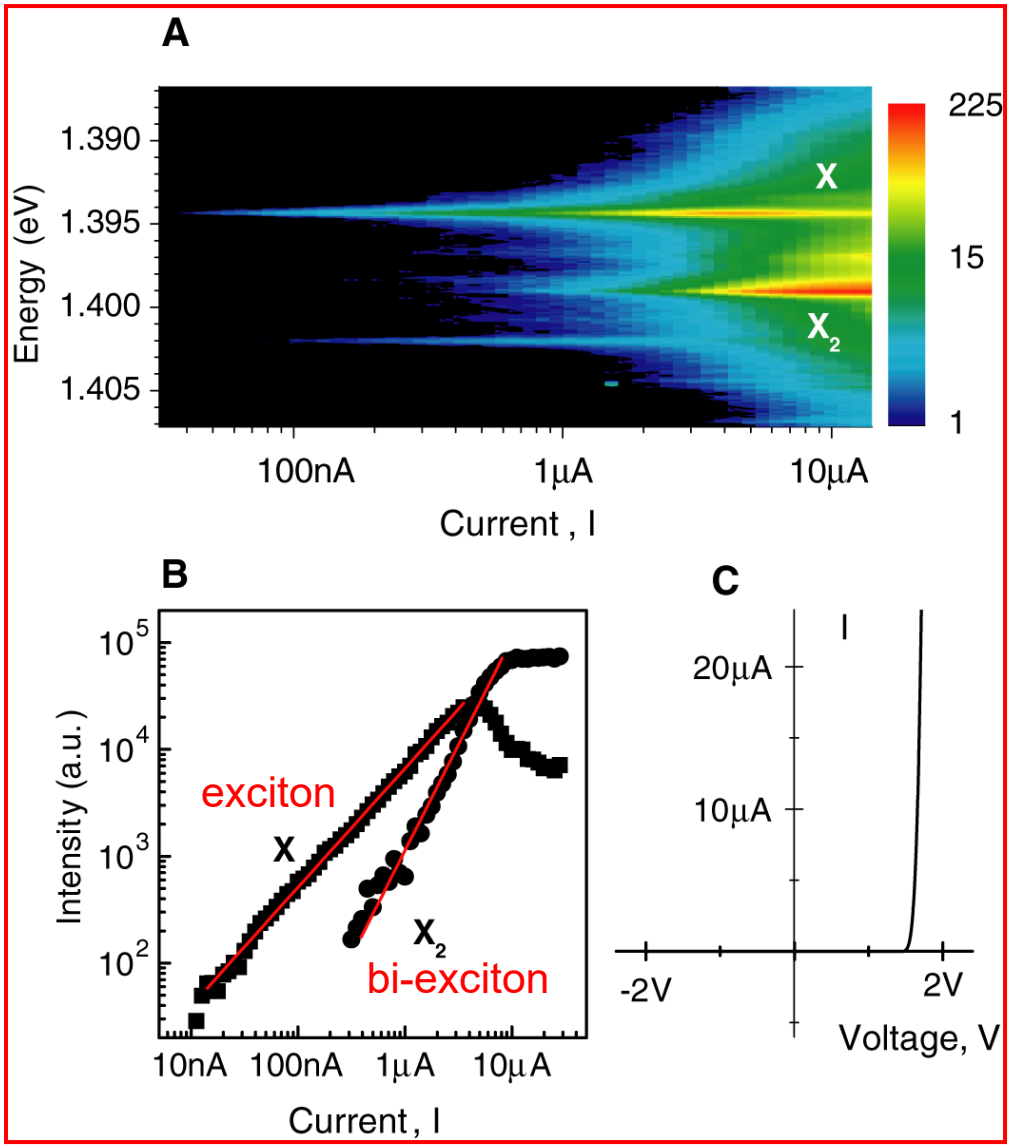




- InAs dots have a narrower bandgap than GaAs – electrons and holes collect in them and recombine emitting a photon.

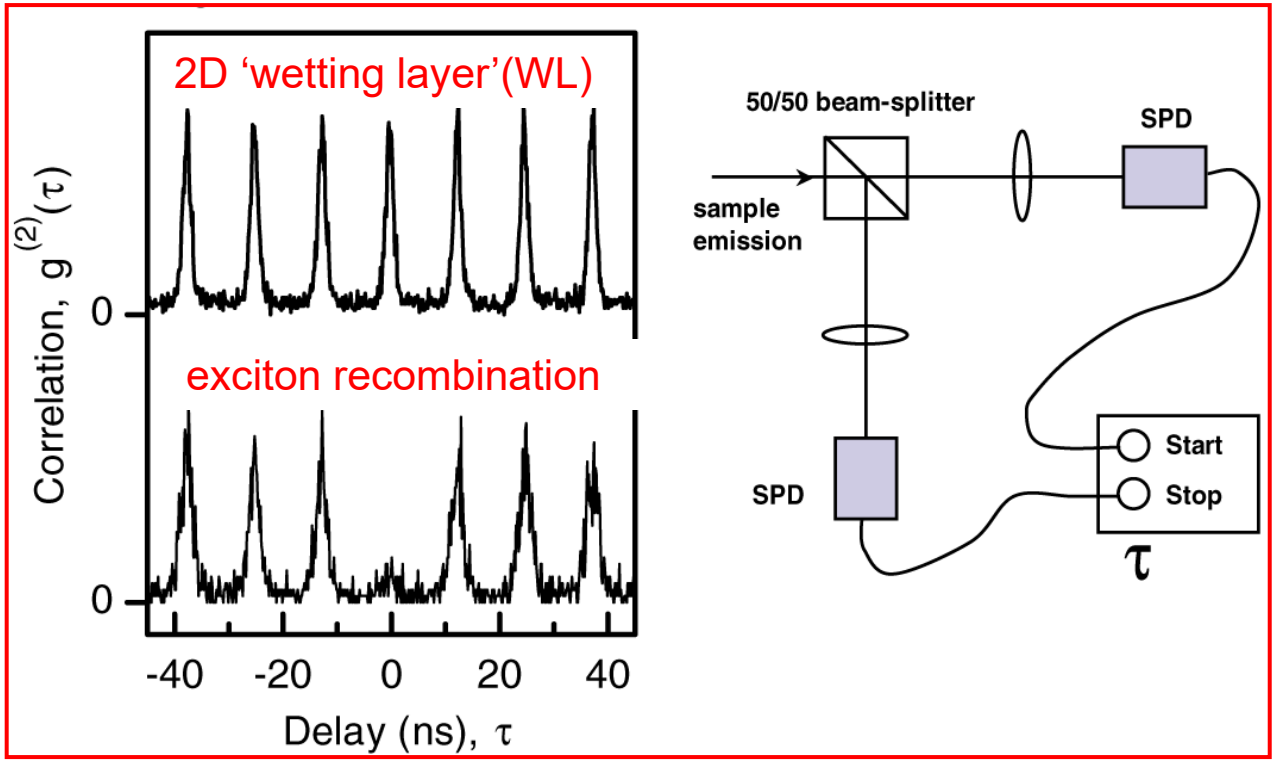
Single Photon Source (3)

- Near ideal diode IV characteristics with turn on at 1.5V.
- Luminescence emitted due to one electron and one hole recombining in single dot giving out photon with well defined energy.
- Emission from both ‘exciton’ (1 electron and 1 hole) or ‘bi-exciton’ (2 electrons and 2 holes) states
- Expected variation of intensity with current for both exciton and biexciton – similar to dependence on laser power for photoluminescence.



Single Photon Source (4)

- 'Hanbury-Brown and Twiss' setup for photon pair correlation measurements.
- Beam splitter, two spectrometers and photon counting Si avalanche photodiodes.
- Time delay between photons recorded.



- Sample driven with 1.5V dc plus square pulses of 0.4ns width repeated every 12.5ns (80MHz).
- Exciton lifetime =1.3ns > pulse width - only one exciton created per pulse.
- Low correlation between two photon events for dot (in contrast to WL).
- Single photons emitted – uses in quantum cryptography and computing.

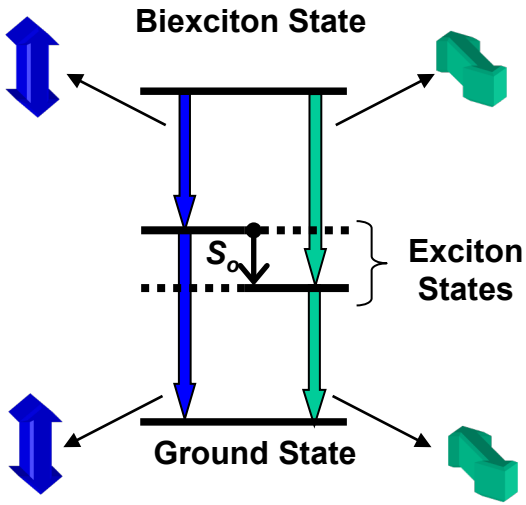
Entangled photon-pair sources

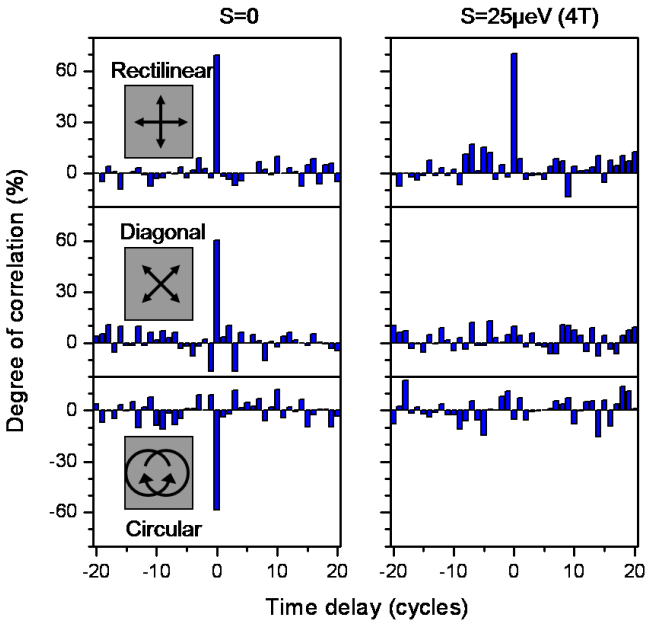
TOSHIBA

- Polarization entangled pair photon sources from biexciton/exciton cascade wavefunction:

$$\frac{1}{\sqrt{2}}\left(|H_1H_2\rangle+|V_1V_2\rangle\right)\equiv\frac{1}{\sqrt{2}}\left(|D_1D_2\rangle+|A_1A_2\rangle\right)\equiv\frac{1}{\sqrt{2}}\left(|L_1R_2\rangle+|R_1L_2\rangle\right)$$

- Non - zero 'fine structure' splitting of exciton level S due to dot anisotropy enables 'which path information' and suppresses entanglement
- Solved by (1) picking the right dot (2) using annealing (3) in plane magnetic field
- Correlation measurements between polarization of exciton and biexciton photons – require good correlations in rectilinear, diagonal bases, anti-correlation in circular basis states
- Best fidelity to ideal state >90%
- Both optically and electrically driven entangled photon sources available
- Applications in quantum teleportation and quantum relays for quantum key distribution, optical quantum computing.

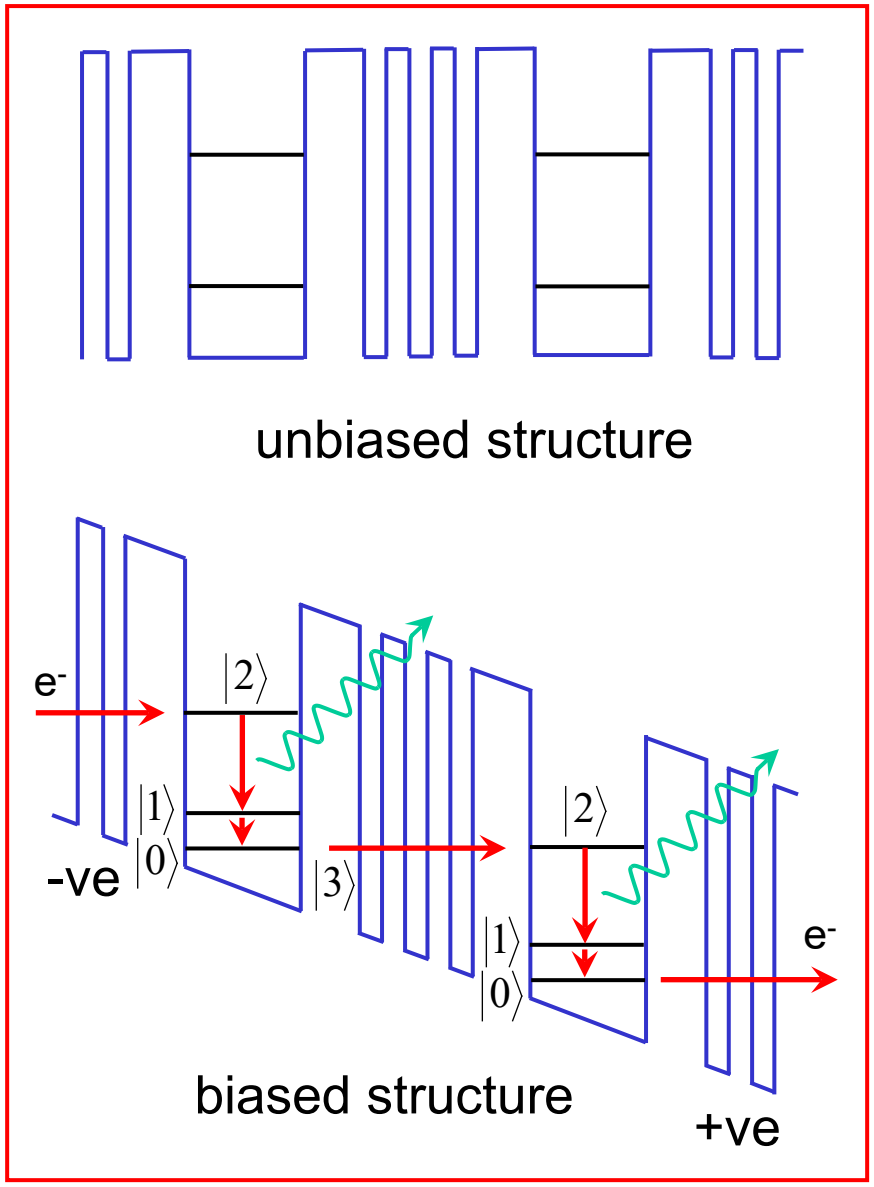




Stevenson *et al*, Nature **439**, 179-182 (2006)
Salter *et al* Nature, **465**, 594–597 (2010)

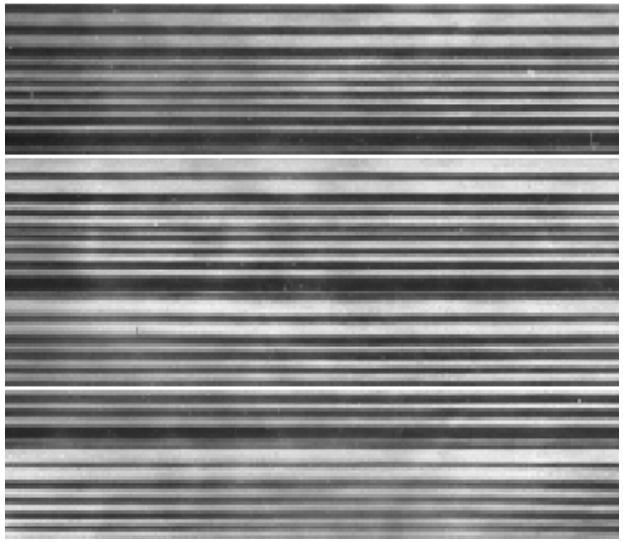
Quantum Cascade Laser

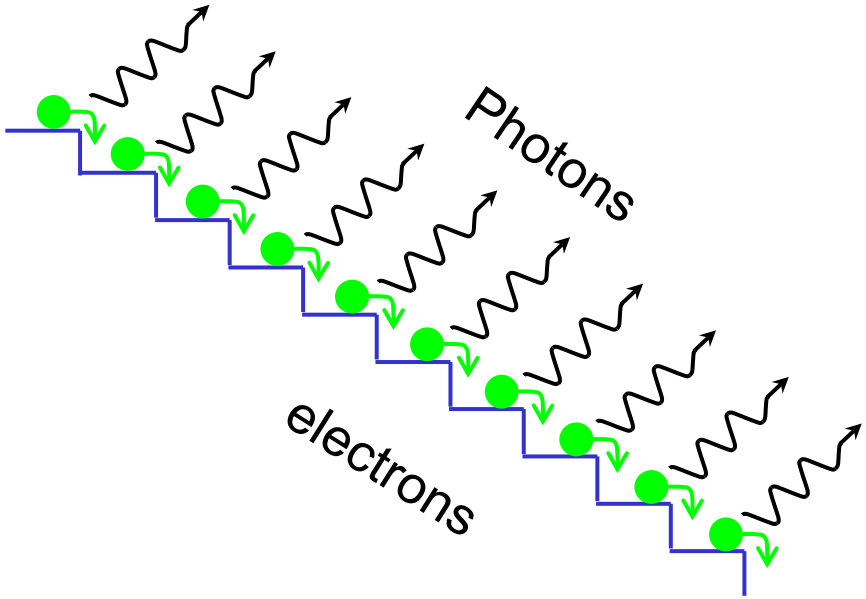
- Most semiconductor lasers consist of forward biased pn junctions where electrons recombine with holes to emit light.
- The quantum cascade laser however makes use of intersubband transitions in quantum wells.
- One difficulty is in pumping the system, this is solved by electrically biasing the structure which allows electrons to tunnel from one well to the next.
- This is a 4 level laser with the lowest level of one well forming the upper level of the next.
- The transition between levels 1 and 0 is phonon assisted – to make it much faster than that between 2 and 1.



Quantum cascade laser (2)

- New type of semiconductor laser – invented at Bell laboratories in 1994[1]
- Semiconductor structure - a sequence of quantum wells and barriers Sequence is repeated many (≈ 80) times - up to 800 individual layers
- In each sequence electrons undergo a transition between subbands of the quantum well, emitting a photon
- With 80 or more of these quantum wells in a laser each electron causes the emission of 80 photons – highly efficient - in conventional semiconductor (diode) lasers each electron causes emission of 1 photon
- Wavelength 3-27μm (infrared) powers up to 1W (pulsed) at room temp

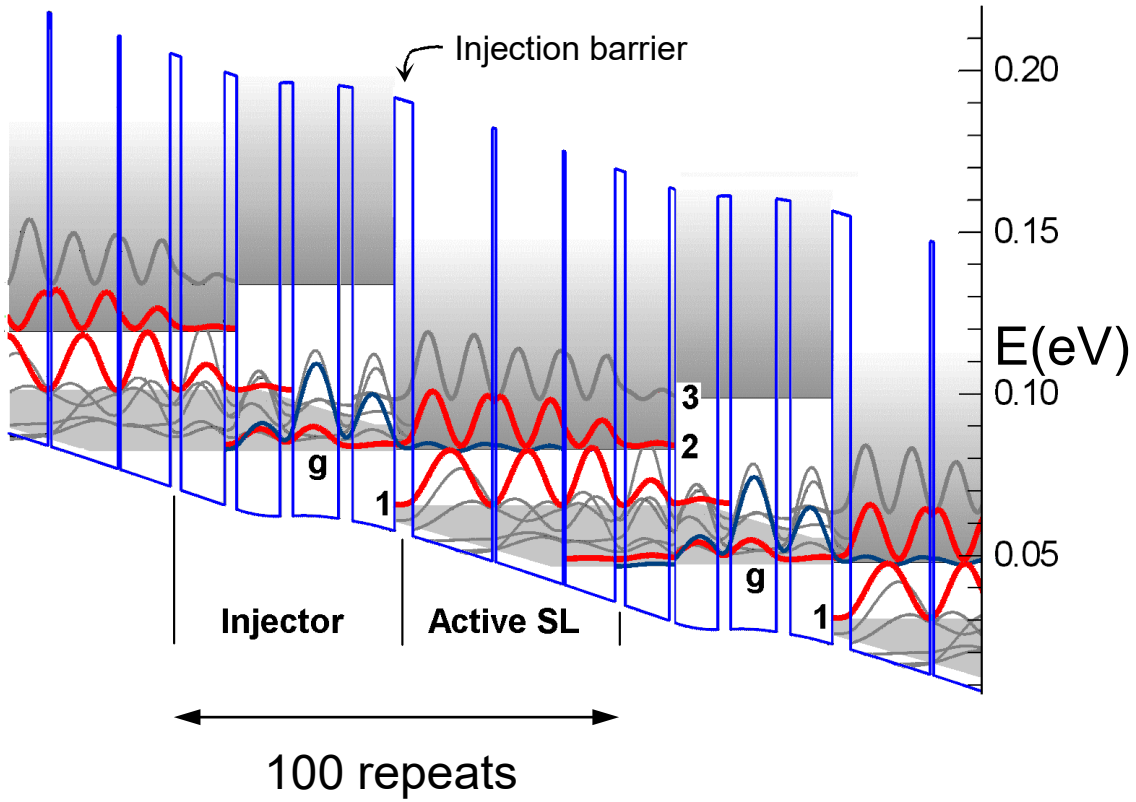




[1]J Faist et al Science **264**,553 (1994)

THz Quantum Cascade Laser (1)

- Since 2002 rapid progress in development of cascade lasers at THz frequencies – wavelengths up to 150μm
- GaAs/AlGaAs quantum well structure – energy level separation controlled by quantum well width
- Control of barrier widths and tunnelling time gives correct lifetimes for states – allows population inversion
- Quantum well structure repeated 100 times - 1 electron passing through device produces 100 photons –high efficiency



Kohler et al Nature **417**(2002) 156-159

- Cascade lasers require waveguide structure to confine radiation and generate optical mode structure

THz Quantum Cascade Laser (2) – Device structure

- Multilayered active region etched into waveguide structure
- Ohmic contacts made to top and bottom of device
- Care taken with heat dissipation

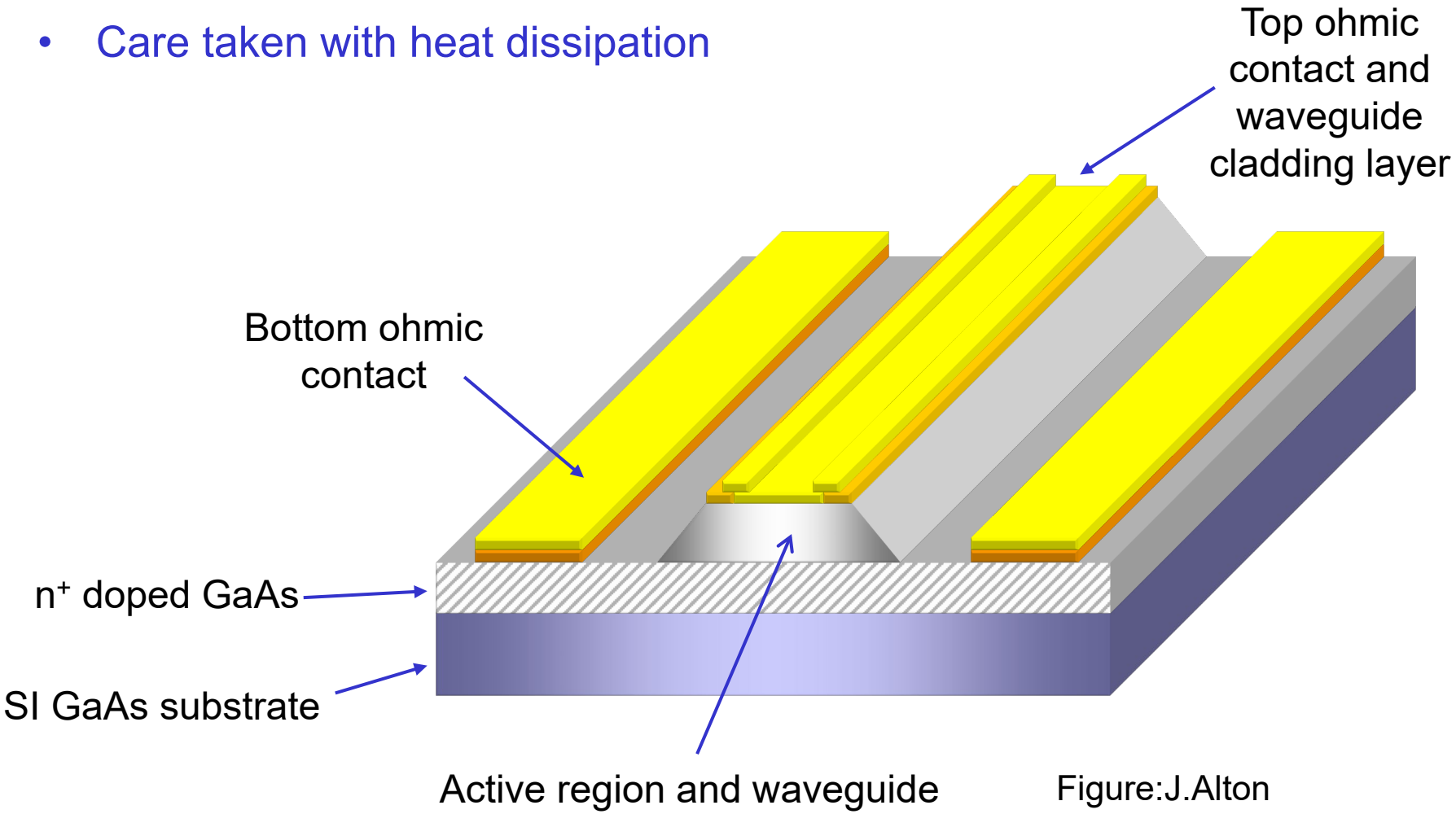


Figure:J.Alton

THz Quantum Cascade Laser (3)

- Performance

Driven by: 200ns pulses, 2□s intervals

2mW output power at 4K and 4.4THz, 0.1mW at 40K, maximum operating T=50K

- Applications:

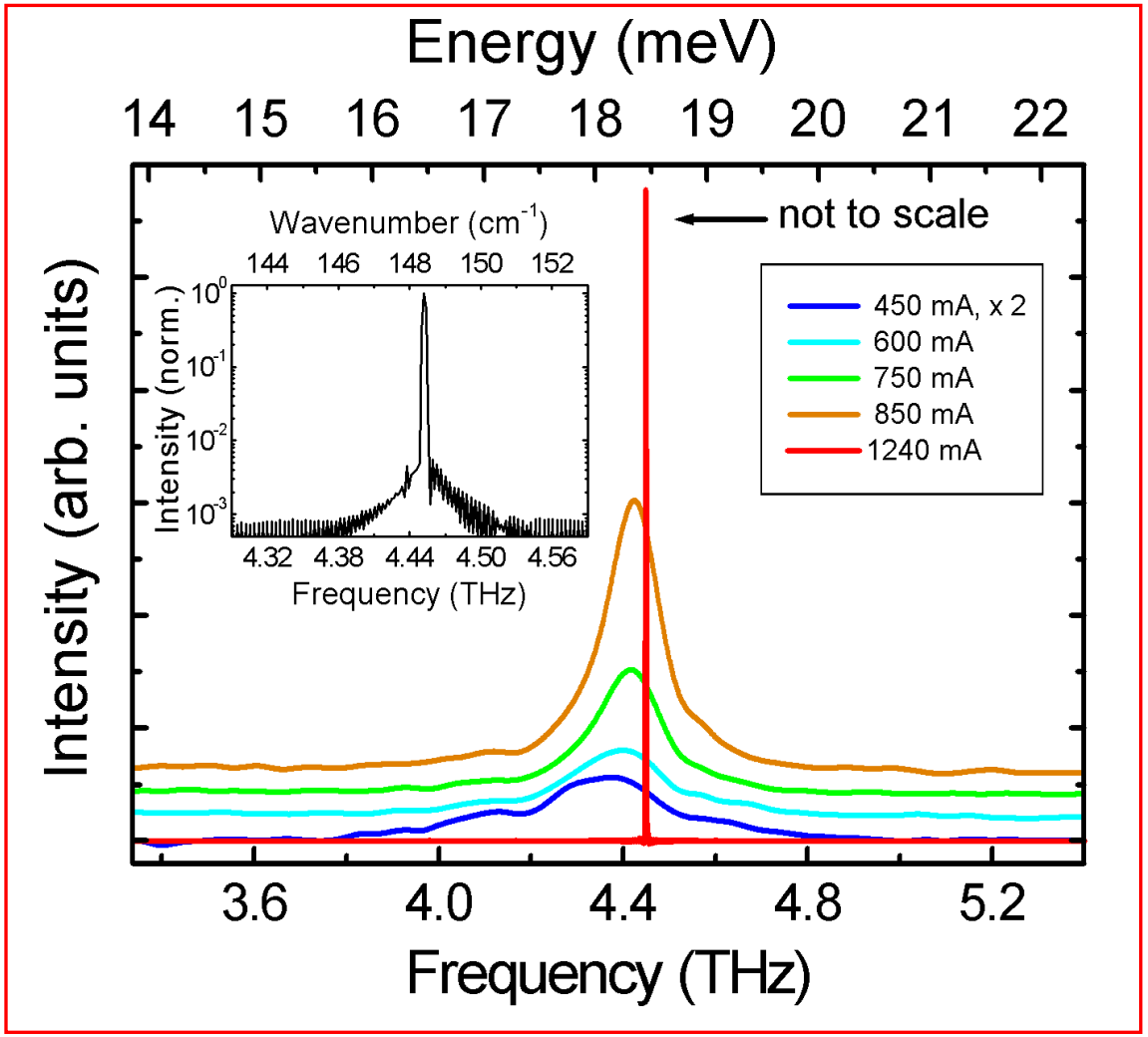
THz spectroscopy

Imaging - security and pharmaceuticals

Gas sensing – emissions

Astronomy- Local oscillators

Quantum control experiments



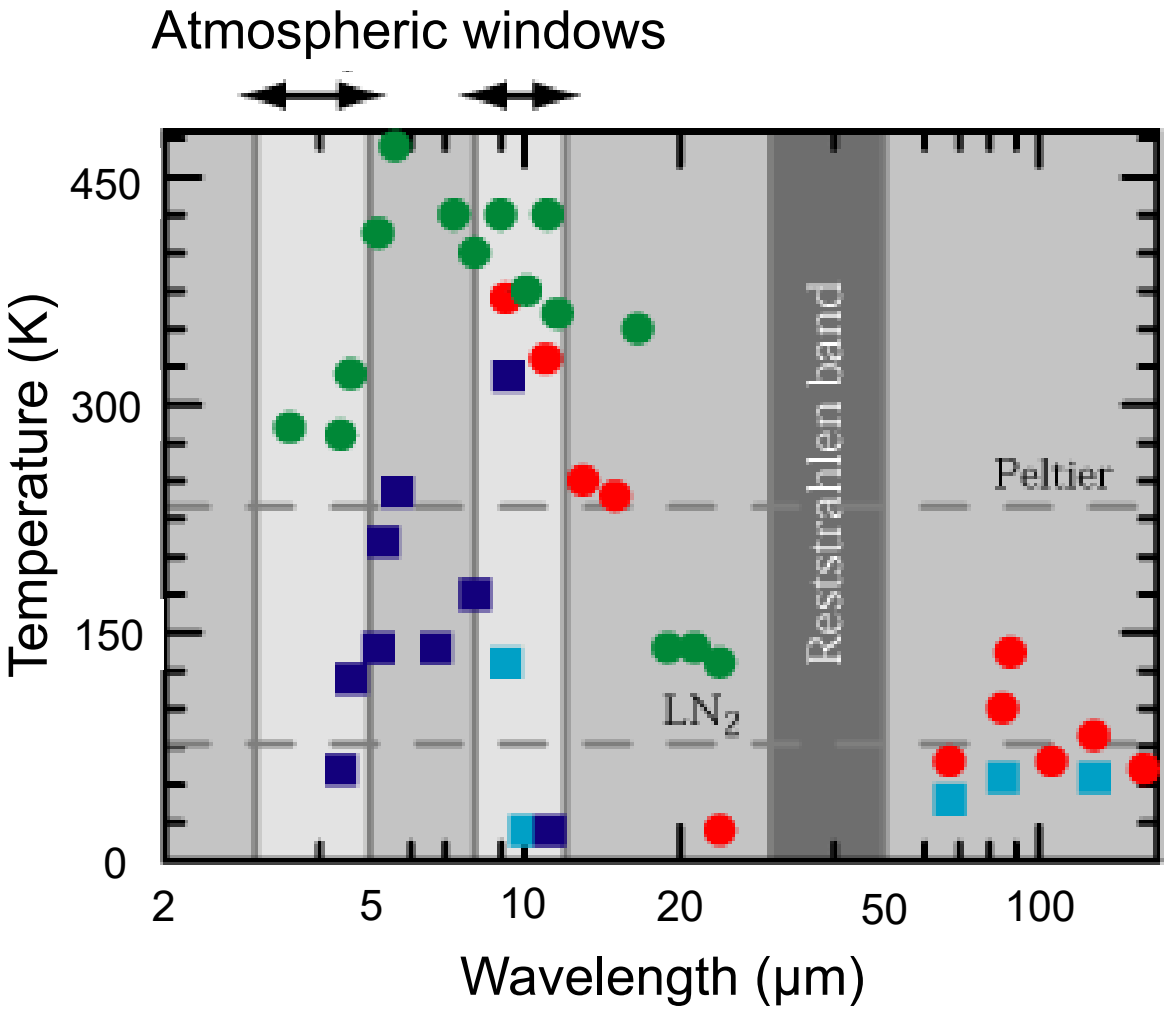
Koher et al Nature **417**,156 (2002)

- Current state-of-the-art -

200K operation at 3.2Thz/94 μm, Fathololoumi et al Opt Ex **20**, 3866 (2012),

1W emission at 3.4THz and T=10K, Li *et al* Elec Lett **50**, 309 (2014)

Quantum Cascade Lasers – wavelength coverage



•Very wide range of wavelengths available due to the use of 'band-gap engineering' of multilayered structures to define energy levels.

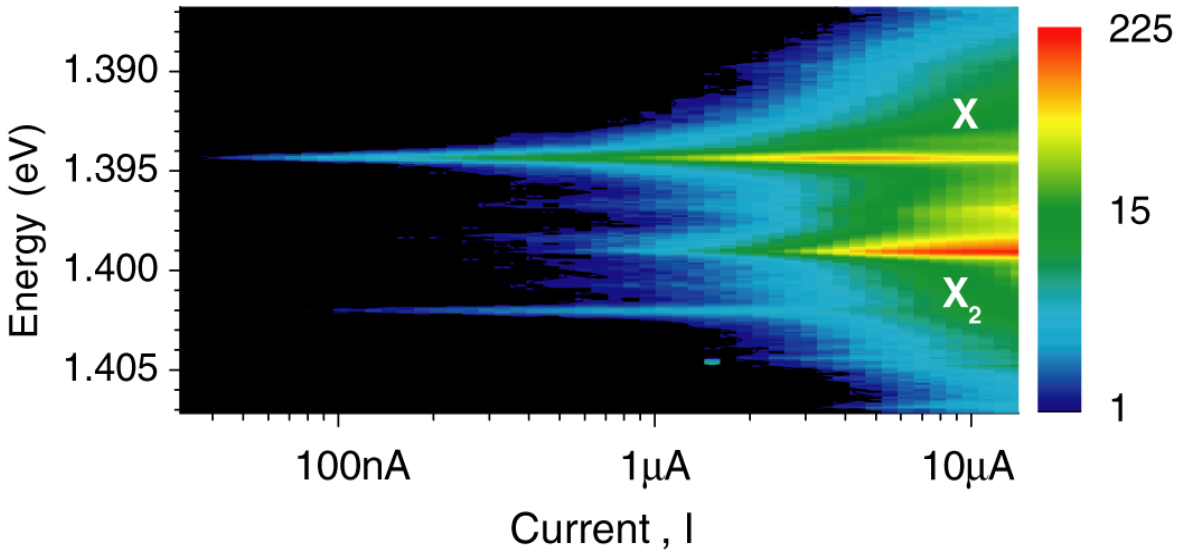
Figure: J Faist, University of Neuchatel

Summary of Lecture 18

- Single electron pumping with application to a current standard
- Single photon sources, made from InAs quantum dots
- Quantum cascade laser

Quantum Condensed Matter Physics

Lecture 18



The End

Quantum Condensed Matter Physics

Lecture 19

David Ritchie

Quantum Condensed Matter Physics: synopsis (4)

5. Electronic instabilities (2L)

The Peierls transition, charge density waves, magnetism, local magnetic moments, Curie Law. Types of magnetic interactions; direct exchange, Heisenberg hamiltonian, superexchange and insulating ferromagnets, band magnetism in metals, local moment magnetism in metals, indirect exchange, magnetic order and the Weiss exchange field.

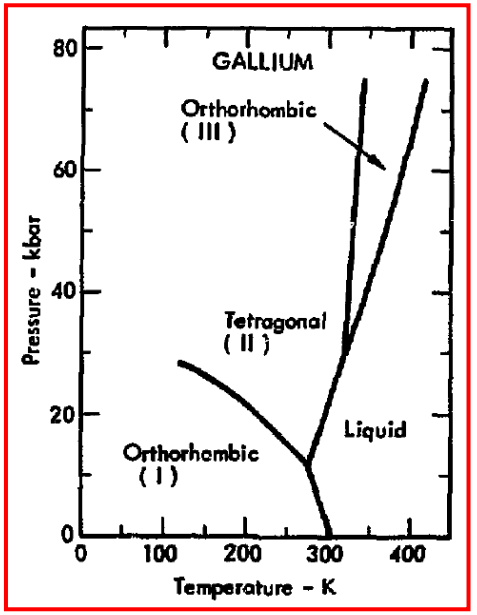
6. Fermi Liquids (2L)

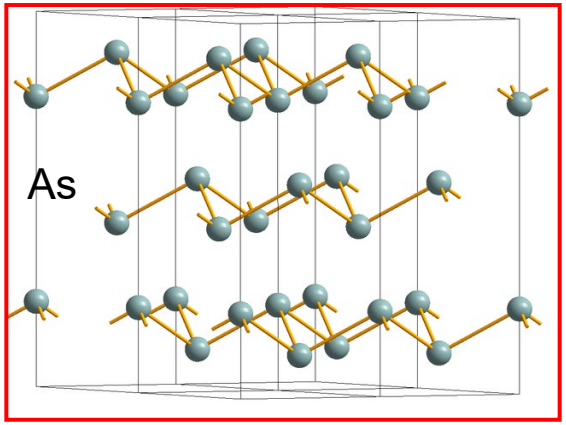
Fermi liquid theory; the problem with the Fermi gas. Liquid Helium; specific heat and viscosity. Collective excitations, adiabatic continuity, total energy expansion for Landau Fermi liquid, energy dependence of quasiparticle scattering rate.

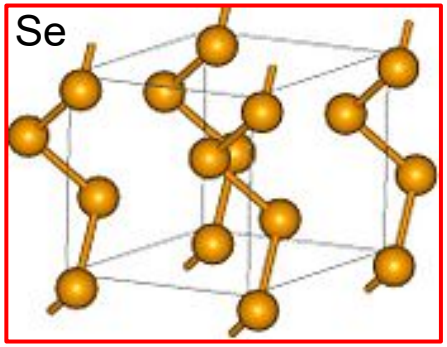
Quasiparticles and holes near the Fermi surface, quasiparticle spectral function, tuning of the quasiparticle interaction, heavy fermions, renormalised band picture for heavy fermions, quasiparticles detected by dHvA, tuning the quasiparticle interaction. $CePd_2Si_2$; heavy-fermion magnet to unconventional superconductor phase transitions.

Electronic instabilities

- Crystal structure of solids much more complex than expected
- Few solids are simple close packed structures
- e.g. Ga metal has several different phases as a function of temperature and pressure
- Se crystallises in a structure which is an array of spiral chains with 3 atoms per unit cell
- As, Sb, Bi, have puckered sheets where each atom has 3 nearest neighbours
- Due to chemical bonding and balance of forces
- Fundamental principle of bonding – by placing chemical potential in a gap, occupied states lowered in energy (and unoccupied states go up)
- Getting chemical potential to lie in a gap involves the Brillouin zone boundary being in the right place – at a momentum containing exactly the correct number of states to account for all the electrons in a solid







The Peierls Transition

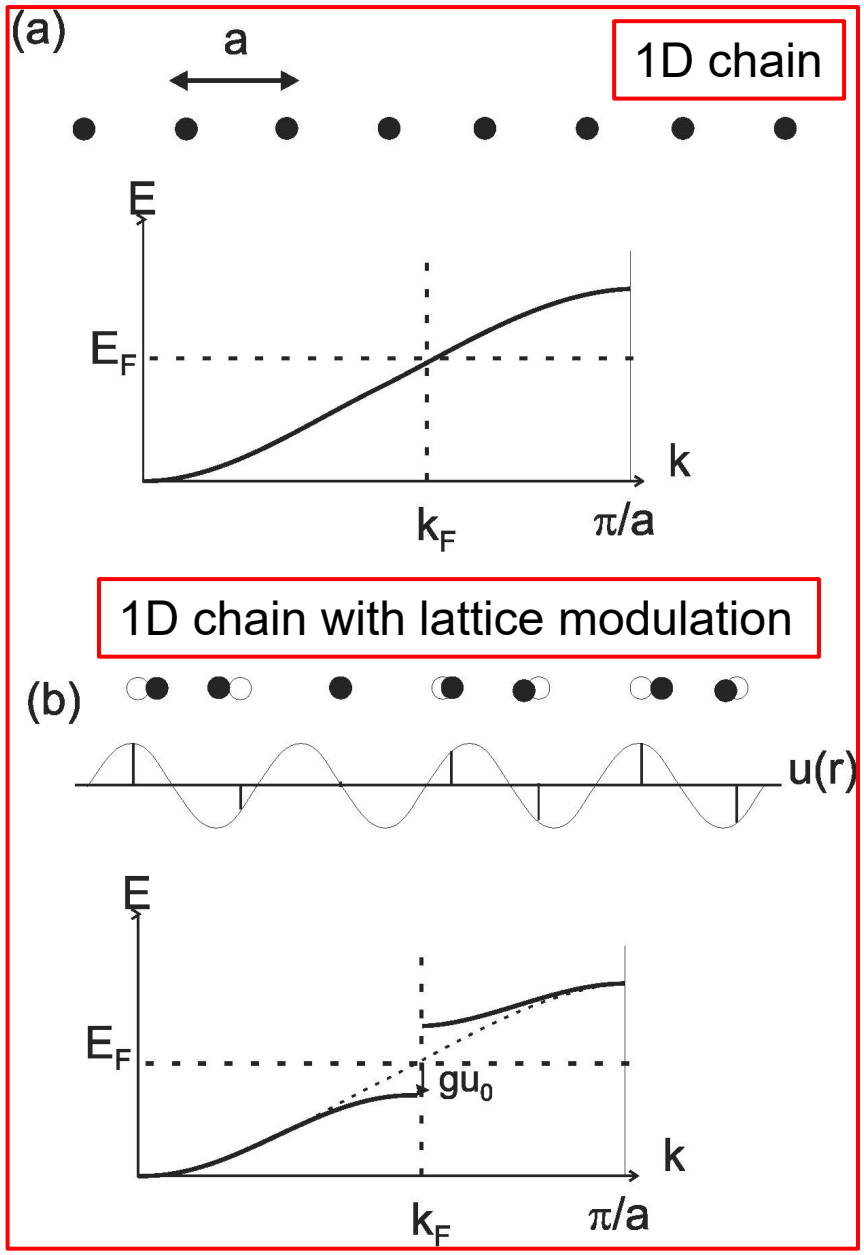
- Consider a 1D chain of atoms
- Lattice constant a, electron density chosen so the Fermi wavevector k_f lies in the middle of the band - a metal
- We can turn this metal into an insulator by applying an external potential with periodicity $2\pi / Q$ where $Q = 2k_f$
- From previous lectures we know a periodic potential $V_0 \cos Qx$ produces Bragg scattering at a wavevector $Q/2$ - a new Brillouin zone boundary
- If $Q/2 = k_f$ there is an energy gap induced on the Fermi surface
- Rather than applying an external potential we can get the same effect by making a periodic lattice distortion (PLD) with the same periodicity
- So move the n^{th} atom in the chain to a new position $R_n = na + u_0 \cos(Qna)$
- Assume the PLD amplitude is small $u_0 \ll a$
- We have already met this situation in the diatomic chain……
- If the atoms have a PLD with periodicity $2\pi / Q$ they will also produce a new potential with the same period which is seen by the electrons
- The amplitude of the Fourier components is proportional to the displacement and we can write $V_Q = g_Q u_0$ with g_Q the electron-phonon coupling constant

The Peierls Transition

- Energy gap on the zone boundary is $|V_Q|$
- Hence an energy level at a momentum just below k_f is lowered by an energy proportional to atomic displacement $|u_0|$ - the unoccupied level just above k_f is raised by the same amount
- Period chosen to be $2\pi / 2k_f$ so that a band gap of $2g_Q u_0$ is introduced at exactly the chemical potential
- Overall there is an energy lowering as a result of the PLD, the magnitude can be calculated (see problem 4.4) by adding up the energy changes of all occupied states giving in the limit $u_0 / a \ll 1$ where A is a constant:

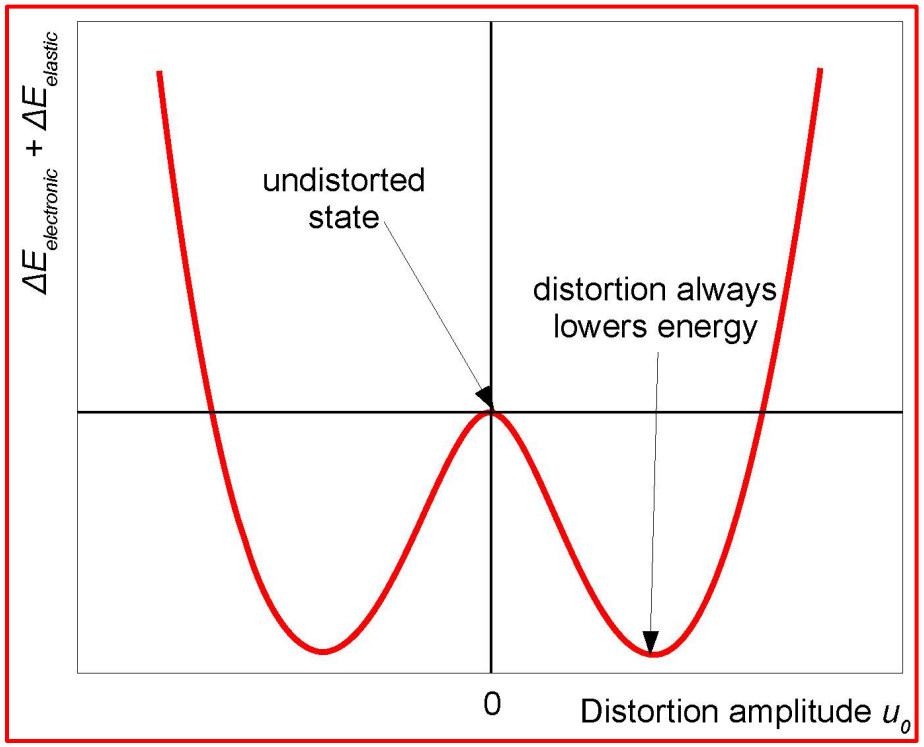
$$E_{elec} = A(u_0 / a)^2 \ln|u_0 / a|$$

- The ln varies a bit faster than the square, it is negative, the energy goes down with the distortion



The Peierls Transition

- So by an extension of the standard band structure result there is an electronic charge modulation accompanying the periodic lattice distortion
- This is usually called a charge density wave (CDW)
- The result $E_{elec} = A(u_0 / a)^2 \ln|u_0 / a|$ is just the electronic contribution to the energy from states close to the Fermi surface
- We can model other interactions between atoms as springs and we can add an elastic energy of the form $E_{Elas} = K(u_0 / a)^2$ giving a potential of the form: $E(x) = Ax^2 \ln|x| + Bx^2$
- This always has a minimum at non-zero displacement
- The system lowers its energy by distorting to produce a PLD and CDW with a period determined by the Fermi wave vector: $2\pi / 2k_f$
- This spontaneous lattice distortion is a *broken symmetry* phase transition named after its discoverer Rudolf Peierls



Charge density waves

- Materials that are strongly anisotropic in electronic structures are prone to spontaneous lattice formation and accompanying charge density wave
- Phase transitions occur on lowering T, corresponding to onset of ordering
- Can be monitored by measuring Bragg peaks in crystal structure using electron, neutron or x-ray scattering
- Figures show electron diffraction images from CDW in $La_{0.29}Ca_{0.71}Mn0_3$
- Top figure – real space shows short scale atomic lattice with periodic modulation
- Bottom figure Fourier transform – widely spaced bright peaks from small unit cell
- Less intense peaks from CDW
- Two periods not related since CDW period determined by fermi surface size and shape, depends on electron concentration

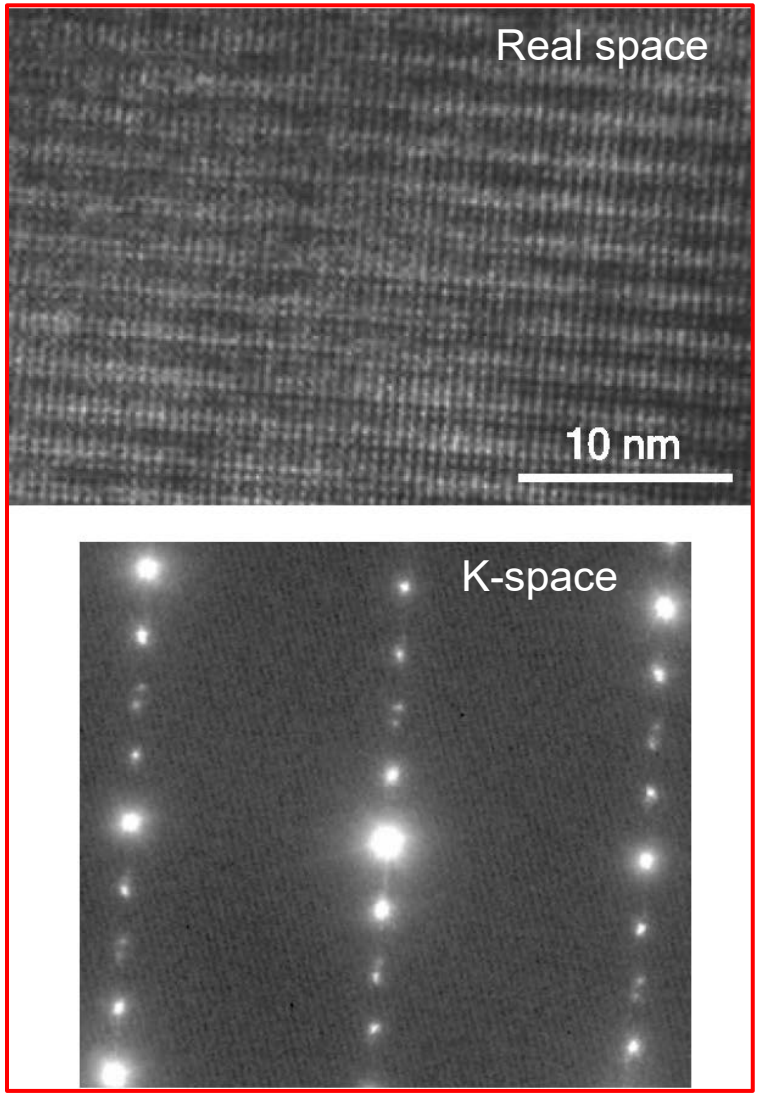
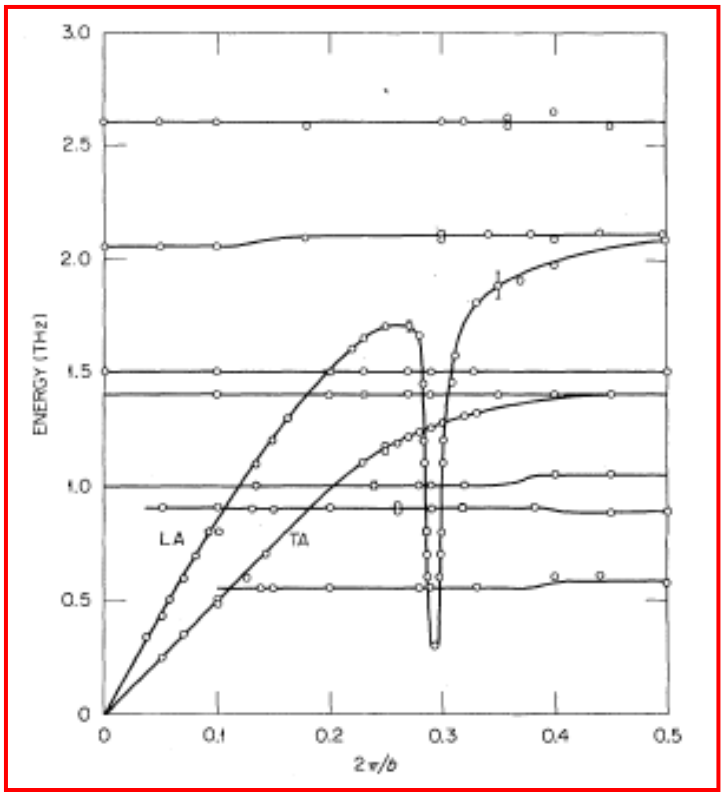


Image from J Loudon, PA Midgeley, ND Mathur

Charge density waves

- The onset of a charge density wave can be seen in the phonon spectrum
- The coefficient of the quadratic term of energy as a function of displacement gives the *phonon stiffness* for a mode of wavevector $2k_f$
- The onset of CDW is when the stiffness becomes zero (-ve below transition)
- At this point there is no restoring force and the phonon spectrum $\omega(q)$ shows a sharp minimum close to $q = 2k_f$
- Figure shows Phonon dispersion curves (measured by inelastic neutron scattering at room T) for quasi 1D organic compound TTF-TCNQ (tetrathiofulvalene tetracyanoquinone)
- Dispersion curve is along the direction of the chains in which there is a *soft phonon* that turns into a periodic lattice distortion at low temperature.
- Figure also shows many non-dispersive optical modes



H A Mook and CR Watson Phys Rev Lett **36**, 801 (1976)

Magnetism

- Defined as capacity of materials to change local magnetic field
- Not possible for classical systems in thermal equilibrium to be magnetic: Bohr-van Leeuwen theorem – see Feynman lectures volume 2
- All magnetic phenomena rooted in protection of orbital or spin angular moment afforded by quantum mechanics
- Distinguish between materials which are diamagnetic, paramagnetic or magnetically ordered
- *Diamagnetic materials* - magnetism induced is opposite to applied field, a relative permeability $\mu < 1$ and magnetic susceptibility $\chi = \mu - 1 < 0$
- Due to motion of charged quantum mechanical particles, a weak effect, negligible in many materials exhibiting paramagnetism or magnetic ordering *Examples: Bismuth* (χ = -16.6x10^{-5}), copper (χ = -1x10^{-5}), water (-9.1x10^{-6}), superconductors (-1) 'perfect' diamagnets
- Diamagnets can be levitated and held in a stable equilibrium in a strong magnet with no power consumption, total (magnetic+gravitational) energy having a minimum.
- Experiment – high water content allow a frog to be levitated in a 16T field

M V Berry and A K Geim Eur J Phys **18**, 307 (1997)

Magnetism

- *Paramagnetic materials* - magnetism induced is in direction of applied field
- Observed in systems with partially filled atomic shells or unpaired electrons. Orbital and spin angular momentum give rise to paramagnetic response significantly greater than any diamagnetic effect due to paired electrons.
- Permeability $\mu > 1$ Magnetic susceptibility $\chi > 0$
- Paramagnetic effects quite small $10^{-1} > \chi > 10^{-6}$
- Examples: Oxygen, sodium ($\chi = 7.2\text{x}10^{-6}$), aluminium ($\chi = 2.2\text{x}10^{-5}$), calcium, uranium.

Motion of liquid oxygen in a magnetic field

- As temperature is reduced in a paramagnet, below a critical value magnetic dipoles may be ordered
- *Ferromagnetism* – dipoles aligned giving a permanent magnetic field
- *Antiferromagnetism* – dipoles anti-aligned
- Magnetic ordering due to quantum mechanical exchange interaction - magnetic dipole-dipole interaction much smaller

Magnetic moments - paramagnetism

- A semiclassical description of paramagnetism (corresponds to $J = \infty$)
- Consider magnetic moments $\boldsymbol{\mu}$ at an angle θ to the applied field
- Energy $E = -\boldsymbol{\mu} \cdot \mathbf{B} = -\mu B \cos\theta$ Boltzmann factor $\exp\left(\mu B \cos\theta / k_B T\right)$
- Probability of angle between θ and $\theta + \mathrm{d}\theta$ is proportional to

$$\exp\left(\mu B \cos\theta / k_B T\right) \times \tfrac{1}{2} \sin\theta \mathrm{d}\theta$$

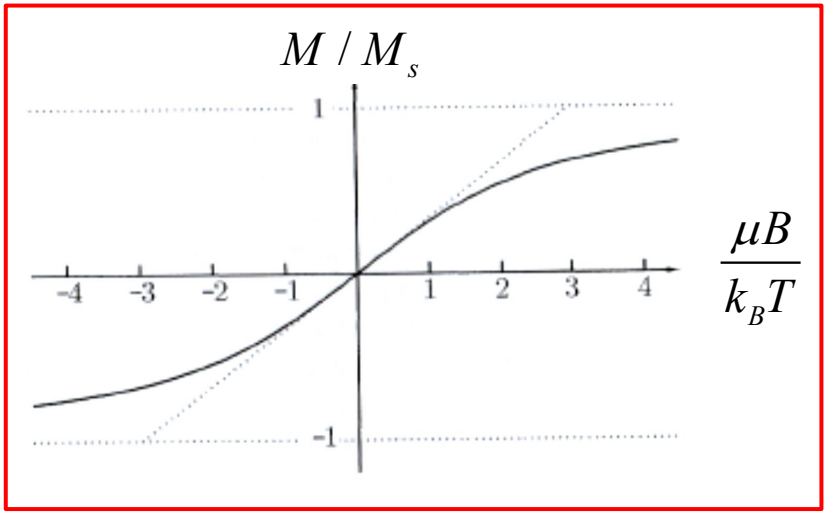
- Average moment given by:

$$\left\langle \mu_z \right\rangle = \frac{\int_0^\pi \mu \cos\theta \exp\left(\mu B \cos\theta / k_B T\right) \tfrac{1}{2} \sin\theta \mathrm{d}\theta}{\int_0^\pi \exp\left(\mu B \cos\theta / k_B T\right) \tfrac{1}{2} \sin\theta \mathrm{d}\theta} = \mu \frac{\int_{-1}^{1} x \exp(yx) \mathrm{d}x}{\int_{-1}^{1} \exp(yx) \mathrm{d}x}$$

- Where $y = \mu B / k_B T, \qquad x = \cos\theta$
- This gives the *Langevin function*

$$\frac{\left\langle \mu_z \right\rangle}{\mu} = \coth y - \frac{1}{y} = \frac{M}{M_s}$$

- The saturation magnetisation $M_s = n\mu$ occurs when all n moments per unit volume are aligned which will happen when $\mu B / k_B T >> 1$

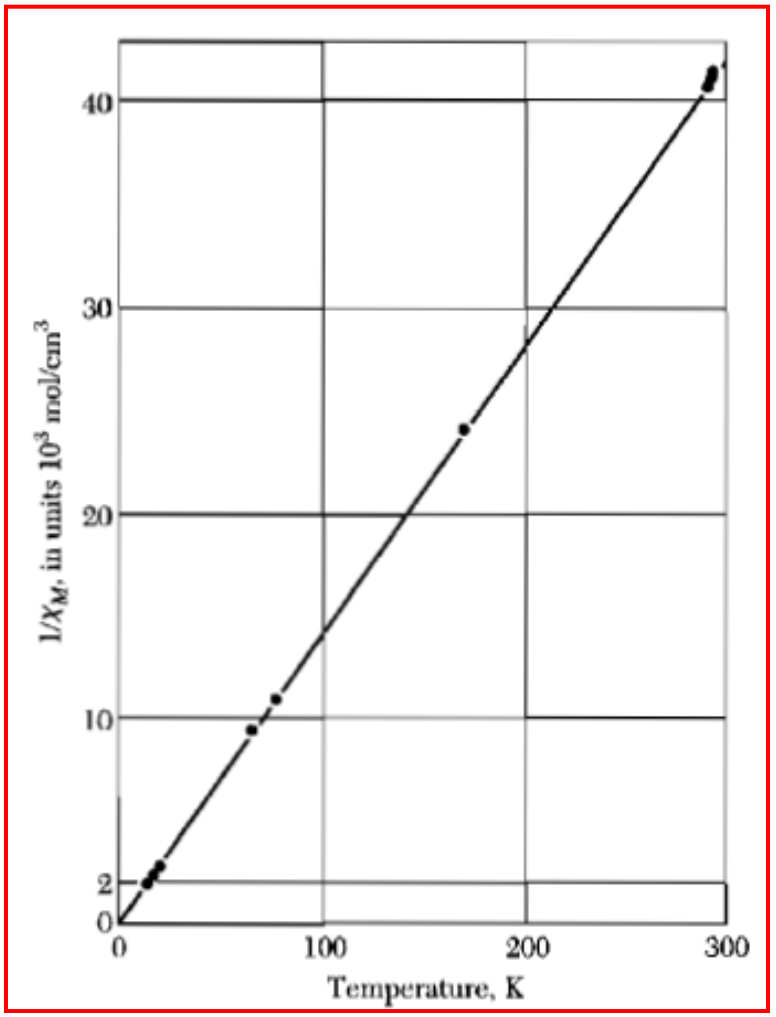


Magnetic moments - paramagnetism

- As $y = \mu B / k_B T \to 0, \qquad \coth y \simeq \frac{1}{y} + \frac{y}{3} \Rightarrow \coth y - \frac{1}{y} \simeq \frac{y}{3}$
- Hence $\frac{M}{M_s} = \frac{\langle \mu_z \rangle}{\mu} \simeq \frac{y}{3} = \frac{\mu B}{3 k_B T}$
- Since in small magnetic fields

$$\chi = M / H \approx \mu_0 M / B, \qquad M_s = n\mu$$

- We obtain $\chi = \frac{n \mu_0 \mu^2}{3 k_B T}$
- This is known as the Curie law of susceptibility, note the inverse temperature dependence.
- Figure shows χ^{-1} plotted against temperature measured for paramagnetic ions in a gadolinium salt $Gd(C_2H_3SO_4).9H_2O$
- The straight line is the Curie law



Jackson and Omnes, Leiden comm. 168a

Magnetic moments - paramagnetism

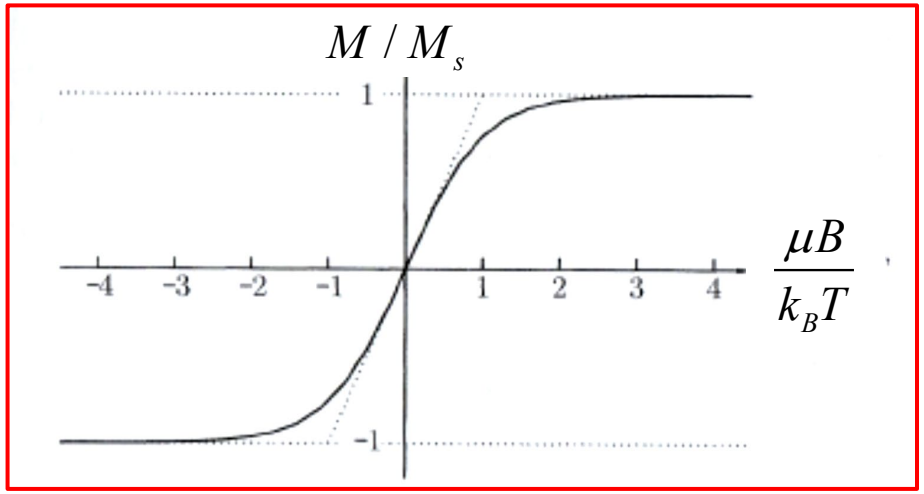
- Calculation repeated for quantum system
- Classical moments replaced by quantum spins with $J = \frac{1}{2} \Rightarrow m_J = \pm\frac{1}{2}$
- Magnetic moments $\mu_B, -\mu_B$ corresponding energies $-\mu_B B,\ \mu_B B$ assuming $g = 2$ hence:

$$\langle g\mu_B m_J \rangle = \frac{\mu_B \exp(\mu_B B / k_B T) - \mu_B \exp(-\mu_B B / k_B T)}{\exp(\mu_B B / k_B T) + \exp(-\mu_B B / k_B T)} = \mu_B \tanh\left(\frac{\mu_B B}{k_B T}\right)$$

- If $y = \mu_B B / k_B T = g\mu_B J B / k_B T \Rightarrow \frac{M}{M_s} = \frac{\langle m_J \rangle}{J} = \tanh y$

- In small fields and with

$$\tanh\left(\frac{\mu_B}{k_B T}\right) \approx \frac{\mu_B}{k_B T} \Rightarrow \chi = \frac{n\mu_0 \mu_B^2}{k_B T}$$



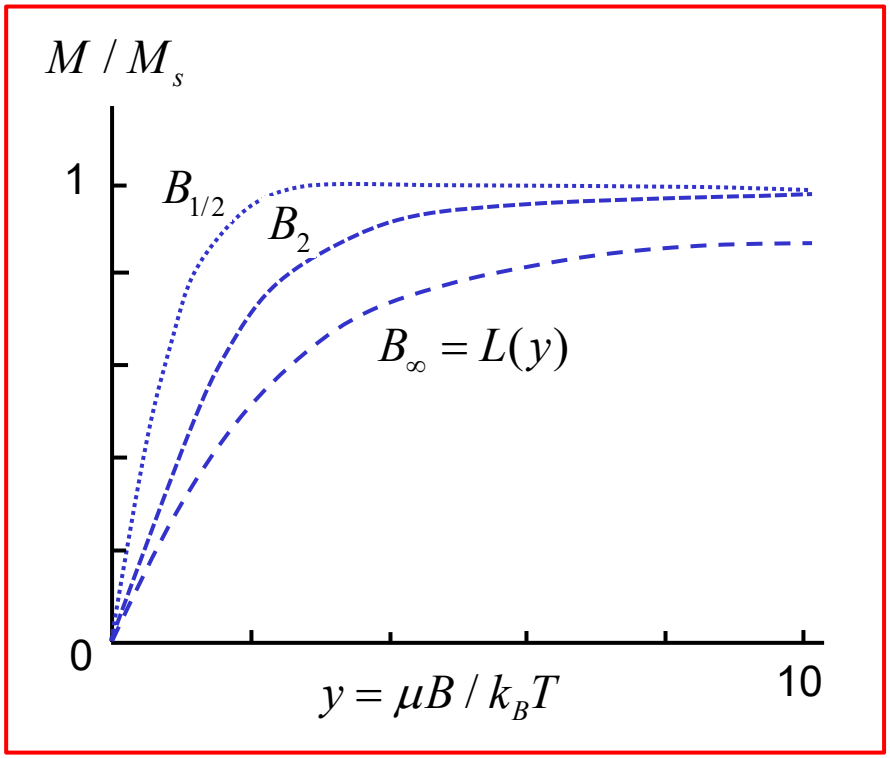
- Can be extended to the general case where J can take any integer or half integer value.

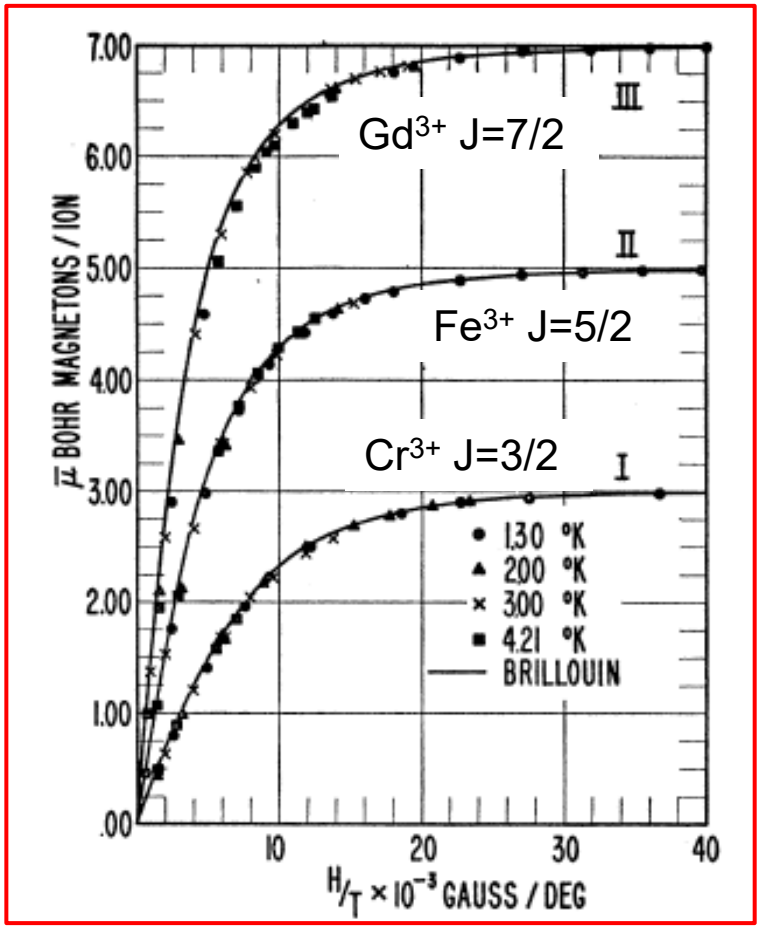
- Can also be derived using free energy – see problem sheet 4 Q6

Magnetic moments - paramagnetism

- We have looked at the semiclassical Langevin theory for $J = \infty$ and the case for $J = \frac{1}{2}$. The general solution is known as the Brillouin function

$$M / M_s = B_J(y) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}y\right) - \frac{1}{2J}\coth\left(\frac{y}{2J}\right), \qquad M_s = ng_J\mu_B J$$





W E Henry Phys Rev **88**, 559 (1952)

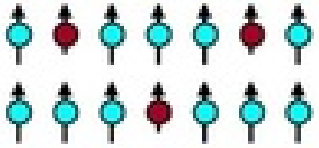
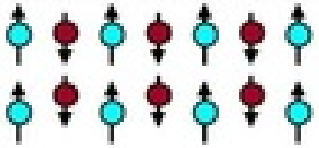
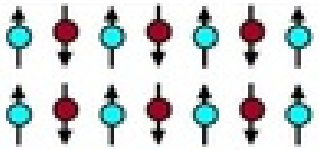
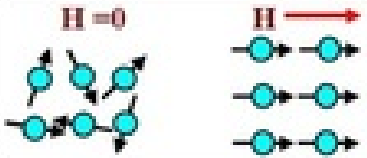
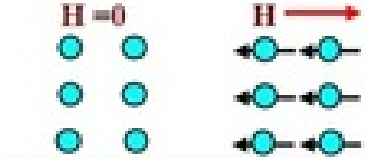
Types of magnetic interactions

- In many materials a finite magnetism is often observed in absence of magnetic field
- Must be produced by interactions coupling to electron magnetic moment
- First idea – moments couple through dipole magnetic fields
- Interaction energy of two magnetic dipoles is of order $\mu_o m^2 / 4\pi r^3$
- Using a magnetic moment of order a Bohr magnetron:

$$U_{dipolar} \approx \frac{\mu_o}{4\pi}\left(\frac{e\hbar}{2m}\right)^2 \frac{1}{r^3} \approx \pi\alpha^2\left(\frac{a_{Bohr}}{r}\right)^3 \text{Ryd.}$$

- Where $\alpha \approx 1/137$ is the fine structure constant
- At typical atomic separations of 2nm this is about $4\times10^{-5} eV$ corresponding to a temperature of less than 1K
- This is far too small to explain ordering magnetic temperatures for Co - 1388K, Fe - 1043K, Ni - 627K
- The real explanation revolves around the symmetry of wavefunctions and the Pauli exclusion principle, the large energies are due to the Coulomb interaction between electrons

Types of magnetic interactions

type	spin alignment	spin in simplified plot	examples
ferromagnetic	all spins align parallel to one another: spontaneous magnetization- $M = a + b$		Fe, Co, Ni, Gd, Dy, $SmCo_5$, Sm_2Co_{17}, $Nd_2Fe_{14}B$
ferrimagnetic	most spins parallel to one another, some spins antiparallel: spontaneous magnetization- $M = a - b > 0$		magnetite (Fe_3O_4), yttrium iron garnet (YIG), $GdCo_5$
antiferromagnetic	periodic parallel-antiparallel spin distribution: $M = a - b = 0$		chromium, FeMn, NiO
paramagnetic	spins tend to align parallel to an external magnetic field: $M = 0$ @ $H=0$, $M>0$ @ $H>0$		oxygen, sodium, aluminum, calcium, uranium
diamagnetic	spins tend to align antiparallel to an external magnetic field $M = 0$ @ $H=0$, $M<0$ @ $H>0$		superconductors, nitrogen, copper, silver, gold, water, organic compounds

Summary of Lecture 19

- Peirels transition
- Charge density waves
- Magnetism
- Local magnetic moments and paramagnetism
- Curie Law
- Types of magnetic interactions

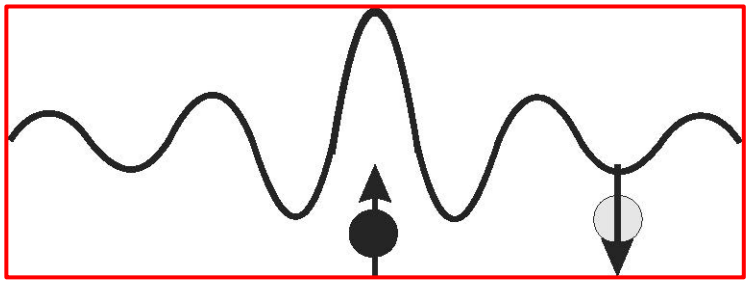
Quantum Condensed Matter Physics

Lecture 19

The End

Quantum Condensed Matter Physics

Lecture 20



David Ritchie

Quantum Condensed Matter Physics: synopsis (4)

5. Electronic instabilities (2L)

The Peierls transition, charge density waves, magnetism, local magnetic moments, Curie Law. Types of magnetic interactions; *direct exchange, Heisenberg hamiltonian, superexchange and insulating ferromagnets, band magnetism in metals, local moment magnetism in metals, indirect exchange, magnetic order and the Weiss exchange field.*

6. Fermi Liquids (2L)

Fermi liquid theory; the problem with the Fermi gas. Liquid Helium; specific heat and viscosity. Collective excitations, adiabatic continuity, total energy expansion for Landau Fermi liquid, energy dependence of quasiparticle scattering rate.

Quasiparticles and holes near the Fermi surface, quasiparticle spectral function, tuning of the quasiparticle interaction, heavy fermions, renormalised band picture for heavy fermions, quasiparticles detected by dHvA, tuning the quasiparticle interaction. $CePd_2Si_2$; heavy-fermion magnet to unconventional superconductor phase transitions.

Types of magnetic interactions – Direct exchange

- Consider two electrons in two orthogonal orbitals $|a\rangle, |b\rangle$ which are eigenstates of the single-particle Hamiltonian $\hat{H}_0$
- The electrons are indistinguishable and the two-body wavefunction is antisymmetric under particle exchange

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = -\Psi(\mathbf{r}_2, \mathbf{r}_1)$$

- The two-body antisymmetric and symmetric spatial wavefunctions can be represented by

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(|ab\rangle - |ba\rangle\right), \quad \Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(|ab\rangle + |ba\rangle\right)$$

- Where the first slot in the Dirac-ket vector is the state occupied by electron 1 and the second slot that occupied by electron 2
- Combining with symmetric and antisymmetric spin wave functions to maintain overall antisymmetry on particle exchange gives

$$\frac{1}{2}\left(|ab\rangle + |ba\rangle\right)\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right), \qquad \frac{1}{\sqrt{2}}\left(|ab\rangle - |ba\rangle\right)\begin{pmatrix} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{pmatrix}$$

- The state on the left is a spin singlet and the one on the right a spin triplet

Direct exchange

- The full Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{H}_{1,2}$,interaction part $\hat{H}_{1,2} = V(\mathbf{r}_1 - \mathbf{r}_2)$
- Introduce shorthand notation $E_0 = \langle ab | \hat{H} | ab \rangle = E_a + E_b + E_{Coul}$

$$E_{Coul} = \langle ab | \hat{H}_{1,2} | ab \rangle = \int |\psi_a(\mathbf{r}_1)|^2 |\psi_b(\mathbf{r}_2)|^2 \, V(\mathbf{r}_1 - \mathbf{r}_2) \mathrm{d}^3\mathbf{r}_1 \mathrm{d}^3\mathbf{r}_2$$

$$E_{ex} = \langle ba | \hat{H}_{1,2} | ab \rangle = \int \psi_b^*(\mathbf{r}_1)\psi_a(\mathbf{r}_1)\psi_a^*(\mathbf{r}_2)\psi_b(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \, \mathrm{d}^3\mathbf{r}_1 \mathrm{d}^3\mathbf{r}_2$$

- E_{Coul} looks like the Coulomb repulsion between charge densities, E_{ex} is of a similar form but the electrons have exchanged places
- For short range interactions such as $V = \delta(\mathbf{r}_1 - \mathbf{r}_2)$, $E_{Coul} \to E_{ex}$
- Singlet state energy is $E_s = \frac{1}{2}\langle ab + ba | \hat{H} | ab + ba \rangle = E_0 + E_{ex}$
- Triplet state energy is lower $E_t = \frac{1}{2}\langle ab - ba | \hat{H} | ab - ba \rangle = E_0 - E_{ex}$
- There is a spin dependant effective interaction in this system.
- The interaction arises because the electrons are constrained to single occupancy of the two orbitals allowing spin flips as the only degree of freedom

Direct exchange

- This simple example reflects a general phenomenon
- The spin triplet is symmetric under electron exchange, its associated spatial wavefunction must be antisymmetric to maintain overall antisymmetry.
- An antisymmetric spatial wavefunction must have nodes when two spatial coordinates are equal i.e. $\psi(....,r_i = r,...r_j = r,...) = 0$
- Hence the particles stay further apart in an antisymmetrised spatial state than in an symmetric state
- This reduces the effect of the repulsive Coulomb interaction
- Thus the combination of the Pauli principle and Coulomb repulsion means that states with antisymmetric spatial states (symmetric spin states which generally have high spin) have lower energy.
- When the orbitals are orthogonal, E_{ex} is positive and the lowest energy state contains the triplet spin state
- If the overlapping orbitals are not orthogonal – as happens for orbitals in neighbouring atoms the interaction *may* be negative and the singlet spin state lowest in energy – an example is molecular hydrogen
- The involvement of the Coulomb interaction explains the high ordering temperatures in Ferromagnetism

Heisenberg Hamiltonian

- We can express the spin-dependant interaction between the electrons in terms of their spin states $\hat{S}_1,\ \hat{S}_2$
- Triplet and singlet states differ in the expectation value of the magnitude of total spin $\hat{S} = \hat{S}_1 + \hat{S}_2$
- The eigenvalue for $\hat{S}^2$ in a spin state S is given by $S(S+1)$
- We can differentiate between singlet and triplet states:

$$\hat{S}^2 = \left(\hat{S}_1 + \hat{S}_2\right)^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1 \cdot \hat{S}_2 = \frac{3}{2} + 2\hat{S}_1 \cdot \hat{S}_2$$

  where for a spin-half state $\hat{S}_i^2 = \frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{3}{4}$
- So for the singlet state $S = 0$ and the eigenvalue of $\hat{S}_1 \cdot \hat{S}_2$ is $-\frac{3}{4}$
- For the triplet state $S = 1$ and the eigenvalue of $\hat{S}_1 \cdot \hat{S}_2$ is $+\frac{1}{4}$
- We can write the spin Hamiltonian as

$$\hat{H}_{spin} = \frac{1}{4}(E_s + 3E_t) - (E_s - E_t)\hat{S}_1 \cdot \hat{S}_2$$

- Where $E_s,\ E_t$ are the energies of the singlet and triplet states
- Defining $J = (E_s - E_t)/2$ and shifting the zero of energy: $\hat{H}_{spin} = -2J\hat{S}_1 \cdot \hat{S}_2$
- Model favours parallel spins if $J > 0$, antiparallel spins if $J < 0$

Heisenberg Hamiltonian

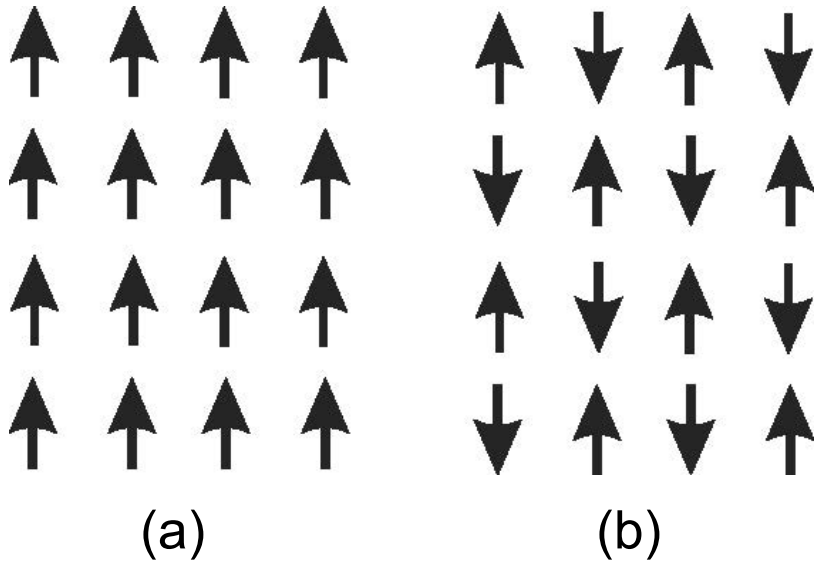
- From the previous slide

$$\hat{H}_{spin} = -2J\hat{S}_1 \cdot \hat{S}_2$$

- We can extend this to cover a collection of spins through the Heisenberg model

$$\hat{H}_{Heisenberg} = -\sum_{ij} J_{ij}\hat{S}_i \cdot \hat{S}_j$$

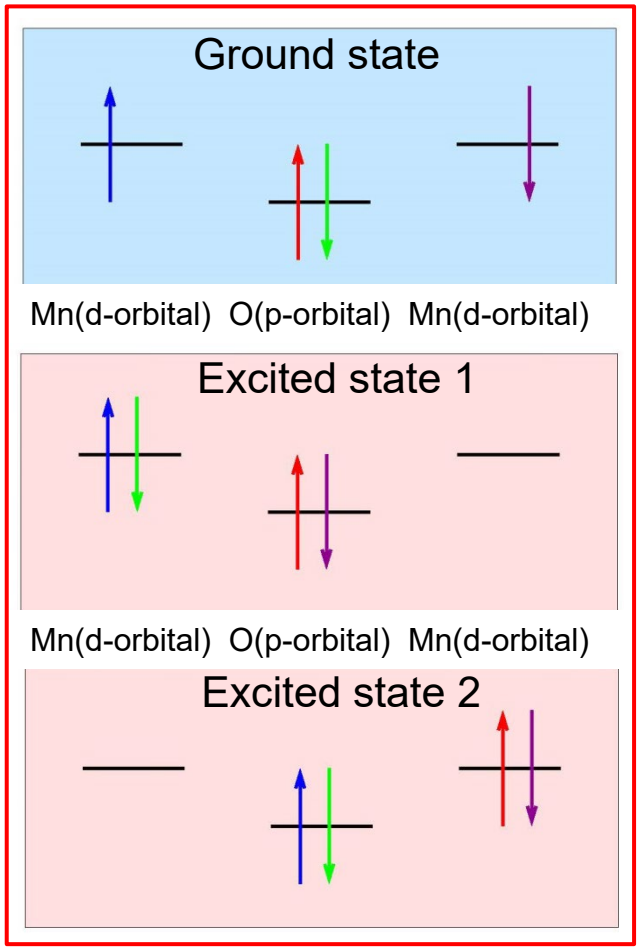
- This takes into account pairwise interactions between the total spins on neighbouring atomic sites $\hat{S}_i, \hat{S}_j$
- The coupling only depends on the relative orientation of the spins and not their direction relative to the crystal
- If the angular momentum of an ion contains both orbital and spin parts, the spin Hamiltonian will include a term that depends on the absolute spin direction



The diagram above shows the ground state of the Heisenberg model for:
(a) A ferromagnet with aligned spins corresponding to $J_{ij} > 0$
(b) An antiferromagnet with anti-aligned spins on neighbouring sites corresponding to $J_{ij} < 0$

Superexchange and insulating antiferromagnets

- With strong overlap between orbitals (covalent bond), advantageous for the system to form fully occupied hybridised molecular orbitals. Singlet state has far lower energy than triplet state and system has no magnetic character
- But - weaker interactions can be important e.g. 2 magnetic moments (Mn) separated by a non magnetic ion (often O^{2-}) in an insulator such as MnO
- Direct exchange is not important - too far apart
- Ground state - each magnetic ion is singly occupied, non-magnetic ion doubly occupied
- If the 2 spins on O^{2-} are anti-parallel, it is possible for an electron to hop onto one of the Mn ions and be replaced by an electron from the other Mn
- The excited state created can be admixed to the initial ground state and will, by 2nd order perturbation theory, cause the new, perturbed ground state energy to be lowered
- The admixture is not possible if the 2 magnetic moments were aligned, hence the ground state depends on orientation of 2 magnetic moments

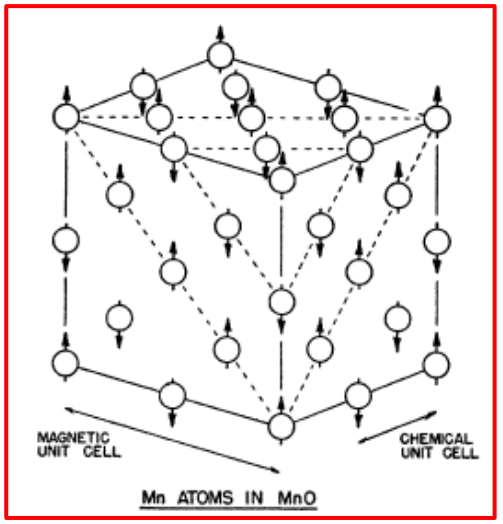


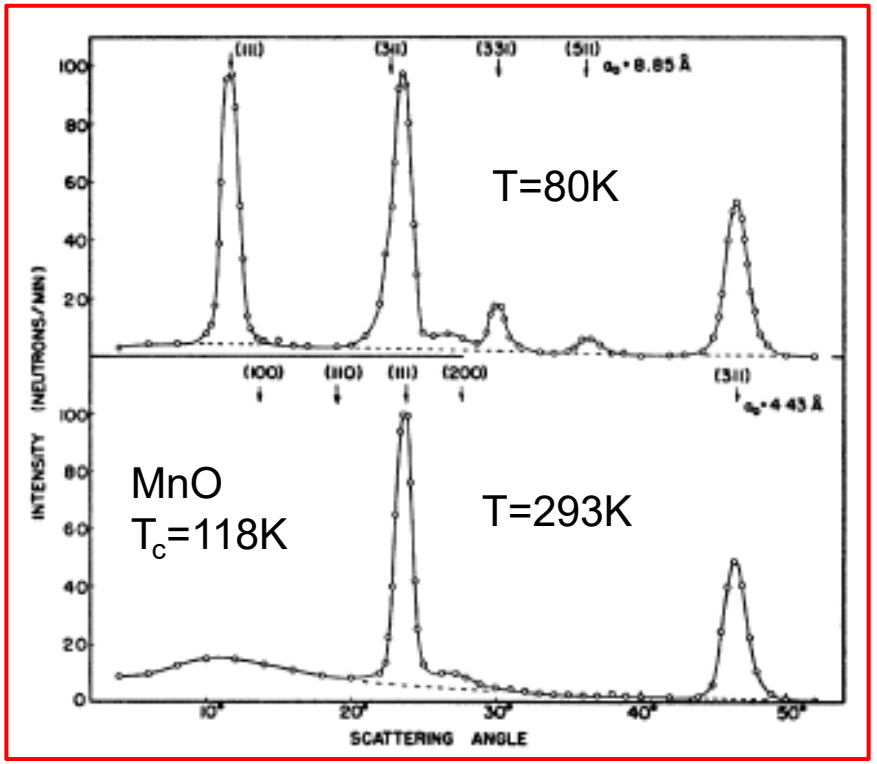
Superexchange and insulating antiferromagnets

- Second order perturbation theory suggests that this *superexchange* interaction is of order $J \sim -t^2 / U < 0$ where t is the matrix element governing hopping between the magnetic moment (Mn) and the non magnetic ion (O). U is the Coulomb repulsion energy on the magnetic moment
- When extended to a lattice it favours an antiferromagnetic state in which alternate sites have antiparallel spins
- On complicated lattices, very complex arrangements of spins can result
- The magnitude of this interaction is often quite small, from a few K to a few hundred K.
- This system will often exhibit phase transitions from a magnetic ordered state to a disordered paramagnetic state at room temperature or below

Magnetic order in MnO – Neutron scattering

- Neutron magnetic moments can couple to atomic magnetic moments
- Amplitude of scattering depends on direction of atomic moment so arrangement in crystal can be determined.
- At 293K two peaks are seen due to different nuclear scattering for Mn and O ions in FCC lattice – confirms structure determined by x-ray diffraction
- Below 118K no change in nuclear scattering peaks but additional peaks due to Mn magnetic moment alignment
- In crystal (111) planes of Mn spins point in the same direction which reverses in adjacent (111) planes
- The magnetic unit cell is double the size of the chemical unit cell
- Amplitude of peaks can be used to determine magnetic order as a function of temperature





Shull et al Phys Rev B **83**, 333 (1951)

Band magnetism in metals

- Pauli paramagnetism is the response of a metal to a magnetic field
- We have a Fermi gas with energy dispersion $\epsilon_{\mathbf{k}}$ in magnetic field $B_a = \mu_0 H$
- spin up and spin down will be split by the Zeemen effect

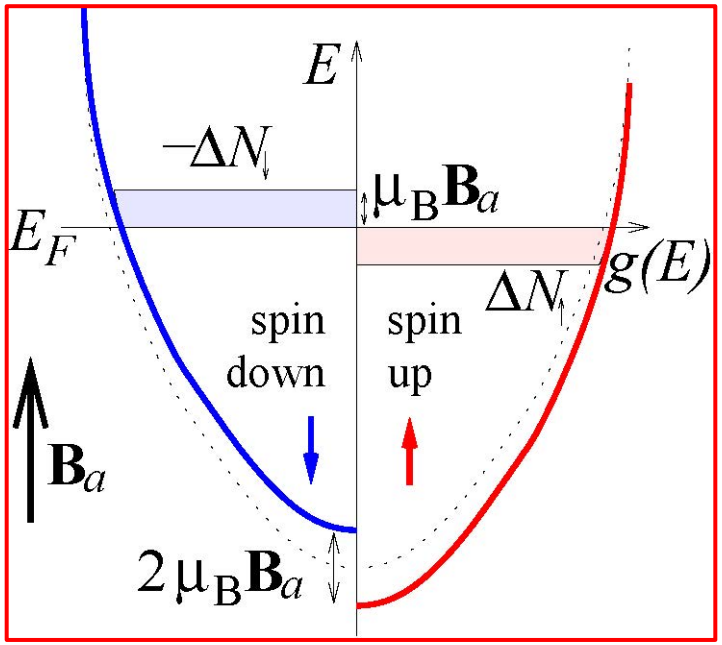
$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}} - \mu_B B_a \,, \qquad \epsilon_{\mathbf{k}\downarrow} = \epsilon_{\mathbf{k}} + \mu_B B_a$$

- The chemical potential (and E_F) is the same for both spins so there is a transfer of carriers from the minority spin band to the majority spin band
- This produces a population imbalance between the 2 spin species:

$$n_\uparrow - n_\downarrow = \mu_B B_a g_v(E_F)$$

- Where $g_v(E_F)$ is the density of states at the Fermi level per unit volume
- We assume that the splitting is small enough so the DoS is constant
- Magnetisation is $M = \mu_B(n_\uparrow - n_\downarrow)$ and $B_a = \mu_0 H$ giving static spin susceptibility:

$$\frac{M}{H} = \chi_\sigma = \mu_0 \mu_B^2 g(E_F)$$



Band magnetism in metals

- From the last slide the Pauli susceptibility is $\chi_\sigma = \mu_0 \mu_B^2 g(E_F)$
- We compare this result to the Curie law susceptibility obtained from local moments obtained before $\chi(T) = \frac{1}{3}\mu_0 \mu^2 \frac{N}{V}\frac{1}{k_B T}$
- The Curie law susceptibility is strongly temperature *dependent*
- The Pauli susceptibility is largely temperature *independent* – particularly at low temperatures where the thermal broadening of the Fermi distribution is not important
- Similarities – both depend on the square of the fluctuating moment and both have an energy scale in the denominator – given that $g(E_F) \simeq \frac{N}{V}\frac{1}{E_F}$
- For Curie law energy scale is thermal energy $k_B T$
- For Pauli susceptibility energy scale is the Fermi energy E_F
- From a different angle – remember that when calculating the electronic specific heat, only a fraction $k_B T / E_F$ contribute to the specific heat
- Here we argue that this fraction of electrons can act like local moments, multiplying the Curie law by the fraction $k_B T / E_F$ transforms it (to a constant of order 1) into the Pauli susceptibility for metals

Band magnetism in metals

- Now to include interactions
- The Stoner-Hubbard model includes an energy penalty U for lattice sites that are doubly occupied – those holding both an up- and down-spin electron

$$\hat{H}_{int} = \sum_{sitesi} U n_{i\uparrow} n_{i\downarrow}$$

- Treating this interaction as a mean-field approximation we get a shift in the energies of the two spin bands

$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}} + U\overline{n}_{\downarrow} - \mu_0\mu_B H, \qquad \epsilon_{\mathbf{k}\downarrow} = \epsilon_{\mathbf{k}} + U\overline{n}_{\uparrow} + \mu_0\mu_B H$$

- So the presence of spin-down electrons increases the energy of spin-up electrons in the same way as a magnetic field pointing down would
- The interactions between electrons appears in the same way as an additional magnetic field
- This is called an *exchange field*, it is not physical in the sense that it could deflect a compass needle, it is a 'book-keeping' device to handle the effects of the Coulomb interaction between electrons

Band magnetism in metals

- Using the same approximation as before – the DoS is taken to be a constant, we determine the average spin density

$$\frac{N}{V}(\bar{n}_\uparrow - \bar{n}_\downarrow) = [U(\bar{n}_\uparrow - \bar{n}_\downarrow) + 2\mu_0\mu_B H]\frac{1}{2}g_v(E_F)$$

- The magnetisation is $M = \mu_B(n_\uparrow - n_\downarrow)$ which then gives us the static spin susceptibility

$$\chi_\sigma = \mu_0 \frac{\mu_B^2 g(E_F)}{1 - \frac{Ug(E_F)}{2}}$$

- In this expression g is the density of states per atom, in contrast to $g_v = \frac{N}{V}g$ which is density of states per unit volume.
- In comparison to the non-interacting state the magnetic susceptibility is enhanced and will diverge if U is large enough so the Stoner criterion is satisfied:

$$Ug(E_F)/2 > 1$$

- This marks the onset of Ferromagnetism in this model

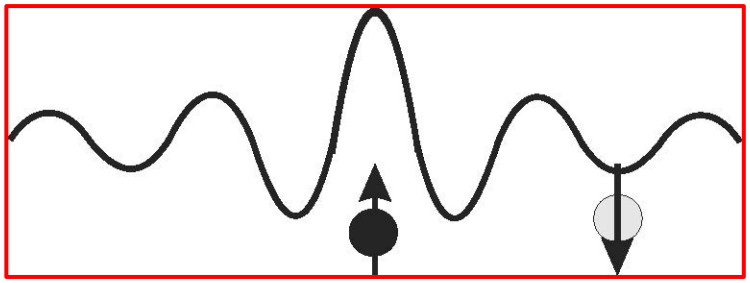
Band magnetism in metals

- The Stoner criterion for ferromagnetic order $Ug(E_F)/2 > 1$ has a fundamental interpretation
- Because the density of states per atom is of order $1/E_F$ the Stoner criterion expresses the balance between the interaction energy U and the kinetic energy E_F
- If the kinetic energy of the electrons is high, they will not form a magnetically ordered state
- If the interaction strength is higher than the kinetic energy the electron system can lower its energy by aligning its spins
- Variations on this criterion appear in many other areas of correlated electron physics

Local moment magnetism in metals – indirect exchange

- In a d-band metal such as iron or f-band metals such as gadolinium or erbium there are both localised electrons with a moment derived from the tightly bound orbitals as well as itinerant electrons from the sp bands
- The itinerant bands are only weakly spin-polarised, if at all because the exchange interactions are small and the kinetic energy large
- But – the itinerant electrons acquire an induced spin polarisation due to its interaction with the core spins on one atom
- This spin polarisation can be transmitted to a neighbouring ion where it attempts to align the neighbouring spin
- There is then an interaction between the localised electron spins which is mediated by itinerant electrons - often called RKKY

In metals, a local moment will polarise the conduction electron spins, producing a spin density that decays with distance and oscillates in sign with period $1/2k_F$. The interaction of the induced spin density with a neighbouring local moment produces the RKKY interaction.



Magnetic order and the Weiss exchange field

- An alternative approach to the problem of magnetism could start with a phenomenological equation of state, linking magnetism and magnetic field

$$H = aM + bM^3$$

  where we neglect the vector nature of H, M

- In this equation of state, a takes the role of the inverse susceptibility $\chi^{-1} = dH / dM$ and b ensures that the magnetisation bends over towards saturation for high fields
- For a materials to be ferromagnetic, we require a finite M, a remanent magnetisation, even for zero H.
- This appears to be possible only if a is negative
- But - systems of non-interacting electrons do not exhibit a negative susceptibility – the Curie law for isolated moments gives $a \propto T$
- In metals the Pauli susceptibility is positive and only very weakly temperature dependant – so we need to introduce a further term which captures the effect of interactions between the electrons
- The simplest way to incorporate these interactions is to introduce an *exchange molecular field*, h into the equation of state

$$H + h = aM + bM^3$$

Magnetic order and the Weiss exchange field

- The exchange molecular field, h is not a real magnetic field (which could deflect a compass needle….etc)
- It represents, using a *mean field* technique the effect of the exchange interaction produced by many electrons on a particular test electron
- We assume that the exchange field is proportional to the overall magnetisation with constant of proportionality λ, this is known as the *Weiss molecular field concept*
- We arrive at a feedback equation:

$$H + \lambda M = aM + bM^3$$

- This can be re-written in the form of the original equation of state with a modified linear coefficient $a^* = a - \lambda$ as:

$$H = (a - \lambda)M + bM^3 = a^* M + bM^3$$

- Although the non-interacting susceptibility is finite, interactions between the electrons give a feedback effect which boosts the magnetic susceptibility

$$\chi = 1/a^* = 1/(a - \lambda) = \chi_0/(1 - \lambda\chi_0)$$

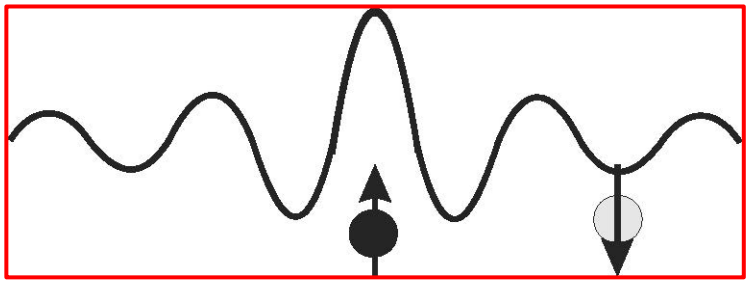
- Where $\chi_0 = 1/a$ is the non-interacting susceptibility.
- This leads to a magnetic instability if $\lambda\chi_0 > 1$ which is a more general form of the Stoner criterion

Summary of Lecture 20

- Types of magnetic interactions
- Direct exchange
- Heisenberg hamiltonian
- Superexchange and insulating ferromagnets
- Band magnetism in metals
- Local moment magnetism in metals – indirect exchange
- Magnetic order and the Weiss exchange field

Quantum Condensed Matter Physics

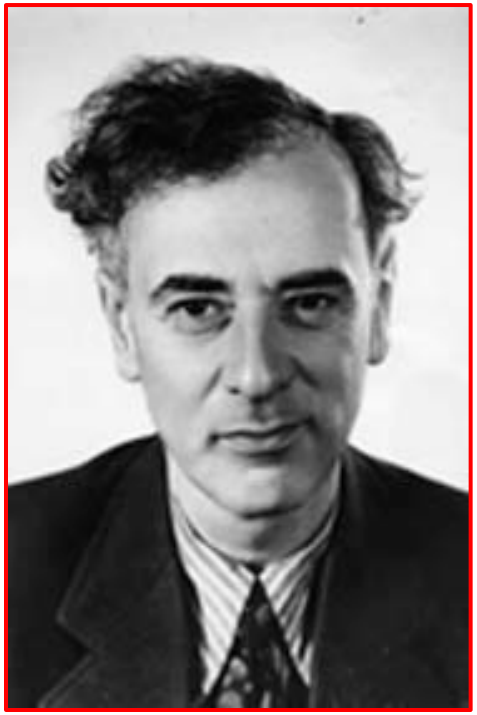
Lecture 20



The End

Quantum Condensed Matter Physics

Lecture 21



David Ritchie

Quantum Condensed Matter Physics: synopsis (4)

5. Electronic instabilities (2L)

The Peierls transition, charge density waves, magnetism, local magnetic moments, Curie Law. Types of magnetic interactions; direct exchange, Heisenberg hamiltonian, superexchange and insulating ferromagnets, band magnetism in metals, local moment magnetism in metals, indirect exchange, magnetic order and the Weiss exchange field.

6. Fermi Liquids (2L)

Fermi liquid theory; the problem with the Fermi gas. Liquid Helium; specific heat and viscosity. Collective excitations, adiabatic continuity, total energy expansion for Landau Fermi liquid, energy dependence of quasiparticle scattering rate.

Quasiparticles and holes near the Fermi surface, quasiparticle spectral function, tuning of the quasiparticle interaction, heavy fermions, renormalised band picture for heavy fermions, quasiparticles detected by dHvA, tuning the quasiparticle interaction. $CePd_2Si_2$; heavy-fermion magnet to unconventional superconductor phase transitions.

Fermi liquid theory – the problem with the Fermi gas

- Up to now our modelling of electrons in solids has been fairly simple-minded
- We *have not* looked for eigenstates of many particle systems.
- We *have* calculated the eigenstates of single particle Hamiltonians (subject to a periodic lattice potential, filled these states with electrons, treating our system as a degenerate Fermi gas
- This separation of a many particle problem into single-particle states relies on being able to separate the many-body wavefunction into an antisymmeterised product of single particle wavefunctions
- e.g. for a two-particle wavefunction:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}\left(\psi_{\mathbf{a}}(\mathbf{r}_1)\psi_{\mathbf{b}}(\mathbf{r}_2)-\psi_{\mathbf{a}}(\mathbf{r}_2)\psi_{\mathbf{b}}(\mathbf{r}_1)\right)$$

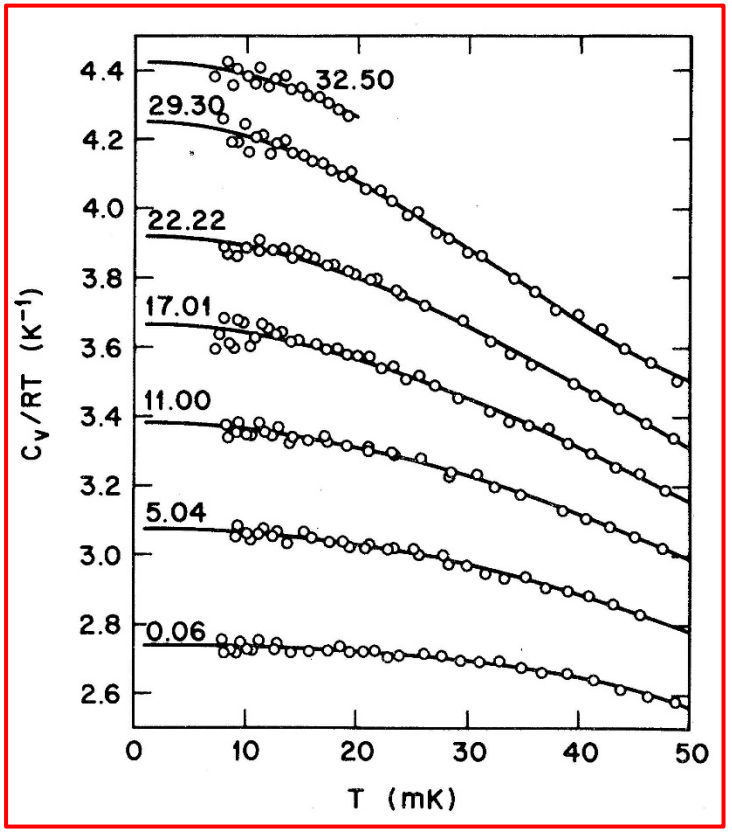
- These product states ignore correlations between electrons – we find that the expectation values of products such as $\langle \mathbf{r}_1\mathbf{r}_2 \rangle$ decompose into the products of expectation values $\langle \mathbf{r}_1 \rangle \langle \mathbf{r}_2 \rangle$
- In the presence of strong electron-electron interactions the electron motion must be correlated
- For example in the Thomas Fermi approximation, the electrons in a Fermi gas react to the introduction of a charged impurity so as to screen the impurity at long distances

Fermi liquid theory – the problem with the Fermi gas

- Taking this to the next level – for any electron the other electrons in a metal execute a correlated screening motion, reducing their density in the vicinity of the first electron
- This will reduce the electron density on the vicinity of the first electron and reduces the effective range of the Coulomb potential due to the first electron and implies that the electrons undergo correlated motion…..
- But – correlations are not included in the single particle picture
- The band structure approach has been very successful explaining many properties of materials – transport properties, thermodynamic properties such as the heat capacity, semiconductors, quantum oscillations etc etc
- The extreme case of ^{3}He at low temperatures is an illustration of this…..

Liquid Helium 3 – specific heat

- The isotopes of ^{4}He (bosons) and ^{3}He(fermions) do not solidify down to zero temperature unless placed under significant pressure (around 33bar)
- This is caused by very weak mutual interaction and low mass boosting quantum mechanical zero point motion.
- They are examples of quantum fluids and ^{3}He is an uncharged analogue of electrons in solids
- Because of hard-core repulsion at small separation and weak Van der Waals interaction, picture helium atoms at low T as a close-packed assembly of hard spheres - not a solid but clearly strongly correlated
- Measurements of all key properties show good agreement with Fermi gas theory
- e.g. the molar heat capacity of a degenerate fermi gas $C_m / T \to const$ at low temperatures – just as found in ^{3}He
- Figure shows measurements of heat capacity of ^{3}He at low temperatures for different pressures



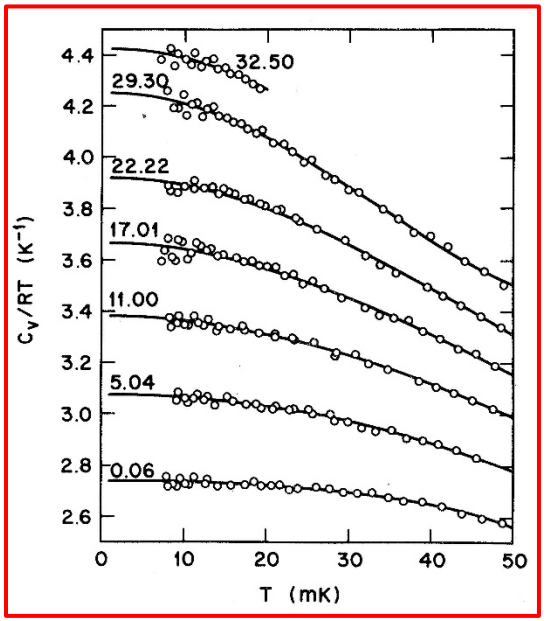
Greywall Phys Rev B **27**, 2747 (1983)

Liquid Helium 3 – specific heat

- Looking more closely – while the general form of the heat capacity and other properties – thermal conductivity, viscosity are the same as a Fermi gas the detailed prefactors may be different
- In a Fermi gas as we saw earlier in the course the specific heat

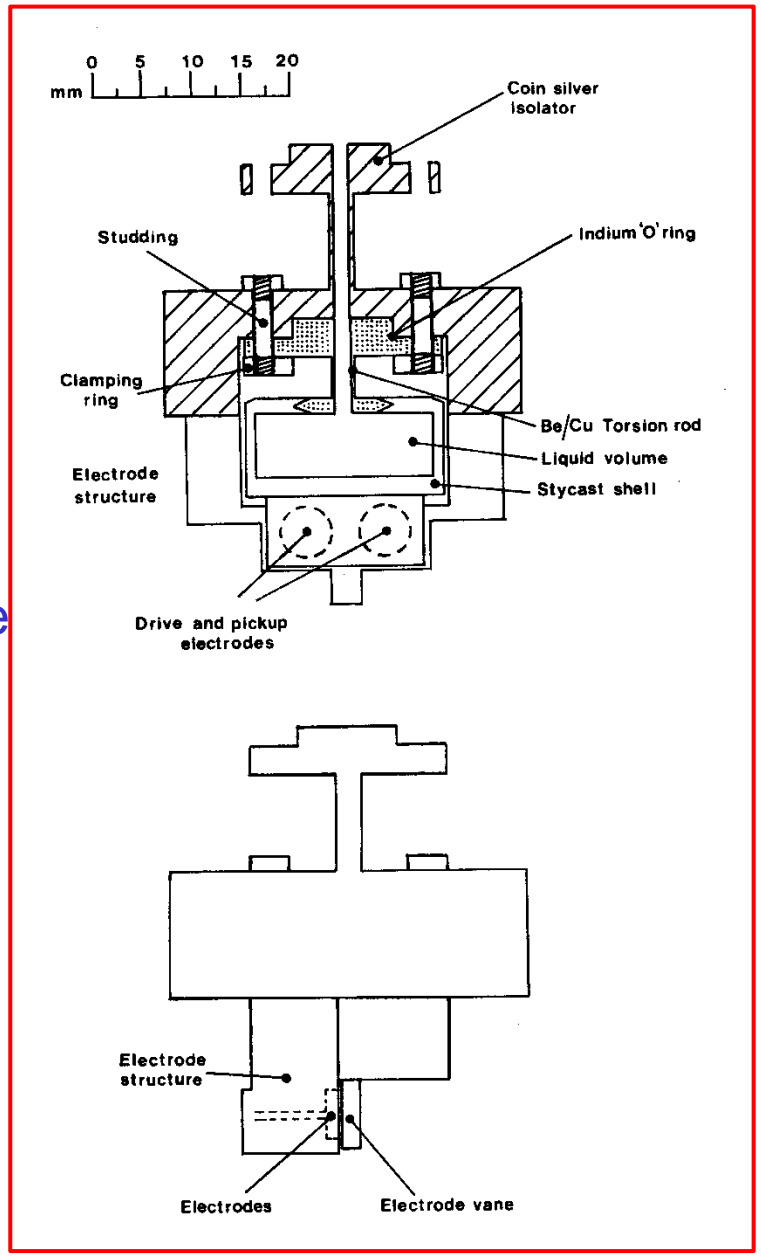
$$c_v = \frac{\pi^2}{2}\frac{T}{T_F}nk_B, \quad T_F = \frac{E_F}{k_B} = \frac{\hbar^2}{2mk_B}\left(3\pi^2 n\right)^{2/3}$$

- where T_F is the Fermi temperature – which is determined by the number density, n, and mass, m, of the particles
- The specific heat per mole, C_m is given by $C_m / T \simeq \frac{\pi^2}{2}\frac{R}{T_F}$ where R is the gas constant
- These equations predict an increase in T_F with increasing pressure as the number density n rises
- Gives a reduction in C_m / T with increasing pressure
- Opposite to dependence observed in experiments
- 'Explained' by change in *effective mass* of ^{3}He atoms from $2.76m_3$ at low pressure to $5.65m_3$ at 33 bar
- Changes in m_3^* with pressure larger than in dilute mixtures of ^{3}He in ^{4}He (L3) – greater interactions



Liquid Helium - viscosity

- Torsional oscillator measurements of liquid helium viscosity
- Cylindrical volume filled with liquid helium, hanging from hollow torsion rod
- Oscillation about vertical axis, motion damped by liquid helium
- Frequency 2kHz, background Q factor >10^5
- Oscillator driven by voltage applied to fixed electrode, motion detected by measuring voltage on second electrode (oscillator vane at constant 400V)
- Driven at peak of resonance with constant amplitude (10-100nm) of motion, drive voltage required $\propto$ dissipation
- Experiment mounted on ^{3}He/^{4}He dilution refrigerator. Measurements over a temperature range 3mK-1K
- Period and dissipation measured as a function of T



Liquid Helium - viscosity

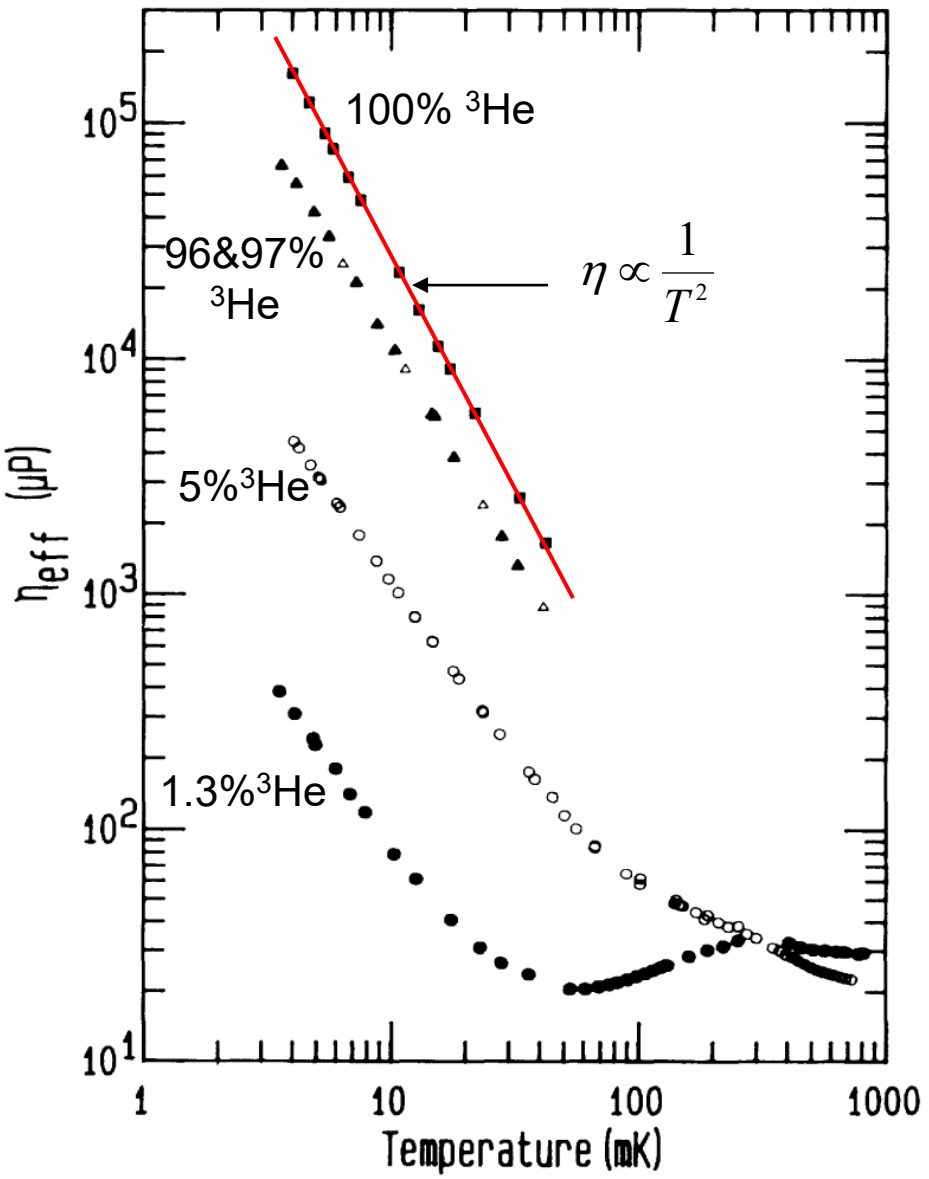
- From kinetic theory, viscosity

$$\eta = \frac{1}{3} n m v_f \lambda$$

- Number density n, mass m Fermi velocity v_f, mean free path $\lambda = v_f \tau_\eta$ between collisions where τ_η is the quasiparticle viscosity scattering time
- For gas or liquid of fermions, scattering time

$$\tau_\eta \propto \frac{1}{T^2} \Rightarrow \eta \propto \frac{1}{T^2}$$

- Correct temperature dependence observed for pure ^{3}He
- Mixtures of ^{3}He and ^{4}He don't give correct T dependence due to surface effects
- Internal dimensions of oscillator $\gg \lambda$



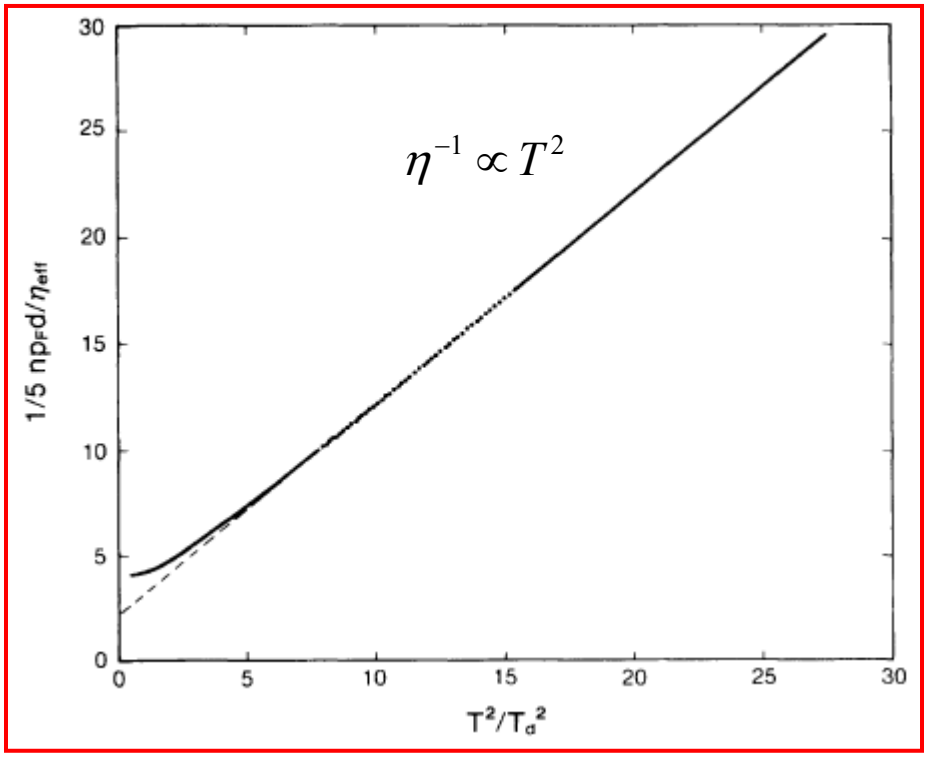
Ritchie et al Phys Rev Lett **59**, 466 (1987)

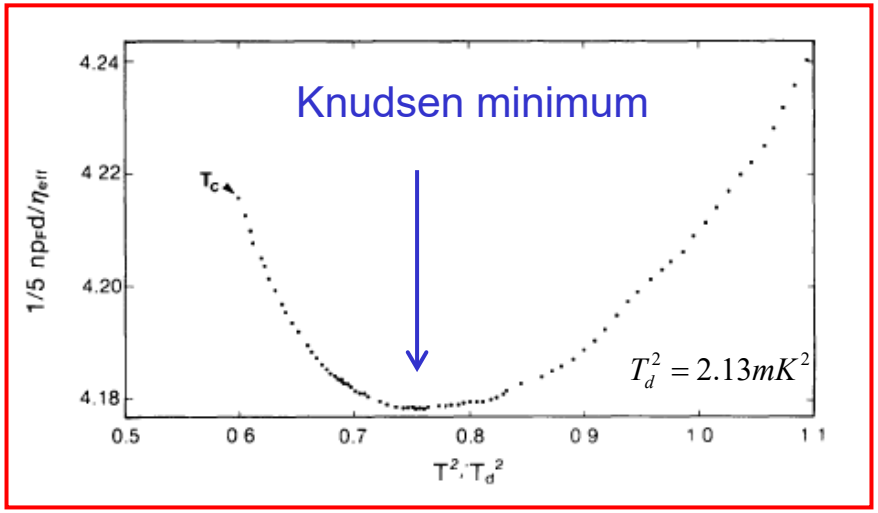
^{3}He – viscosity mean free path

- So what happens if we reduce internal dimensions of oscillator?
- Height reduced from 6mm to 45μm
- Inverse viscosity plotted vs T^2
- Linear as expected but deviation from linearity at lowest T
- Passes through minimum at a temperature of 1.26mK before passing through superfluid transition at 1.13mK
- Minimum in inverse viscosity is signature of mean free path being equal to size of oscillator so

$$\lambda \approx 45\,\mu m$$

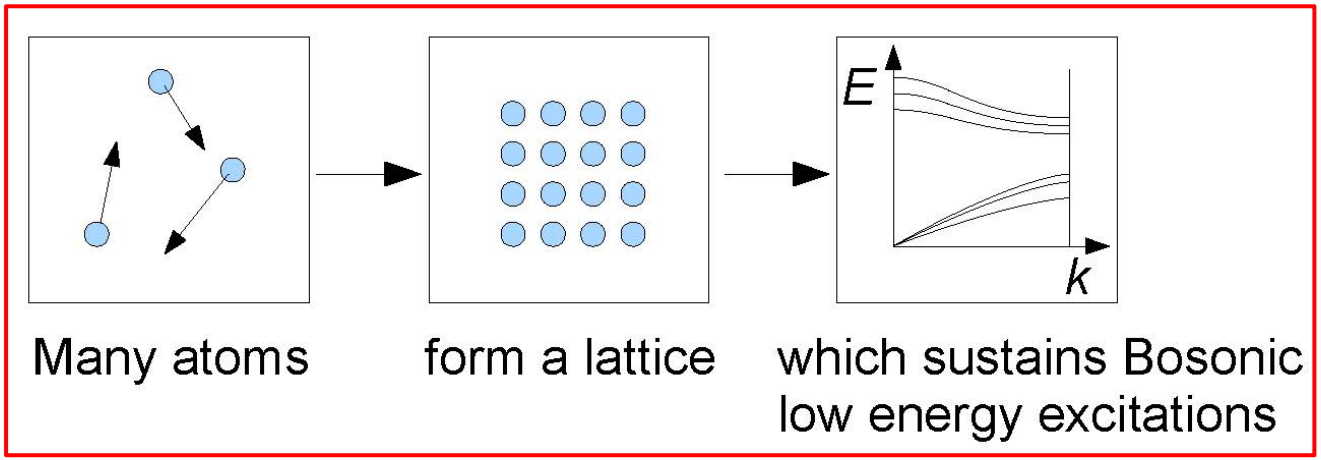
- Known as *Knudsen minimum*
- Very long mean free path given close packed nature of ^{3}He atoms





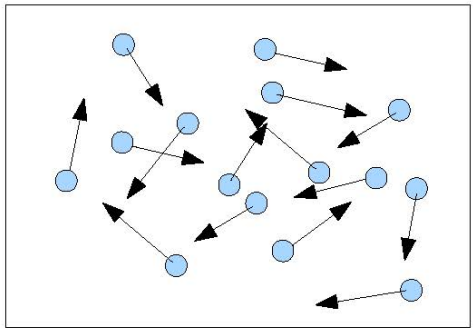
Parpia and Rhodes Phys Rev Lett **51**, 805 (1983)

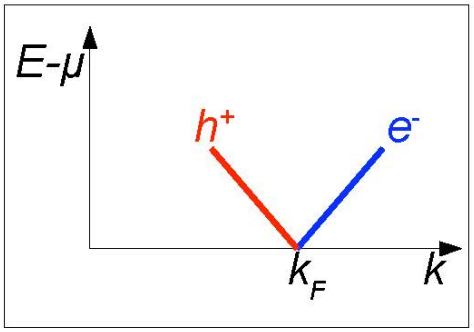
Collective excitations – remember phonons



- In a lattice we concentrate on deviations of the system from its ground state
- These excitations are deformations of the lattice, we decompose them into normal modes labelled with a wavevector and frequency of vibration
- Since we have harmonic oscillations we can use creation and annihilation operators to generate an excited state – 'creating' a phonon
- Commutation relations between creation and annihilation operators cause phonons to follow Bose statistics
- We can create multiple excitations of the same k-state
- So a collection of atoms - which may be fermions or bosons can form a lattice and the low energy excitations can behave like a Bose gas
- This is a tremendous simplification of original problem

Collective excitations in a Fermi liquid





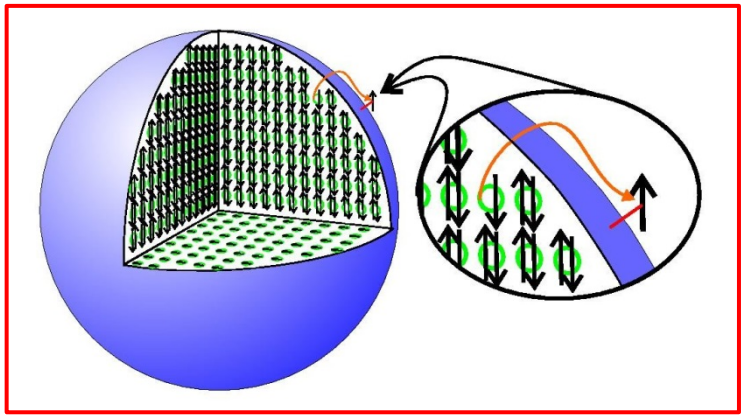
Many interacting Fermions form a liquid

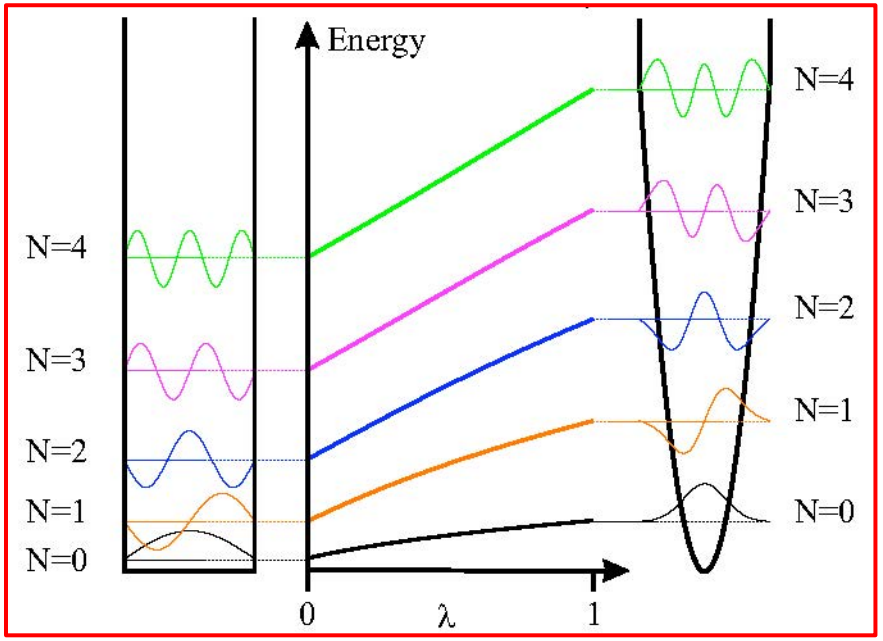
which sustains Fermionic low energy excitations

- Perhaps something analogous happens when fermions form a liquid
- Could the low energy excitations of the liquid formed from strongly interacting fermions (e.g. electrons) behave like a gas of weakly interacting fermions?
- This would explain why a single-particle description works so well in many materials
- In many cases the properties of the electrons making up the liquid carry over with only slight modifications to the properties of the fermionic excitations of the Fermi liquid
- The idea behind Landau's Fermi liquid theory…..

Adiabatic continuity

- Imagine an assembly of non-interacting electrons
- Electron system forms a Fermi gas, ground state of system represented by filled electron states within Fermi surface, empty electron states above it
- Gradually turn on interaction between electrons and follow evolution of energy levels in the system
- Principle of adiabatic continuity suggests we can continue to label the energy eigenstates in the same way as for non-interacting system
- When the system is tuned energy levels shift but labels remain useful
- We assume the excitations of the interacting Fermi system follow the same basic rules as the Fermi gas

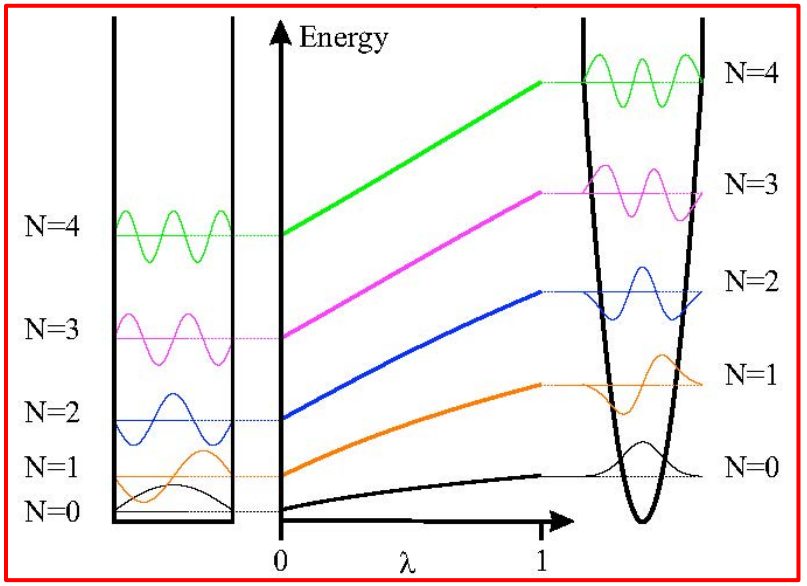




Changing a square well potential into an SHO potential, Schofield, Contemp. Phys. **40**, 95 (1999)

Adiabatic continuity

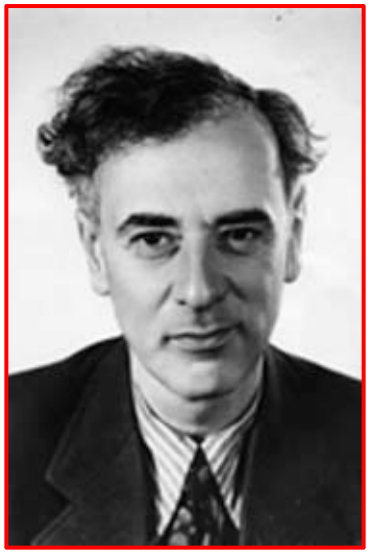
- Important consequence of one-to-one correspondence between quasiparticle states and states of non-interacting system is that the volume of the Fermi surface is unchanged as interaction is turned on - Luttingers's Theorem
- There are a number of pitfalls with this argument
- It only holds if the energy levels *do not* cross as the interaction is turned on
- This is not guaranteed – difficult to find a non-trivial example where this is true for an interacting system
- We can say that for interacting Fermi systems, a Fermi liquid state is possible but not every Fermi system will be described in this way

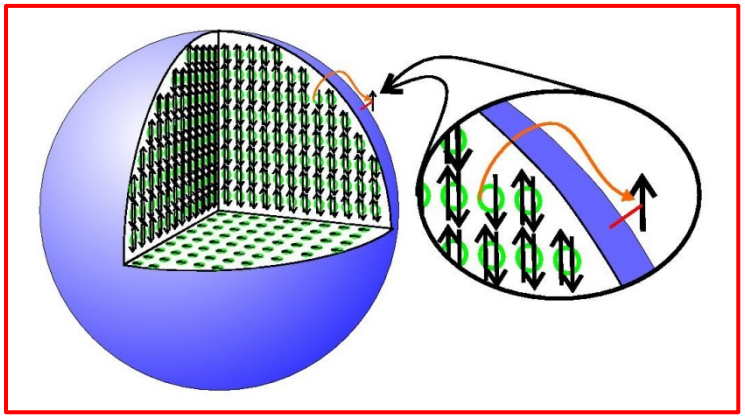


Changing a square well potential into an SHO potential, Schofield, Contemp. Phys. **40**, 95 (1999)

Total energy expansion for Landau Fermi liquid

- Landau's Fermi liquid: label excited states of the interacting system by quantum nos. of non-interacting system: wavevector $\mathbf{k}$, spin, band index, etc
- In analogy with phonons for excited states of lattice vibrations, we refer to an excited state *quasiparticle* of wavevector $\mathbf{k}$
- The quasiparticle lies outside the Fermi surface
- Also *quasiholes* – excitation at wavevectors inside Fermi surface
- We can express the total energy of the interacting system as a function of the occupation number of the various states
- At low temperatures with few excitations this can be approximated by a Taylor expansion





$$E[n_{\mathbf{k}}] = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) n(\mathbf{k}) + \tfrac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} f(\mathbf{k},\mathbf{k}') n(\mathbf{k}) n(\mathbf{k}')$$

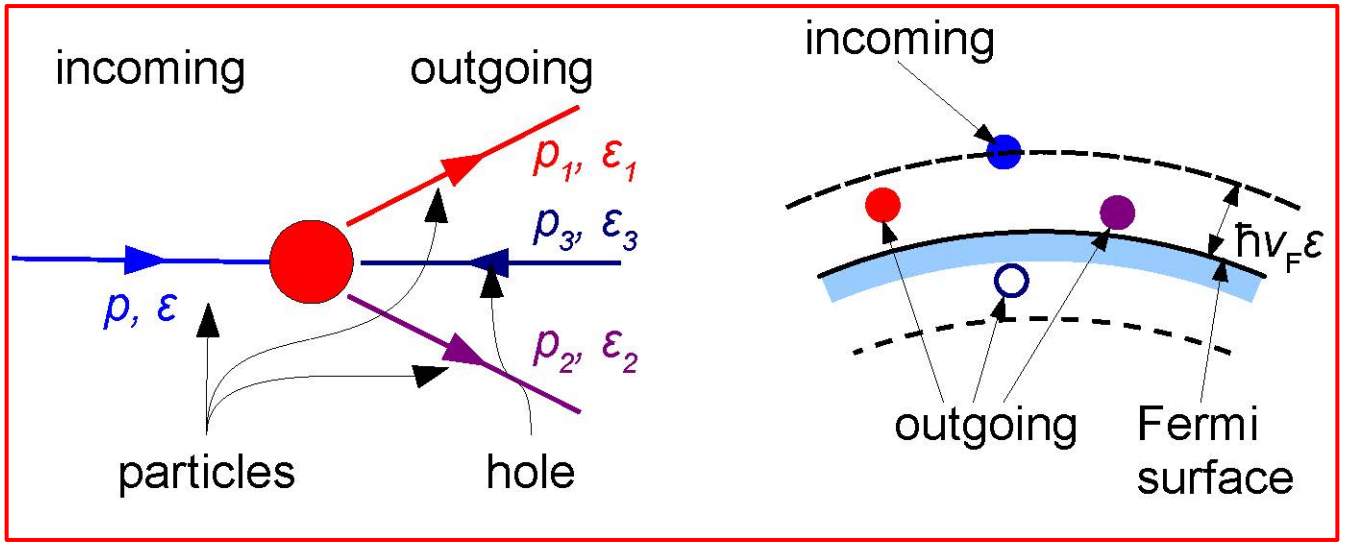
Total energy expansion for Landau Fermi liquid

- From last slide

$$E[n_{\mathbf{k}}] = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) n(\mathbf{k}) + \tfrac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} f(\mathbf{k},\mathbf{k}') n(\mathbf{k}) n(\mathbf{k}')$$

- First term - the energy of having quasiparticles in band states of energy $\epsilon(\mathbf{k})$
- The next term is second order in occupation number $n(\mathbf{k})$ and accounts for interactions between excited states or quasiparticles
- The interaction function is given by $f(\mathbf{k},\mathbf{k}')$
- Hence by using a relatively simple expression for the total energy Landau found a variety of expressions linking material properties such as heat capacity, magnetic susceptibility and compressibility to properties of quasiparticles and the interaction function

Energy dependence of the quasiparticle scattering rate



- Quasiparticle scatters by creating electron-hole pair
- Particle with energy e, momentum p comes in, 2 particles and 1 hole come out
- By Pauli exclusion principle all outgoing particles must have energy (referenced to E_F) >0. Remember the hole energy $= -\epsilon_3$
- By conservation of energy $\epsilon = \epsilon_1 + \epsilon_2 - \epsilon_3$ is fixed
- ϵ_1 and ϵ_2 can be chosen freely from the range 0 to ϵ which fixes ϵ_3
- Hence number of available final states for scattering event rises with increasing incident quasiparticle energy and is $\propto \epsilon^2$

Energy dependence of quasiparticle scattering rate

- Hence the scattering rate $\Gamma \sim \epsilon^2$
- Therefore quasiparticles with energy $\epsilon \to 0$ i.e. close to the Fermi surface, scatter extremely rarely and are long-lived
- Despite the fact that they travel through a strongly interacting and dense liquid, these quasiparticles can travel long distances before they scatter.
- Their free motion is protected by the Pauli exclusion principle because there are very few empty states into which they can scatter
- This is a key result from Landau's Fermi liquid theory, particles interact but do not scatter and therefore are long-lived
- In metals this effect explains why the mean free path can be very long in copper if the temperature is low enough
- The electrical current is carried by a quasiparticle excitation that is a collective mode of the Fermi system
- In the language of perturbation theory the quasiparticle is a dressed excitation involving a correlated motion of the added electron with the many particle background

Energy dependence of quasiparticle scattering rate

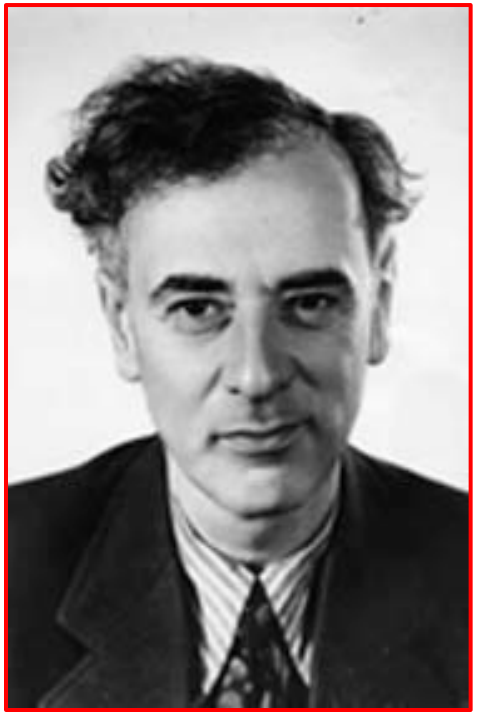
- Conversely with increasing $\epsilon = E - E_F$ the scattering rate grows more quickly than ϵ
- When the scattering rate exceeds $\epsilon / \hbar$ the quasiparticles are no longer well defined because they scatter before their wavefunction can undergo a full oscillation
- Hence the quasiparticles become *overdamped*
- Landau's Fermi liquid theory only applies to low energy excitations and only works well when $k_B T \ll E_F$
- This is still as very wide range – in most metals E_F is thousands of Kelvin

Summary of Lecture 21

- Fermi liquid theory – the problem with the Fermi gas
- Liquid Helium – specific heat and viscosity
- Collective excitations
- Adiabatic continuity
- Total energy expansion for Landau Fermi liquid
- Energy dependence of quasiparticle scattering rate

Quantum Condensed Matter Physics

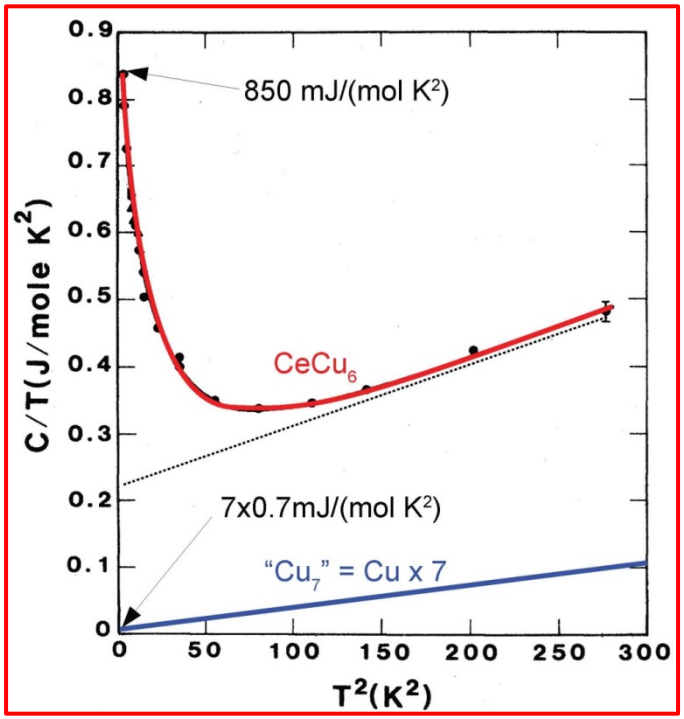
Lecture 21



The End

Quantum Condensed Matter Physics

Lecture 22



David Ritchie

Quantum Condensed Matter Physics: synopsis (4)

5. Electronic instabilities (2L)

The Peierls transition, charge density waves, magnetism, local magnetic moments, Curie Law. Types of magnetic interactions; direct exchange, Heisenberg hamiltonian, superexchange and insulating ferromagnets, band magnetism in metals, local moment magnetism in metals, indirect exchange, magnetic order and the Weiss exchange field.

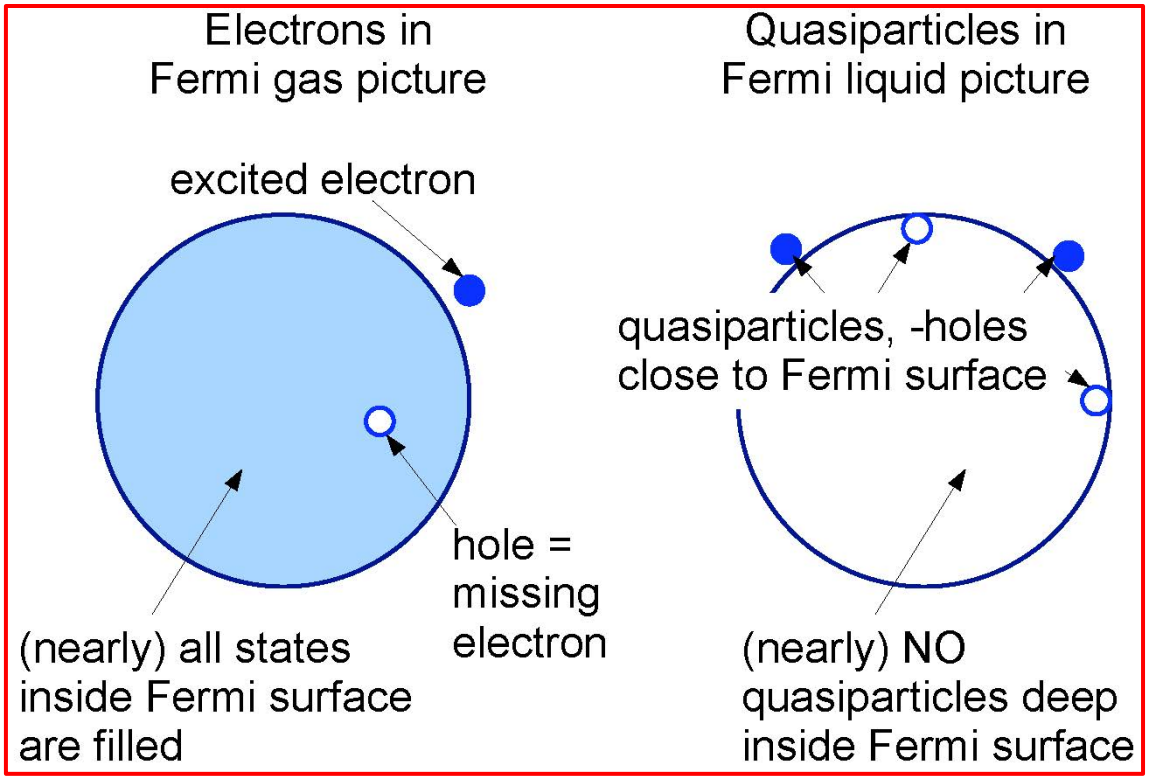
6. Fermi Liquids (2L)

Fermi liquid theory; the problem with the Fermi gas. Liquid Helium; specific heat and viscosity. Collective excitations, adiabatic continuity, total energy expansion for Landau Fermi liquid, energy dependence of quasiparticle scattering rate.

Quasiparticles and holes near the Fermi surface, quasiparticle spectral function, tuning of the quasiparticle interaction, heavy fermions, renormalised band picture for heavy fermions, quasiparticles detected by dHvA, tuning the quasiparticle interaction. $CePd_2Si_2$; heavy-fermion magnet to unconventional superconductor phase transitions.

Quasiparticles and holes live near the Fermi surface

- Fermi liquid quasiparticles are only defined close to Fermi surface
- We cannot have a filled Fermi sphere of quasiparticles as for the Fermi gas
- For a Fermi liquid the wavevector $\mathbf{k}$ labels the quasiparticle states which are only well defined close to the Fermi surface because only then is the lifetime large enough



- We have an unusual 'vacuum' ground state in which the low energy excitations are fermionic particles and holes which sit on either side of a boundary surface in momentum space

Quasiparticle spectral function

- Think about the fermi liquid in another way - consider the response of the many-particle system to the addition or removal of a quasiparticle
- For a non-interacting system, place a particle into a single-particle eigenstate of the Hamiltonian labelled by momentum $\mathbf{k}$
- The wavefunction evolves in time according to the Schrodinger equation

$$\psi_{\mathbf{k}}(\mathbf{r},t) = \psi_{\mathbf{k}}(\mathbf{r})e^{-i\epsilon_{\mathbf{k}}t/\hbar}$$

- Where $\psi_{\mathbf{k}}$ is the Bloch wavefunction satisfying the time-independent Schrodinger equation
- The time-dependent solution oscillates in time with a frequency $\omega = \epsilon_{\mathbf{k}} / \hbar$
- Looking at this in Fourier space

$$\psi_{\mathbf{k}}(\mathbf{r},\omega) = 2\pi\psi_{\mathbf{k}}(\mathbf{r})\delta(\omega - \epsilon_{\mathbf{k}} / \hbar)$$

- So the wavefunction has spectral weight only at $\omega = \epsilon_{\mathbf{k}} / \hbar$
- We can say that the probability amplitude of finding an electronic state with energy $\hbar\omega$ and momentum $\hbar\mathbf{k}$ is

$$A(\mathbf{k},\omega) = \delta(\omega - \epsilon_{\mathbf{k}} / \hbar)$$

- Where $A(\mathbf{k},\omega)$ is called the *electron spectral function* for the non-interacting system

Quasiparticle spectral function

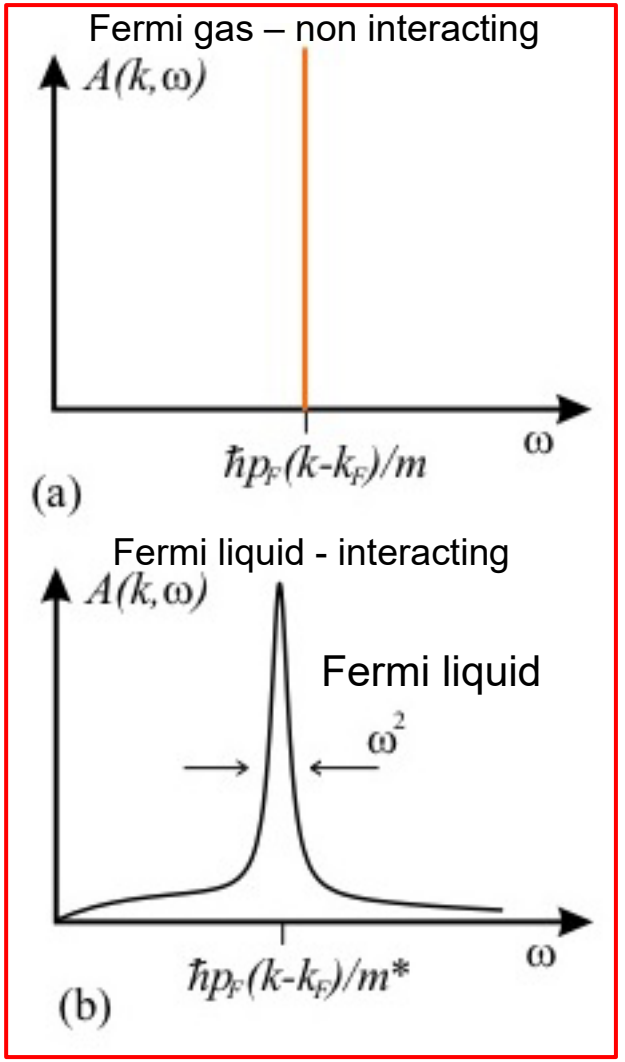
- In an interacting system an electron may take part in a number of eigenstates – so we expect the spectral function to spread out in energy
- Interactions modify the precise form of the dispersion relation so we replace $\epsilon_{\mathbf{k}}$ by a renormalised $\tilde{\epsilon}_{\mathbf{k}}$
- This is often called a mass renormalisation $m^* / m = \epsilon_{\mathbf{k}} / \tilde{\epsilon}_{\mathbf{k}}$
- If we add a quasiparticle it will scatter from other quasiparticles or create other electron-hole pairs
- Because of this the probability amplitude of finding a quasiparticle of momentum $\mathbf{k}$ at time t will decay exponentially at the quasiparticle scattering rate $\Gamma_{\mathbf{k}}$
- These effects change the time dependence of the state to $e^{(i\epsilon_{\mathbf{k}}/\hbar - \Gamma_{\mathbf{k}})t}$
- After a Fourier transform this leads to an *ansatz* for the spectral function in an interacting system of the form

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\Im\left[\frac{1}{\omega - \tilde{\epsilon}_{\mathbf{k}}/\hbar + i\Gamma(\mathbf{k})}\right]$$

- This describes quasiparticles with a dispersion relation $\tilde{\epsilon}_{\mathbf{k}}$ and decay rate $\Gamma_{\mathbf{k}}$
- Notice that if the inverse lifetime $\Gamma_{\mathbf{k}} \to 0$ the spectral function reduces to the non-interacting form $A(\mathbf{k},\omega) = \delta(\omega - \epsilon_{\mathbf{k}}/\hbar)$

Quasiparticle spectral function

- We must take care with the chemical potential
- In equilibrium (and at T=0) we cannot add fermionic excitation at an energy $\hbar\omega < \mu$
- So we will infer that for $\hbar\omega > \mu$ the spectral function we have is for particle like excitations but for $\hbar\omega < \mu$ it is the spectral function for holes
- If $\Gamma_{\mathbf{k}}$ is small the quasiparticles are long-lived and have some real meaning – a quasiparticle resonance at $\hbar\omega = \tilde{\epsilon}_{\mathbf{k}}$ can be resolved if the peak width in the spectral function is less than the centre peak's position
- For interacting system (b) $A(\mathbf{k},\omega)$ has width $2\Gamma_{\mathbf{k}}$
- Phase space argument shows $\Gamma_{\mathbf{k}} \propto \epsilon^2$ quality factor $\tilde{\epsilon}_{\mathbf{k}} / \Gamma_{\mathbf{k}} \propto \tilde{\epsilon}_{\mathbf{k}} / \tilde{\epsilon}_{\mathbf{k}}^2$ which diverges as $\epsilon \to 0$



- Quasiparticles overdamped at high energies but well defined for $E \to E_F$
- Quasiparticle concept is self consistent – possible to have quasiparticles that scatter so rarely so their lifetime is long enough to observe them !

Tuneability of the quasiparticle interaction

- The interaction term in the Landau expansion for the total energy
$$\tfrac{1}{2}\sum_{\mathbf{k}\mathbf{k}'} f(\mathbf{k},\mathbf{k}')n(\mathbf{k})n(\mathbf{k}')$$
causes quasiparticle properties to be changed w.r.t. the free electron value.
- Most importantly - the effective mass m^* can be orders of magnitude larger than the bare electron mass
- The quasiparticle interaction $f(\mathbf{k},\mathbf{k}')$ can be completely different from the Coulomb repulsion, which acts on the underlying electrons
- In particular, $f(\mathbf{k},\mathbf{k}')$ can be spin-dependent
- This is an example of the *tuneability* of correlated electron systems: although the underlying Coulomb interaction is fixed, the effective interaction in the low energy model is highly dependent on details of the system, and can therefore be tuned over a wide range by changing, for example, magnetic field, pressure or doping.

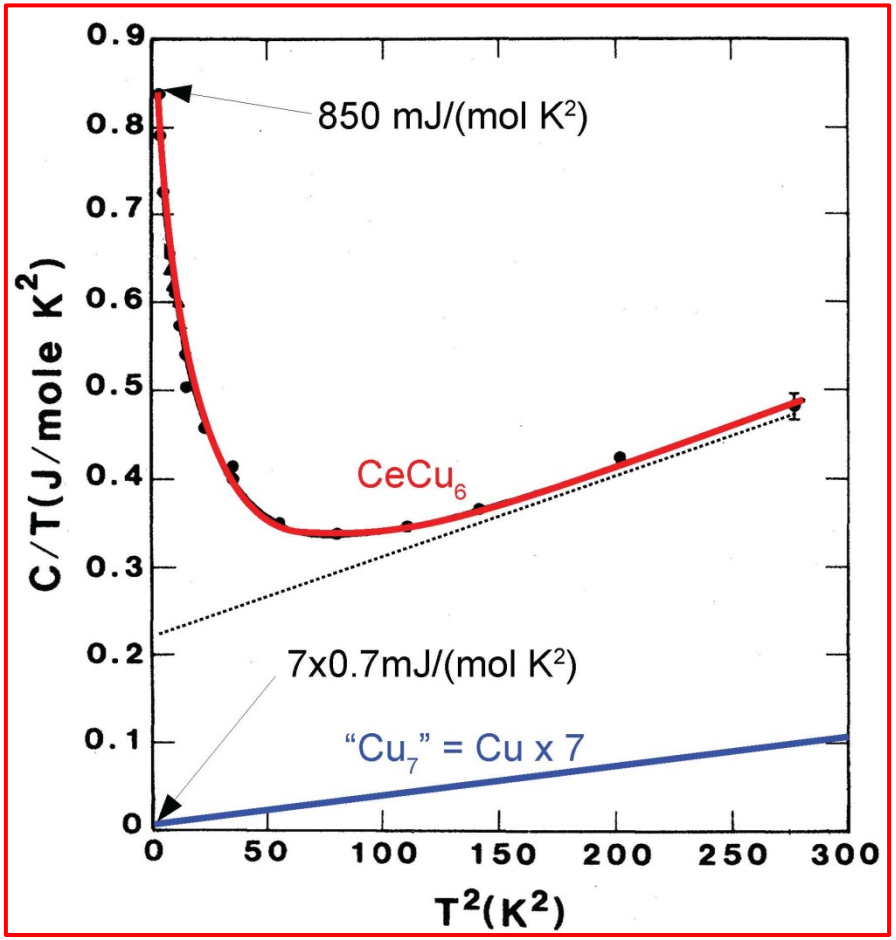
Heavy fermions

- In Fermi liquid theory, quasiparticle mass differs from bare electron mass.
- Strong interactions can cause high effective masses.
- Heavy Fermion materials (at very low temperature) have very high Sommerfeld coefficient of the heat capacity, and high, weakly temperature-dependent magnetic susceptibility.
- This suggests they follow Fermi liquid theory, but the effective quasiparticle masses are strongly enhanced: in some cases up to *1000* times .
- Usually, heavy Fermion materials contain Cerium, Ytterbium or Uranium, which contribute partially filled f-orbitals to the band structure.
- These highly localised states are important, because in a lattice, they lead to very narrow bands. The strong Coulomb repulsion prevents double occupancy of these states.
- There are hundreds of heavy Fermion materials
- Examples: CeCu Si , CeCu , CeCoIn , YbCu Si , UPt .

Heavy fermions – $CeCu_6$

- Figure shows Sommerfeld coefficient of heat capacity C/T for Heavy Fermion material $CeCu_6$
- In the low-T limit C/T approaches 850mJ(molK^2)
- Comparing this value to pure copper, the heat capacity per atom has been boosted by a factor of 150
- So… replacing 14% of the copper atoms in a sample of pure Cu by Ce we increase the low temperature heat capacity by a factor of 150!!!
- We find that (assuming k_F the same)

$$g(E_F) \propto 1/v_F, \; m^* v_F = \hbar k_F \sim \text{const.}$$



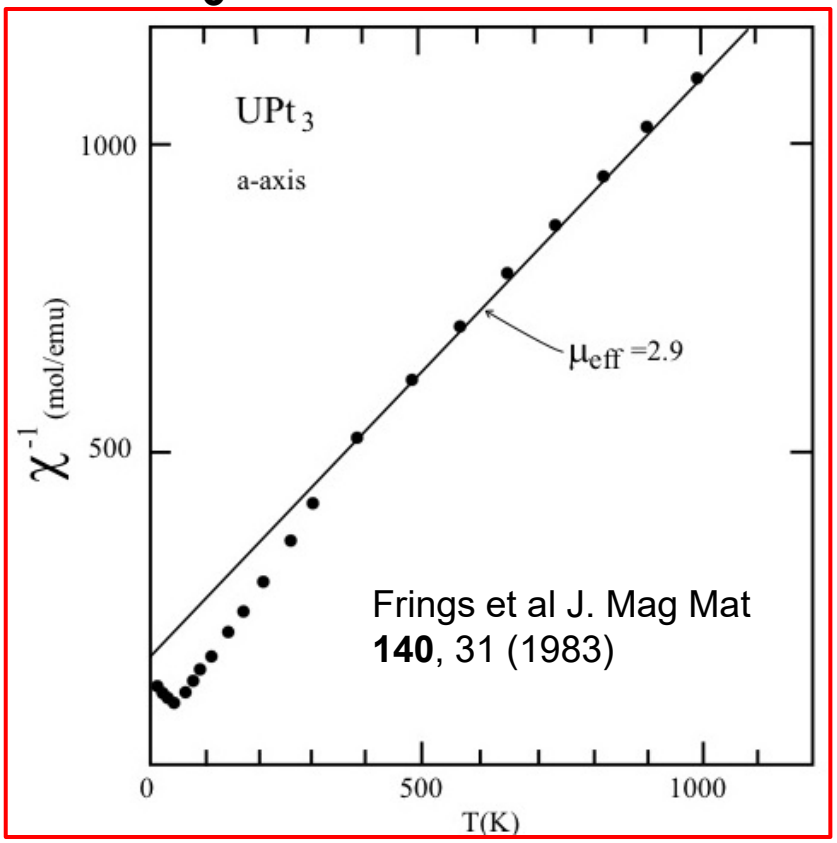
- Hence $m^* \propto g(E_F)$ - so an enhanced DoS at the fermi surface crucial for the properties of these materials
- Note strong upturn in C/T at low T
- Heavy fermion state only develops fully at low temperatures

Heavy fermions – UPt_3

- At low T the behaviour of $CeCu_6$ and other heavy Fermion materials consistent with Fermi liquid theory
- At high T the picture is quite different
- An isolated magnetic moment displays a T dependent Curie law susceptibility

$$\chi^{-1} \propto T$$

- Similar form seen in many heavy fermion materials at high T, often with a slope consistent with a Curie constant expected from electronic configuration of magnetic ions



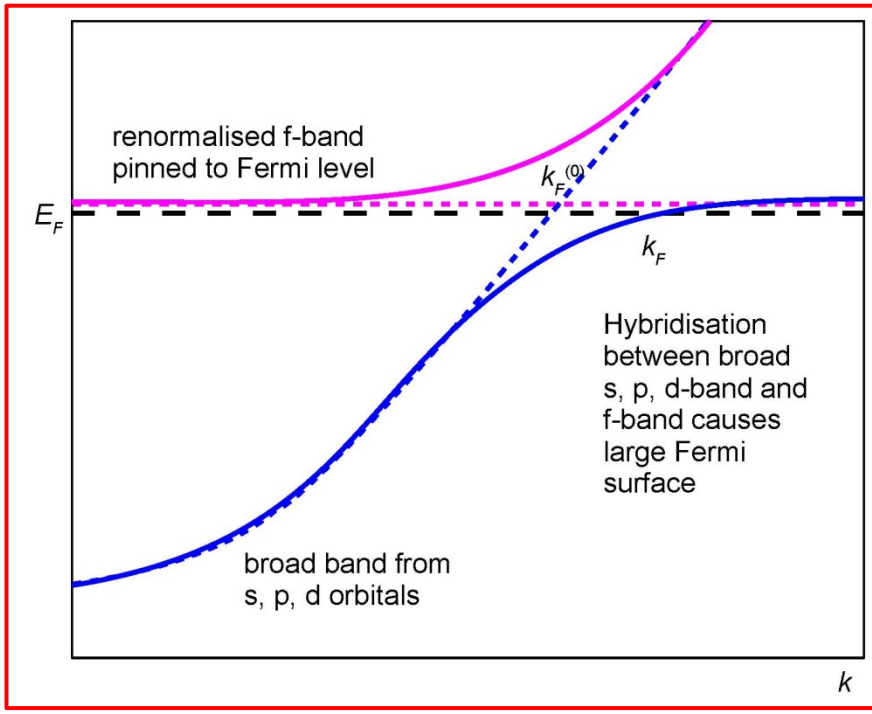
- Figure: UPt_3, electrons in partially filled f-orbitals act as local moments at high T – and obey Curie law susceptibility.
- Curie susceptibility does not extend to zero T but crosses over to a constant value, just as the Sommerfeld coefficient of the heat capacity does
- As T is lowered, free spins start to bind to conduction electrons to make heavy fermions, according to the *Kondo* model

Renormalised band picture for heavy fermions

- To find a qualitative understanding of the origin of the heavy fermion state
- Consider the hybridisation between the bands associated with the more extended s,p,d-orbitals and the bands which arise from the tightly localised f-orbitals
- A partially filled f-orbital will always lie inside filled s,p, and even d-orbitals with a higher major quantum number
- There is negligible hybridisation between f-orbitals on neighbouring atoms – too far apart
- The result is a very flat f-band
- If we consider single-electron states naively, then we find that the f-band formed from the atomic f-orbitals is well below the chemical potential, and should therefore be completely full
- In such a scheme there would be no local moments at high temperature and no heavy fermion behaviour at low temperature
- The scheme fails, because it ignores the strong Coulomb repulsion between electrons sharing the same f-state
- Instead of this naïve picture….

Renormalised band picture for heavy fermions

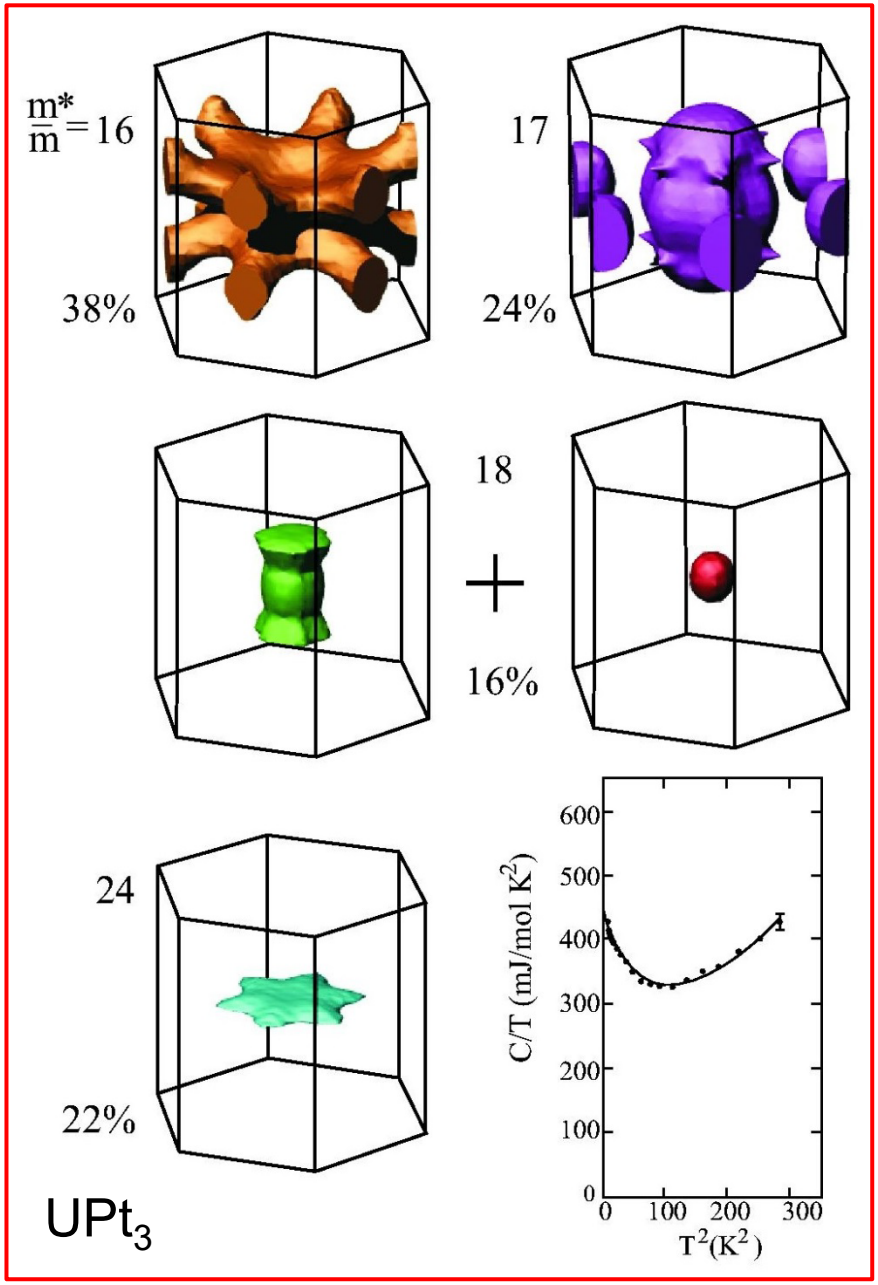
- Once single electron has occupied an f-orbital, energy cost for 2nd electron hopping onto same orbital is very high
- Modify single particle picture to ensure f-orbitals average occupancy is one
- Renormalise energy of the f-states close to the chemical potential, near E_F
- Renormalised, narrow f-band and broad band from atomic s, p, and d-orbitals hybridise, producing anti-crossing very close to E_F



- New dispersion $E(k)$ crosses E_F at much reduced slope compared to the broad s, p, d-bands. As the slope dE/dk gives the Fermi velocity and is inversely proportional to the effective mass, this scheme explains enhanced effective masses observed in materials with partially occupied f-orbitals
- Note that k_F is larger for hybridised system than it would be without hybridisation. Volume of the Fermi surface in heavy fermion systems is large enough to contain not only the electrons on s, p, and d-bands but also the f-electrons

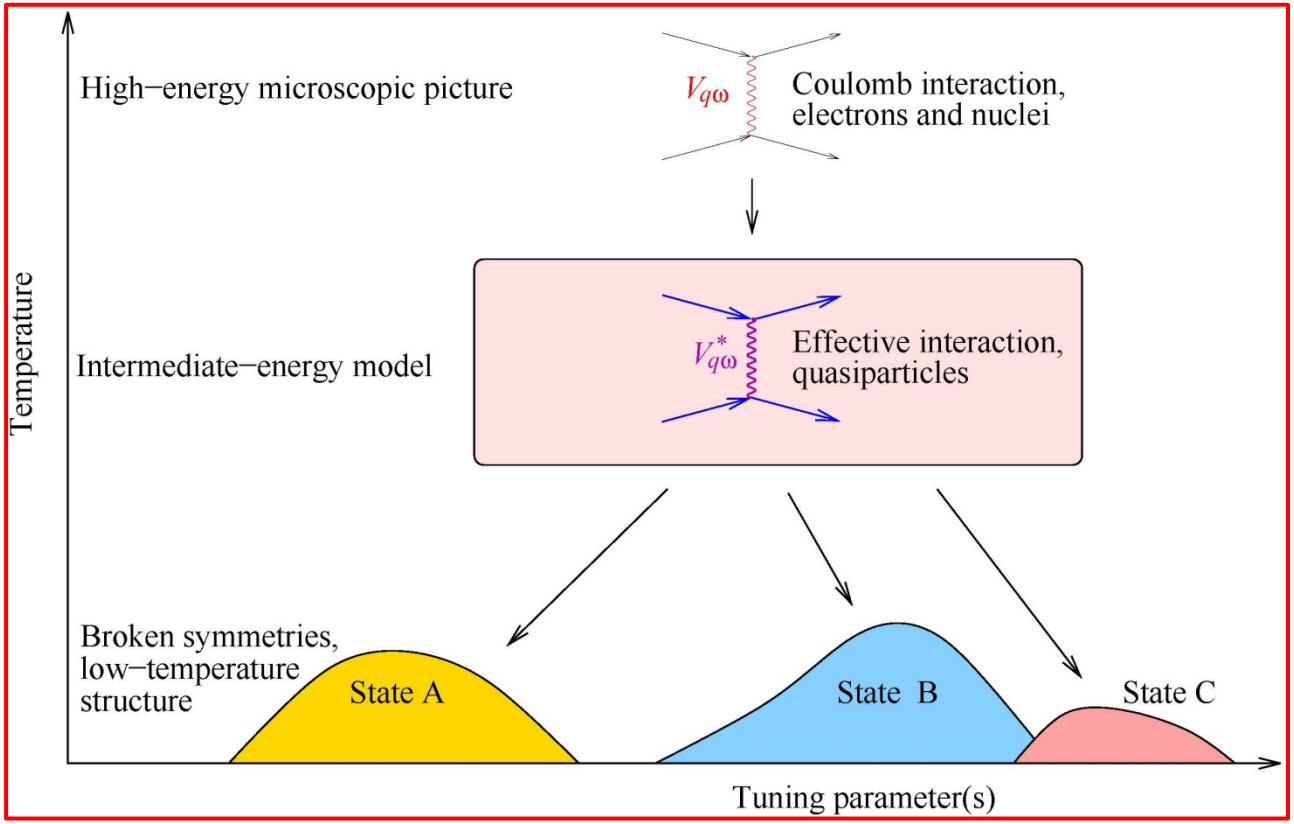
Quasi-particles detected in de Hass-van Alphen experiments

- Quantum oscillations – evidence for heavy fermion liquid state
- Magnetic fields up to 16T
- Several fermi surface sheets
- Volume enclosed by Fermi surface is very stringent criterion, used to decide between the heavy Fermi liquid scenario – in which f- electrons contribute to the Fermi surface – and local moment models
- Temperature dependence of oscillation amplitude leads to effective mass
- Measured effective masses consistent with heat capacity results
- % reflect contributions from quasiparticles in each sheet to specific heat



McMullan et al arXiv:0803.1155

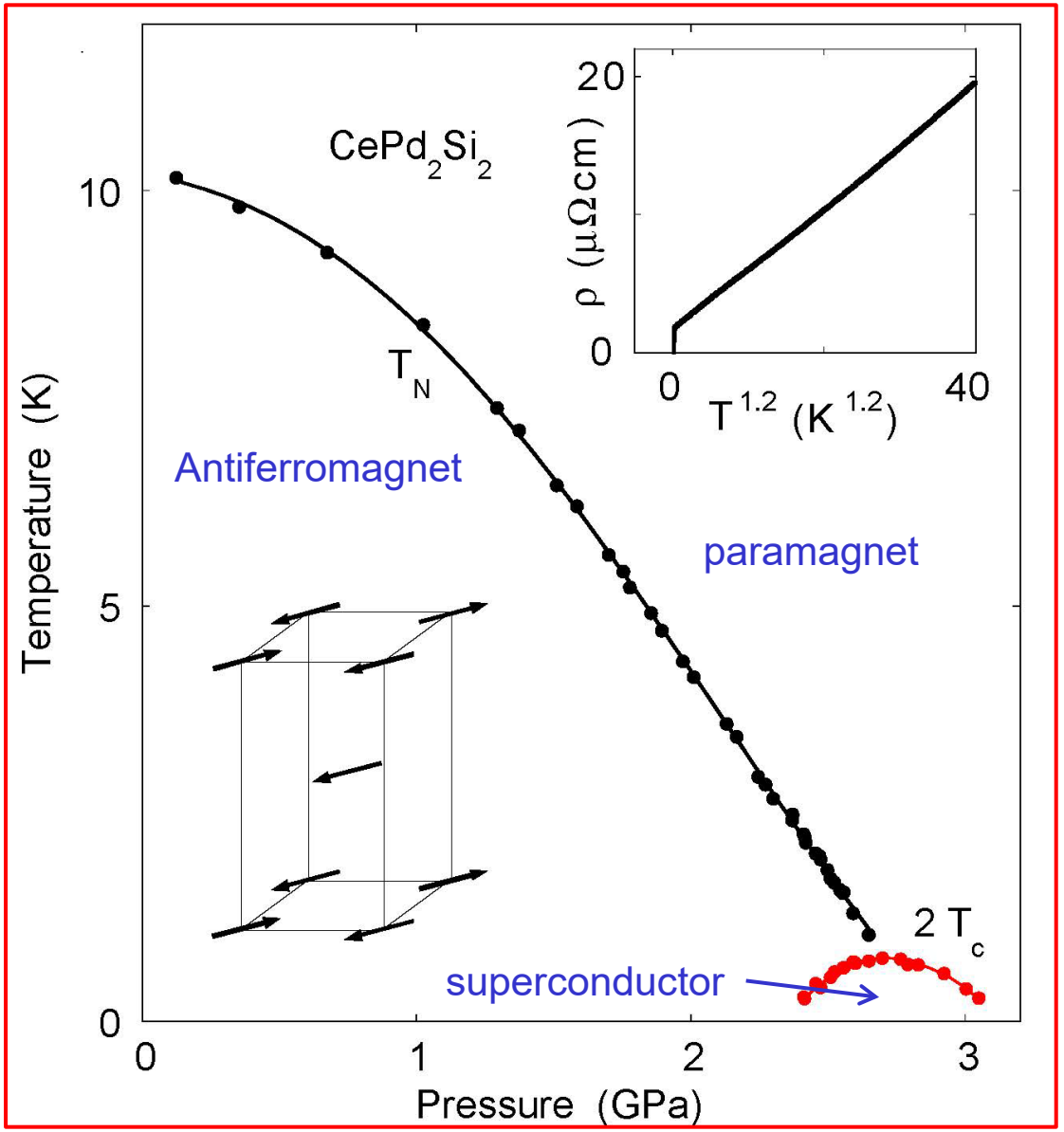
Tuning the quasiparticle interaction



- We cannot tune the Coulomb interaction – but the *effective* interaction, which governs the behaviour of a system at low temperatures, depends on many details and is thereby *highly* tuneable
- By varying the effective interaction, we can select different ground states (magnetism, superconductivity, etc.)

$CePd_2Si_2$: heavy-fermion magnet to unconventional superconductor

- Antiferromagnet below T_N=10K
- T_N depends on pressure.
- Magnetism suppressed near 2.8 GPa
- Anomalous resistivity temperature dependence
- Quantum phase transition: can cross phase boundary at low T, using control parameter other than temperature.



Mathur *et al*, Nature **394**, 39 (1998)

Heavy fermion materials summary

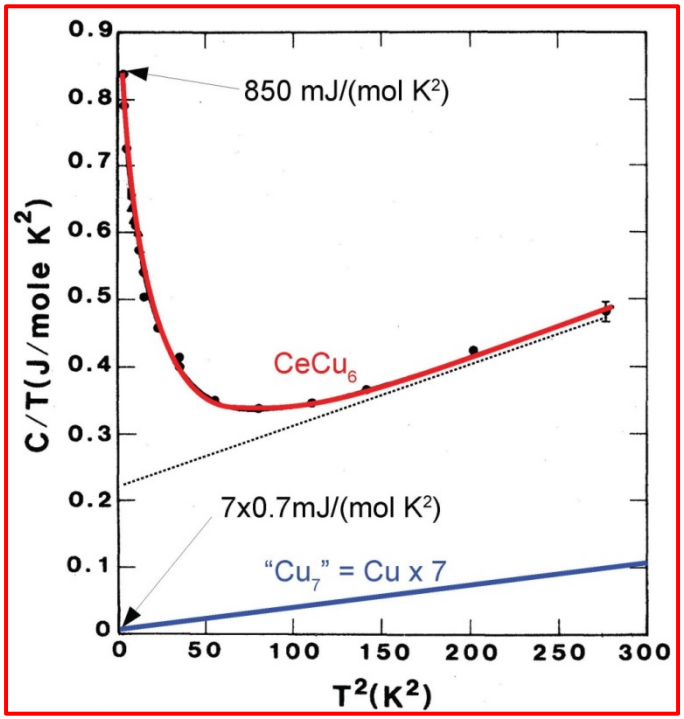
- Usually 4f (Ce, Yb) or 5f (U) intermetallic compounds, such as UPt_3 or $CeCu_2Si_2$
- Low temperature properties consistent with Fermi liquid theory, but very high effective carrier masses
- What is the role of electrons in partially filled f-orbitals? Do they behave like local moments or like conduction electrons?
- Where quantum oscillation studies have been successful, they indicate that the electrons contribute to the Fermi surface, as in a normal metal
- Because $g(E_F)$ is so high in these materials, they tend to order magnetically or even become superconducting.
- There are many different ordered low temperature states in these metals, some simple, some very exotic
- There is an increasing number of materials (e.g., $YbRh_2Si_2$), which do not follow Fermi liquid theory at low T. Are they 'non-Fermi' liquids? Do the f-electrons remain as local moments down to absolute zero in this case, not contributing to the Fermi surface? This is being investigated at the moment

Summary of Lecture 22

- Quasiparticles and holes near the Fermi surface
- Quasiparticle spectral function
- Tuning of the quasiparticle interaction
- Heavy Fermions
- Renormalised band picture for heavy fermions
- Quasiparticles detected by dHvA
- Tuning the quasiparticle interaction
- $CePd_2Si_2$: heavy-fermion magnet to unconventional superconductor
- Heavy fermion materials summary

Quantum Condensed Matter Physics

Lecture 22



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