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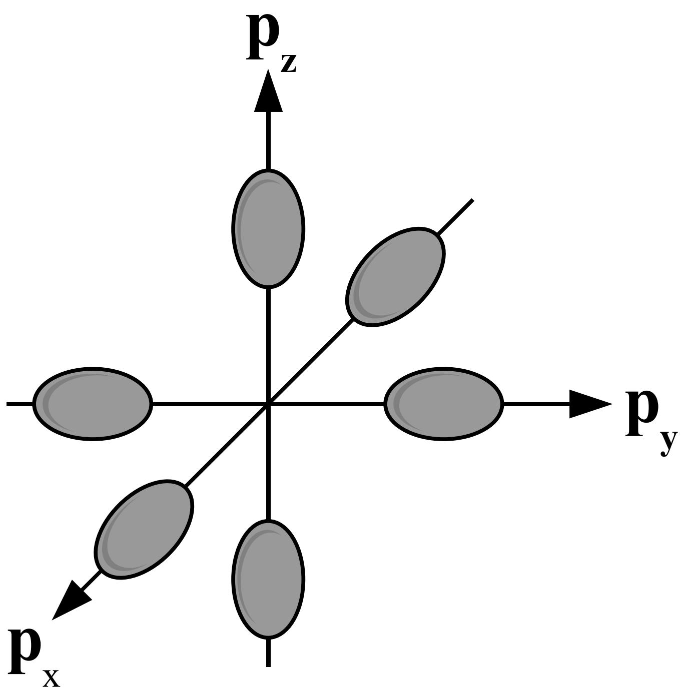
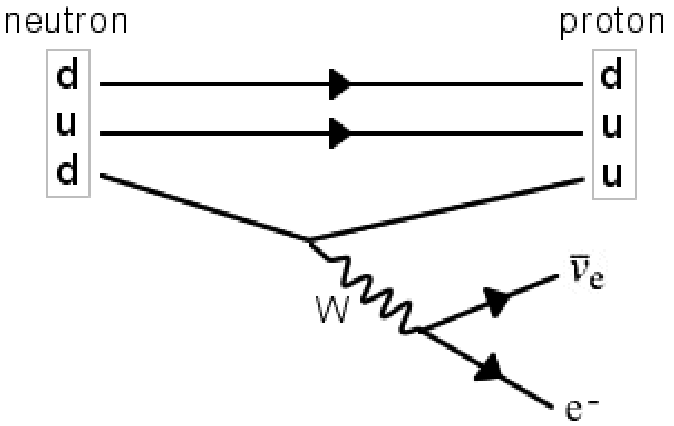
Electron gas of many flavours





Beta radioactive decay via the weak interaction

Work carried out in collaboration with Peter Haynes

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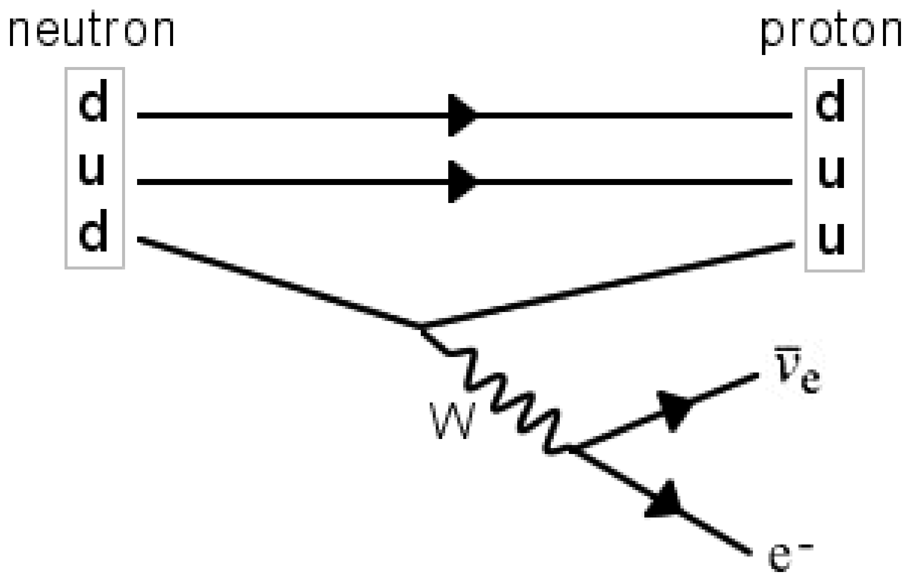
Conference organisers

- Robert Lee & Chris Ko – serving & clearing up
- Jamie Blundell & Fay Tuddenham -- posters
- Mark Dean -- catering
- Andrew Morris – press & publicity
- Alex Silver – Prizes & speaking competition

Abdus Salam

- Quarks exist in six flavours: up, down, strange, charm, bottom and top
- Abdus Salam proposed the weak interaction that allows quark flavour to change



Beta radioactive decay via the weak interaction

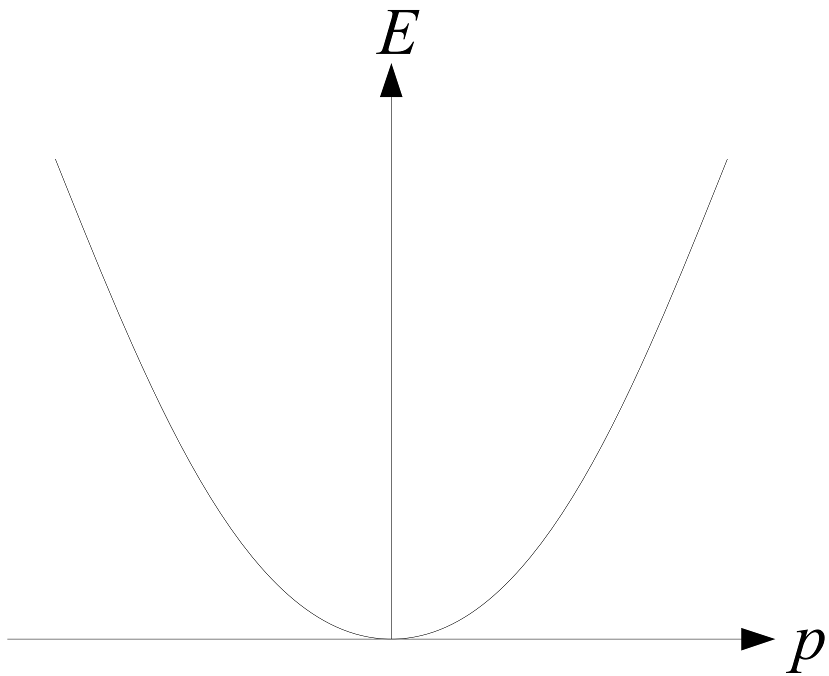
Cambridge 1946-1951
Nobel prize 1979

Condensed matter physics

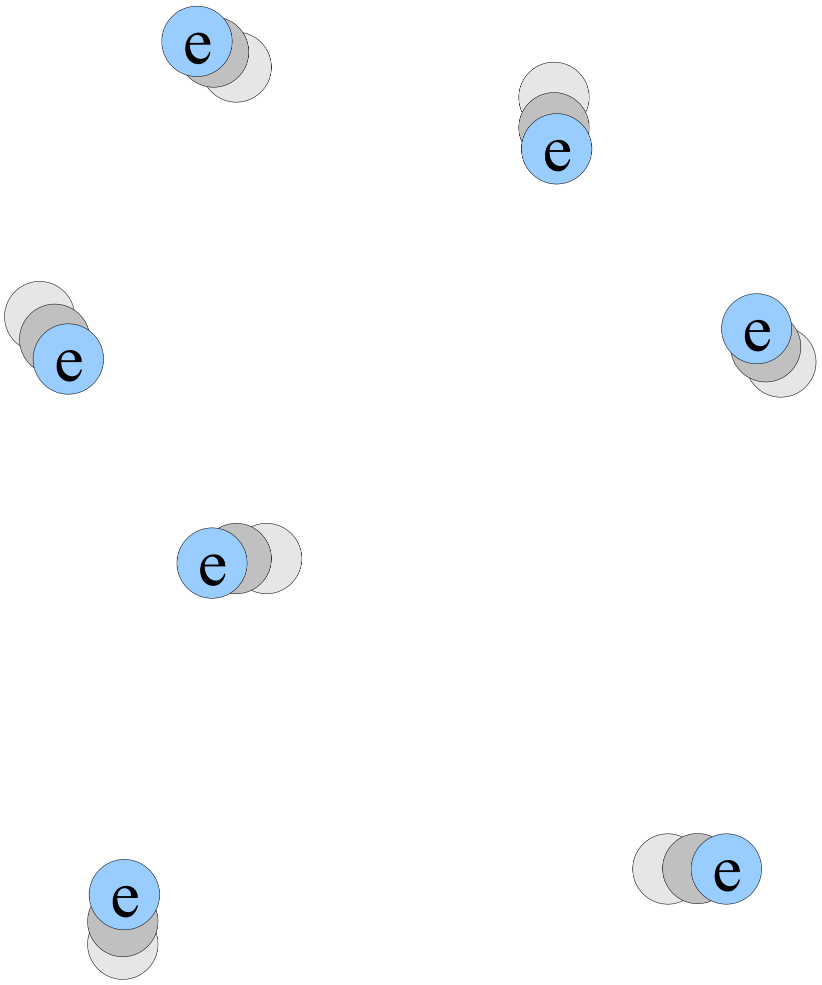
- Abdus Salam was interested in fundamental particles
- Condensed matter physics assumes electrons & nuclei obey well established laws
- Strong Coulomb interactions & quantum mechanics
- Interplay of the two leads to important effects

Free electrons

- Electrons in a vacuum are free to move
- Each electron has kinetic energy $\frac{1}{2}mv^2 = p^2/2m$

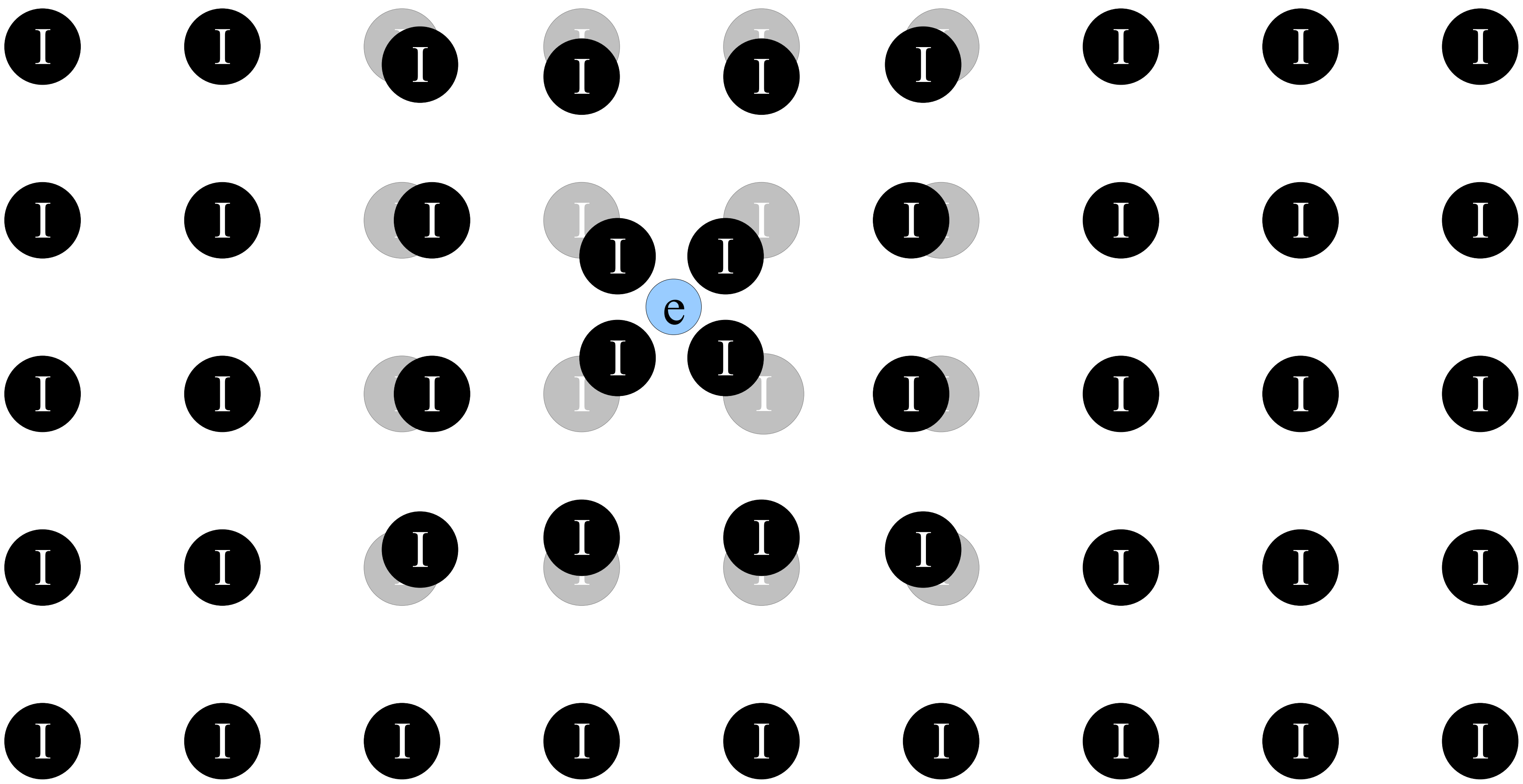


Free electrons



Electrons in a lattice

- In a real materials the electrons *interact* with the ions which alters their dynamics and so their *effective mass*



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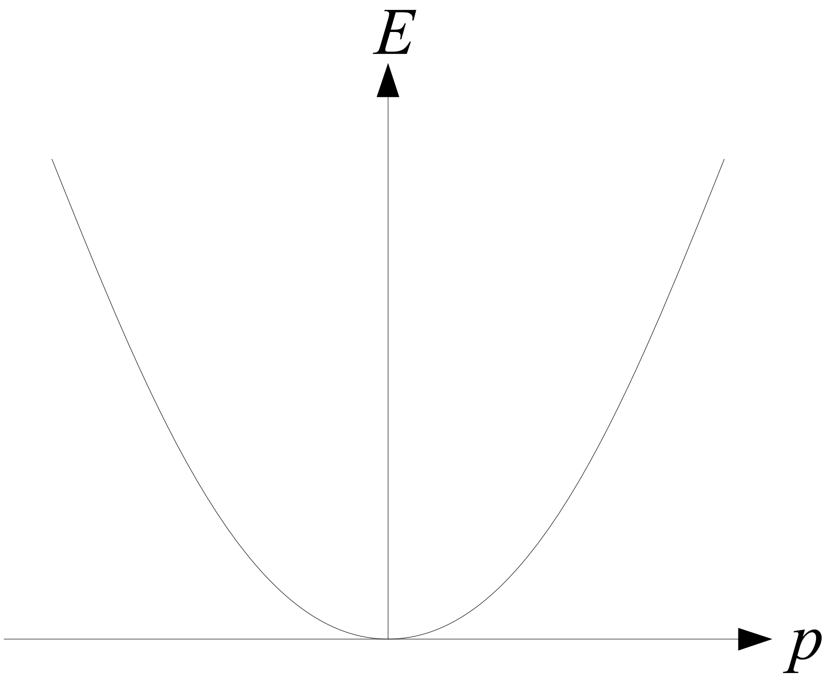
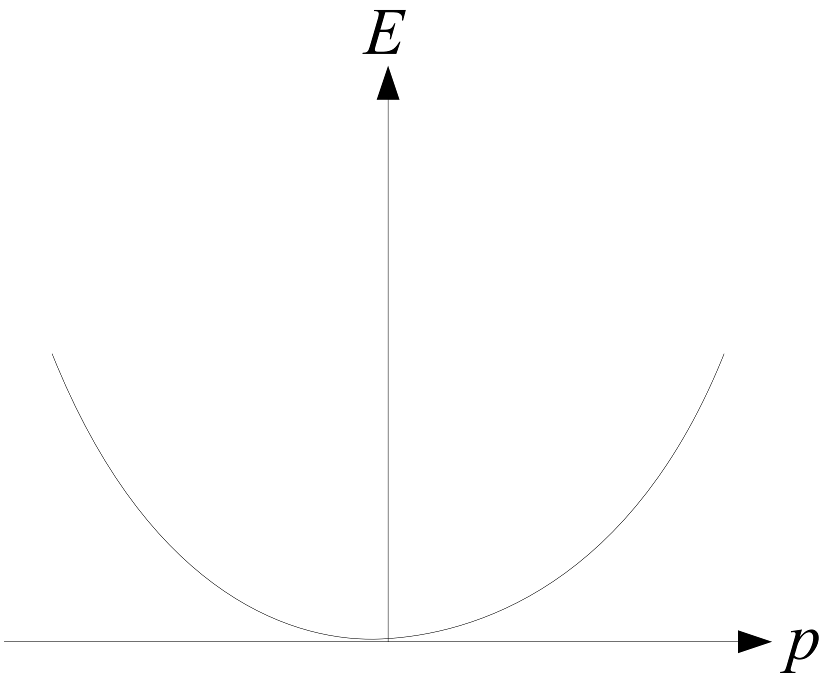
Electrons in metals

- In a metal the electron-ion interaction changes the effective mass of the electrons to m^*



Free electrons

$$E=p^2/2m$$



Metal

$$E=p^2/2m^*$$

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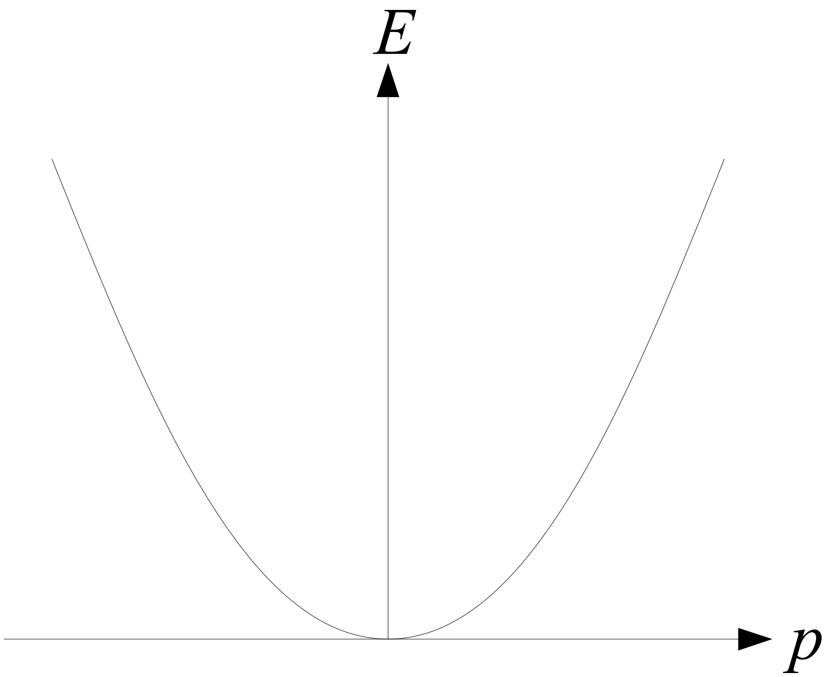
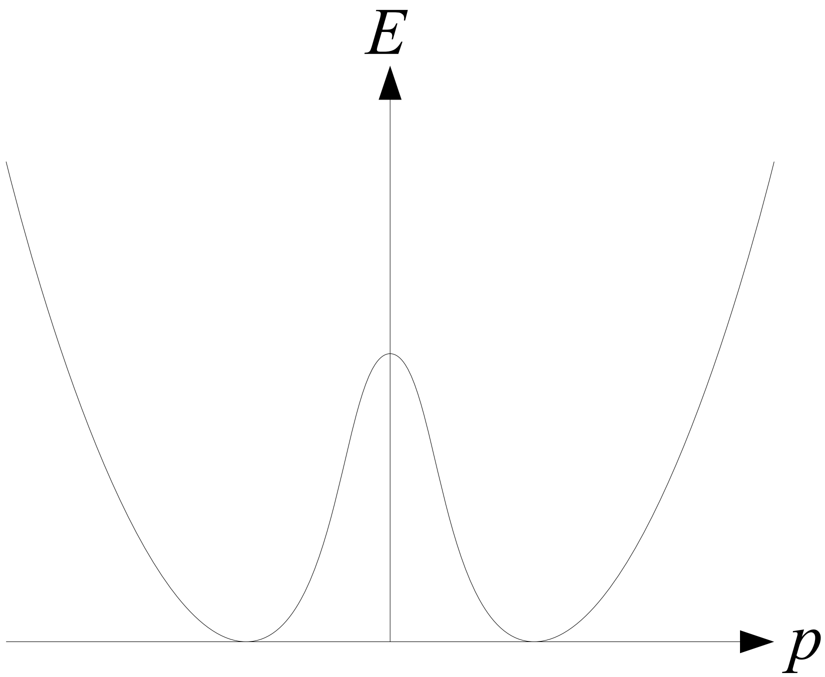
Electrons in semiconductors

- In a semiconductor the change in effective mass dramatically alters the energy dispersion



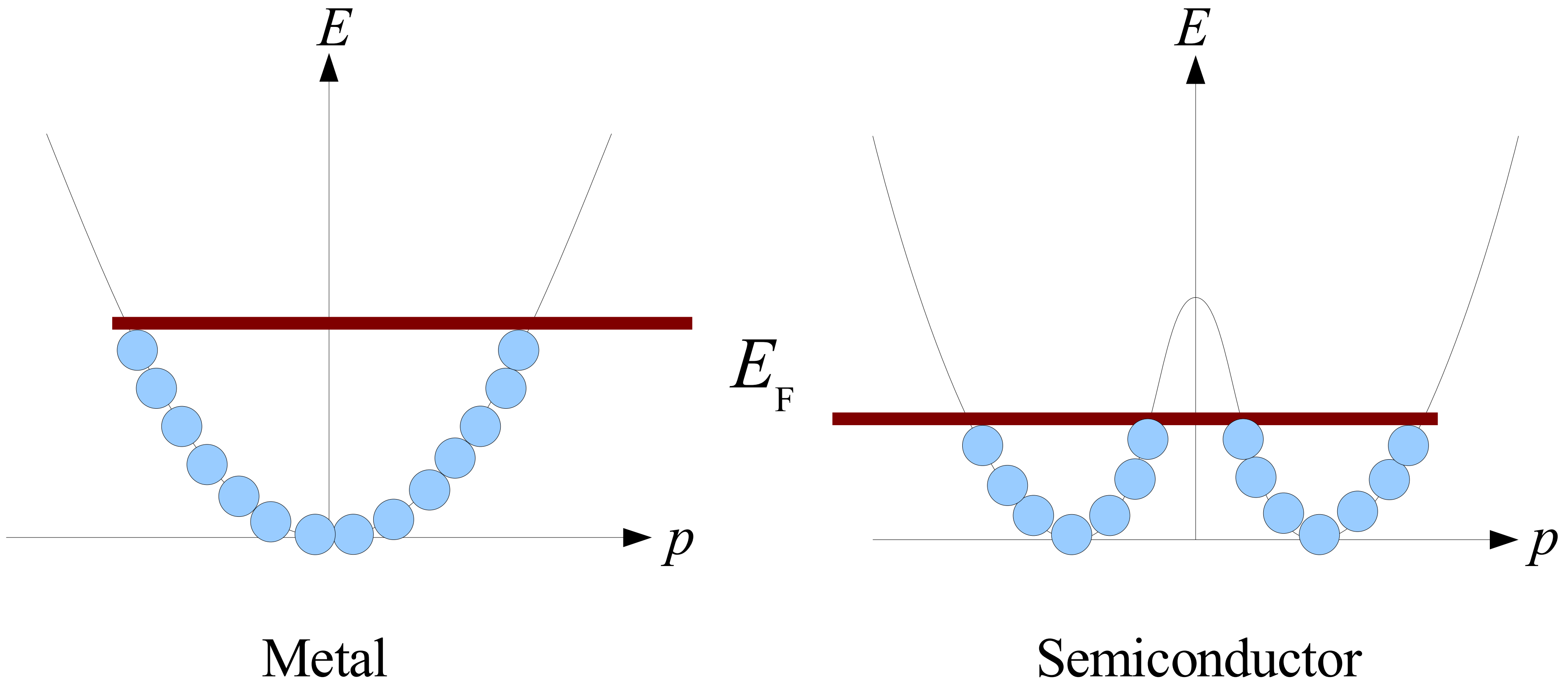
Free electrons



Semiconductor

Fermi surface

- Electrons obey the Pauli exclusion principle so fill the band structure up to the Fermi energy E_F



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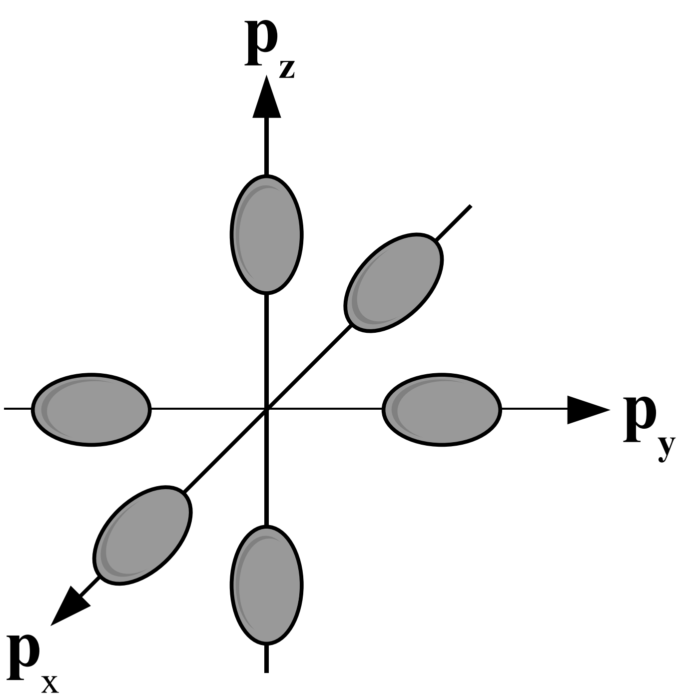
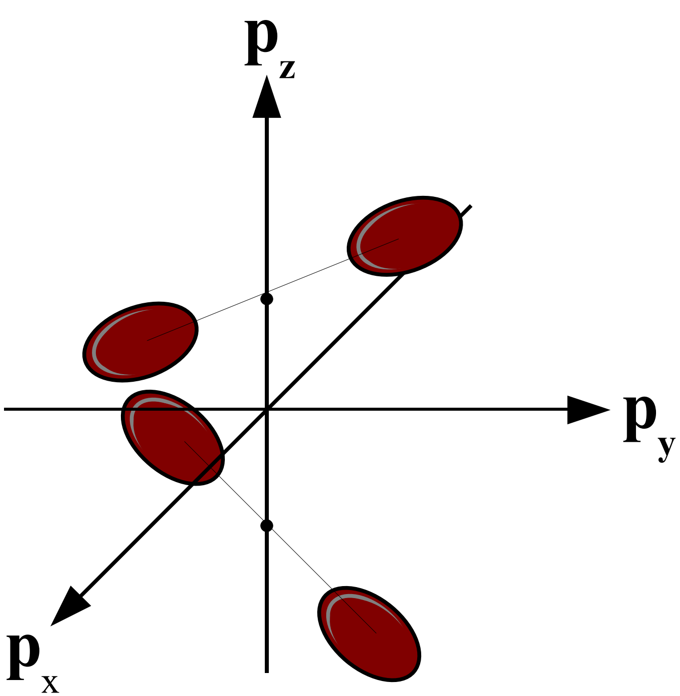
Electron gas of many flavours

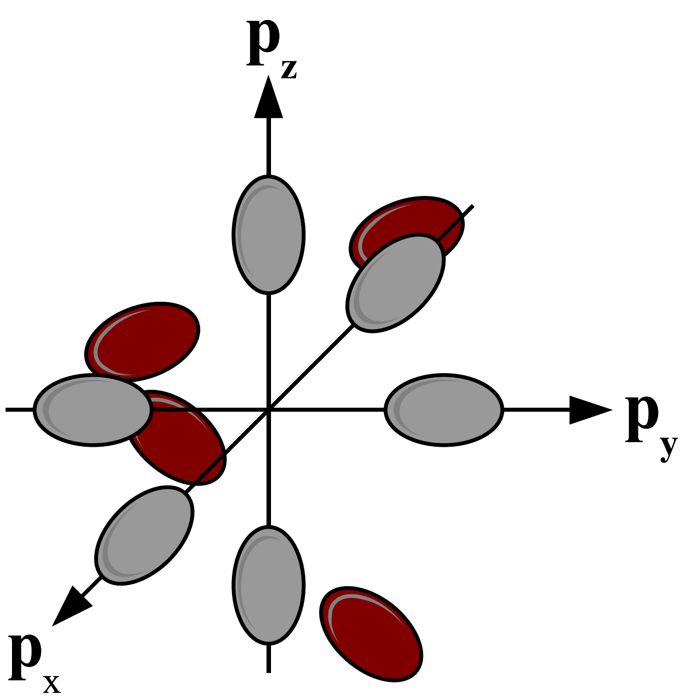
- Silicon on the left has six minima
- Germanium has four minima. A Ge-Si alloy has 4+6=10 minima



Si



Ge



Ge-Si alloy

Motivation to study semiconductors

- Multi-valley semiconductors are found in computers

- Current models for electrons in semiconductors are numerical and material specific
- Valleys can be used as an experimental parameter
- The new approximation is to assume the number of valleys is large which leads to useful analytical results

Electron gas of many flavours

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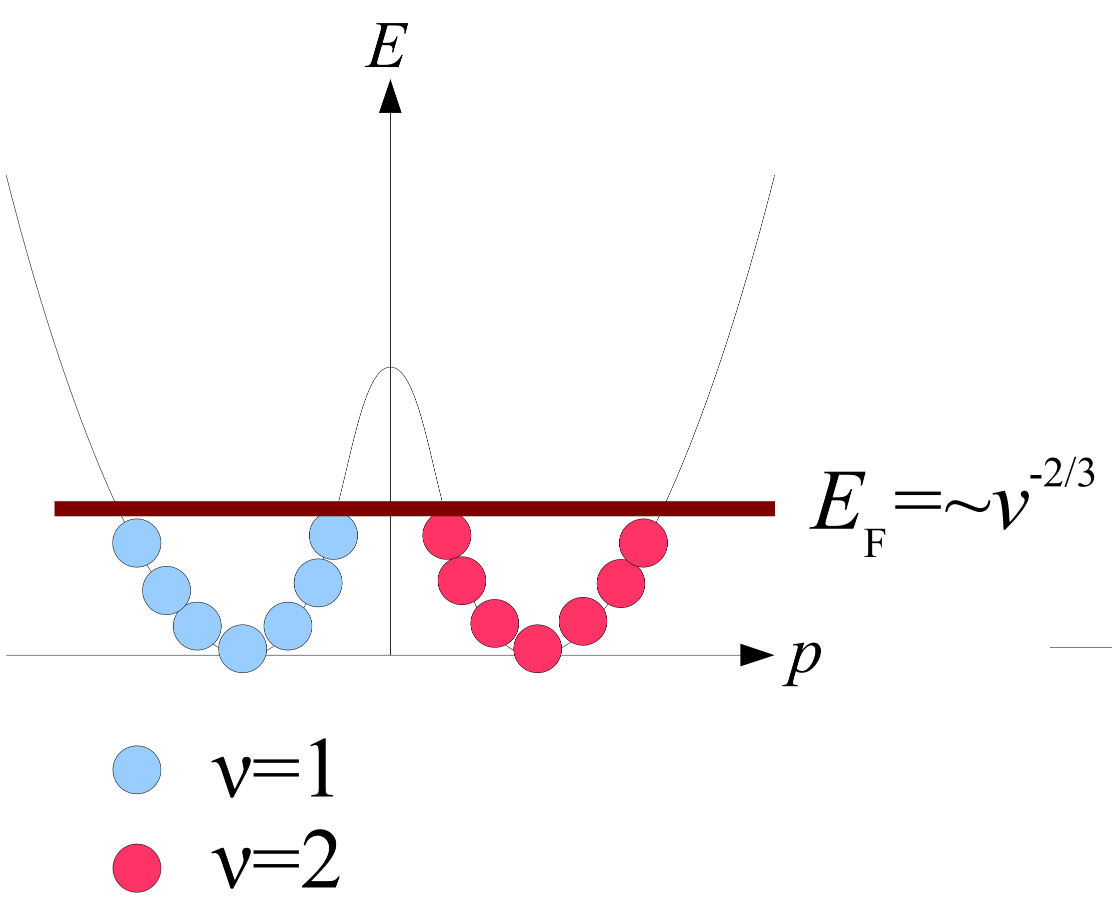
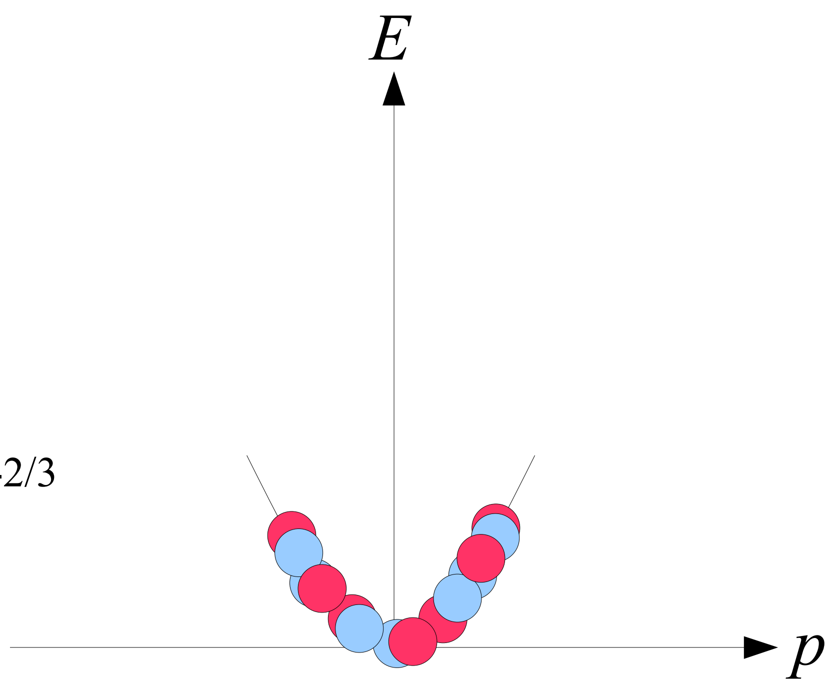
- Each valley looks like a free dispersion $E=p^2/2m$
- Associate a *flavour*, ν, with electrons in different valleys and put them all into one valley





Minimum has characteristic mass m^*

$$E=p^2/2m^*$$

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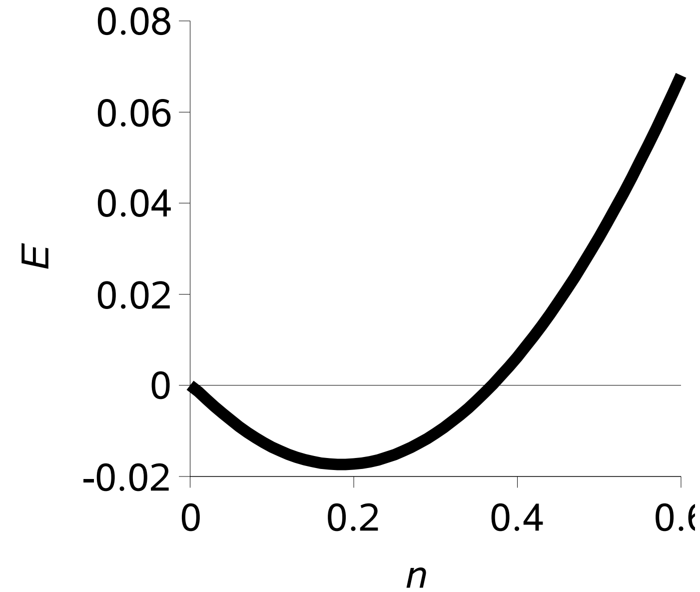
Analytical treatment

- In many flavour limit $\nu \gg 1$ the total energy density of the electron gas is

$$E=\underbrace{\frac{3}{10}\left(3\frac{\pi^2}{\nu}\right)^{2/3}n^{5/3}}_{\text{Non-interacting}}-\underbrace{\frac{32(2\pi)^{1/4}2^{1/2}}{5\Gamma^2(1/4)}n^{5/4}}_{\text{Interacting}}$$

- Minimum in the energy as a function of density



Many-flavor electron gas approach to electron-hole drops, GJC, Phys. Rev. B **78**, 035111 (2008)

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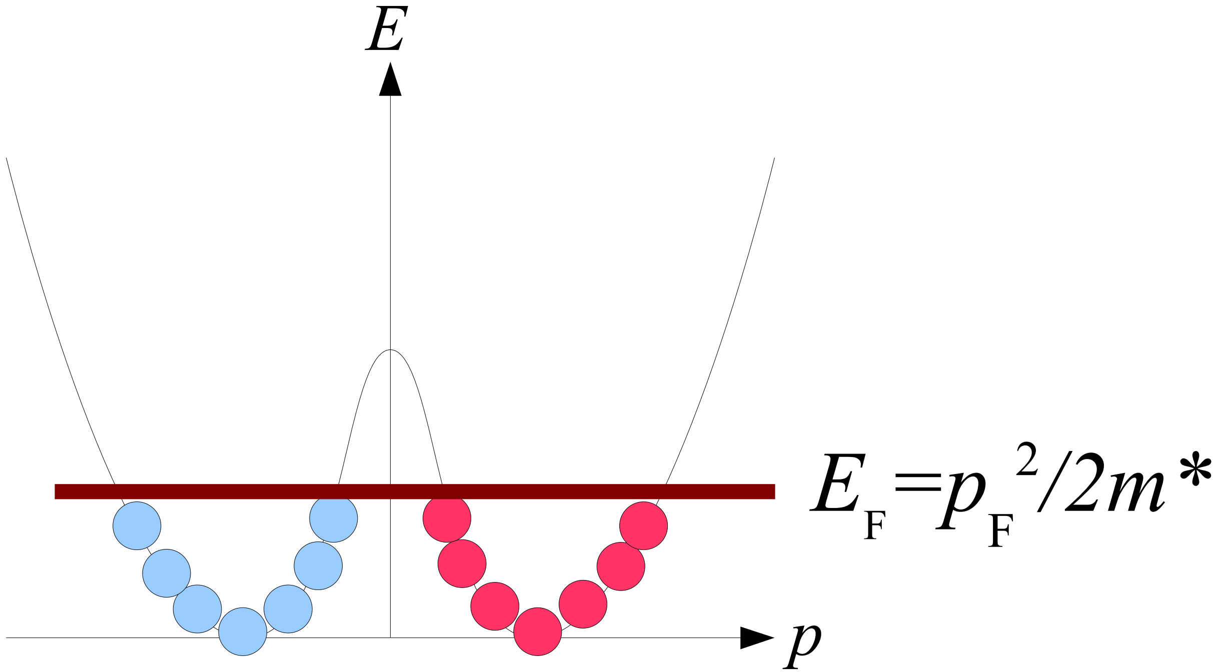
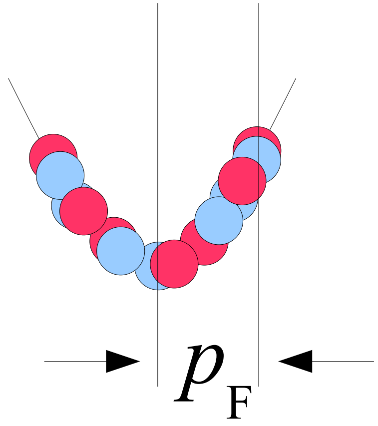
Gradient expansion

- The Fermi momentum is small so the electrons have a long characteristic de Broglie wavelength $\lambda=h/p_F$
- Electron density is expected to spatially vary slowly motivating a gradient expansion





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Analytical treatment

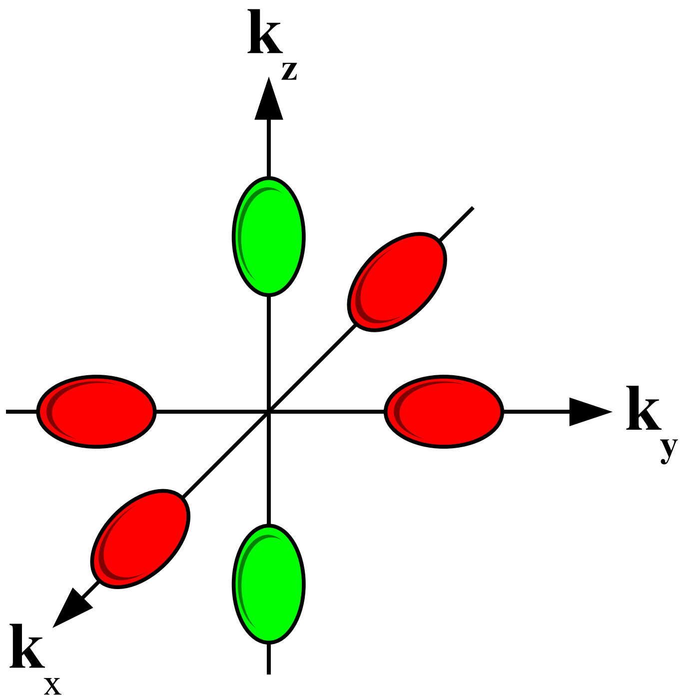
- Including the gradient term correction we get

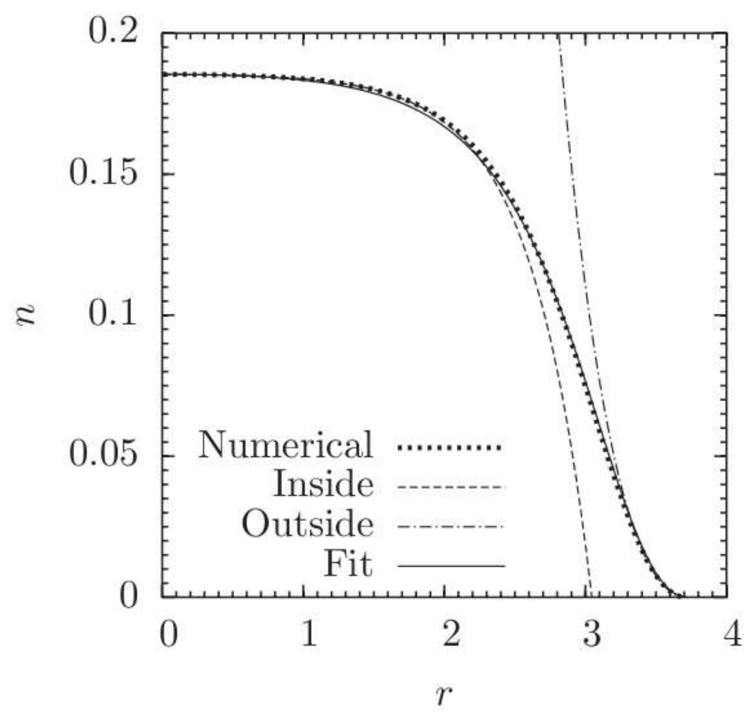
$$E = \frac{3}{10}\underbrace{\left(3\frac{\pi^2}{\nu}\right)^{2/3} n^{5/3}}_{\text{Non}-\text{interacting}} - \frac{32(2\pi)^{1/4}2^{1/2}}{5\Gamma^2\underbrace{(1/4)}_{}}\, n^{5/4} + \frac{(\nabla n)^2}{\underbrace{8\text{n}}_{\text{Gradient}}}.$$

- The formalism can now be applied to situations where density changes

Electron-hole drops

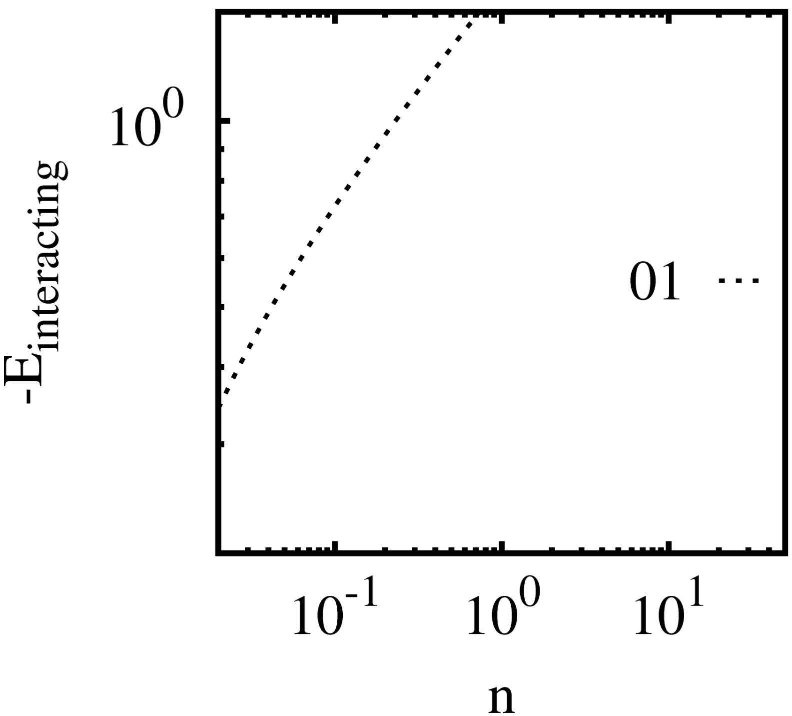
- If stress is applied to a semiconductor the number of valleys changes, e.g from 6 to 2
- The many-flavour theory provides a natural link to such experiments





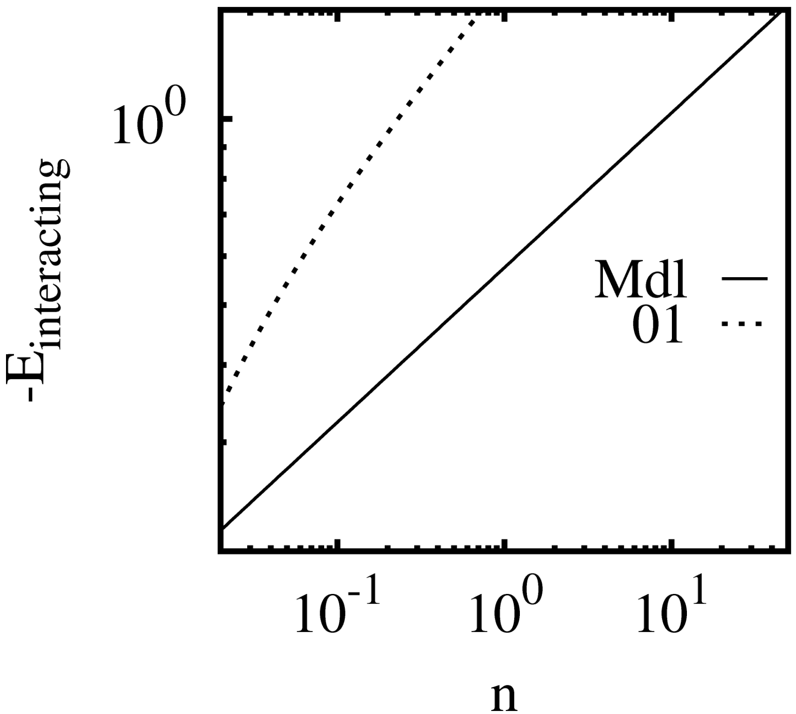
Uniform electron gas

- Computationally verify term for interacting energy using CASINO
- Graph shows interacting energy of electron gas with a single flavour



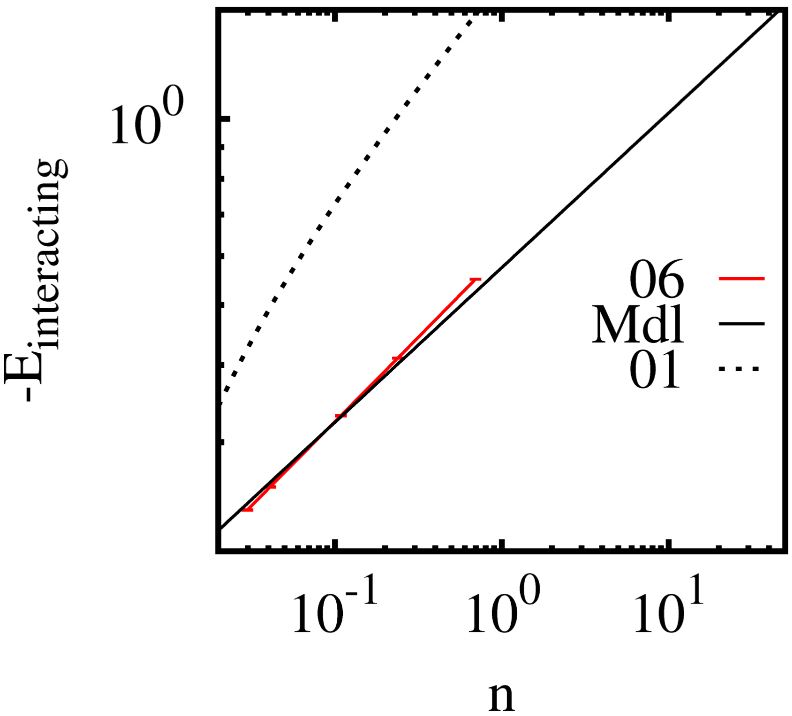
Uniform electron gas

- The solid line shows the analytical interacting energy, independent of number of flavours



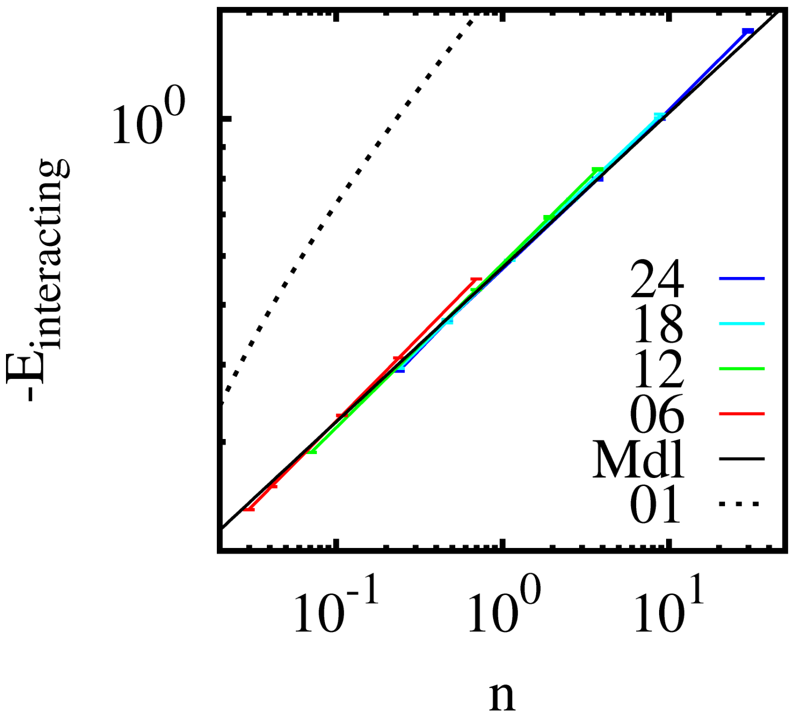
Uniform electron gas

- The red points show results for the interacting energy for simulations with six flavours
- The trendline passes through the analytical prediction



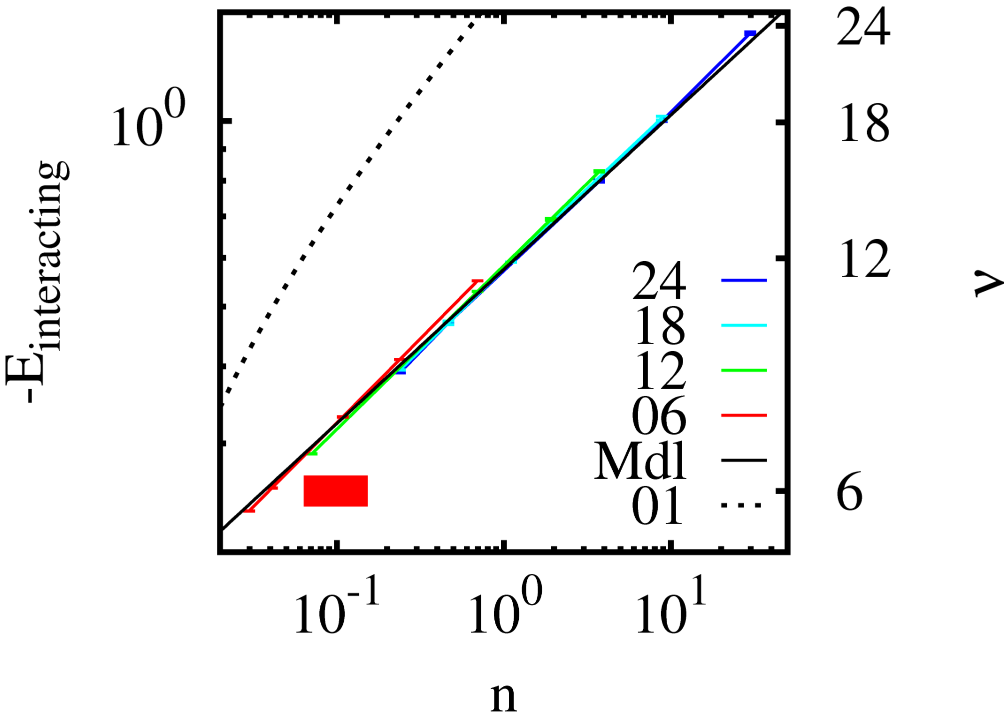
Uniform electron gas

- Green, light and dark blue correspond to results for 12, 18, and 24 flavours



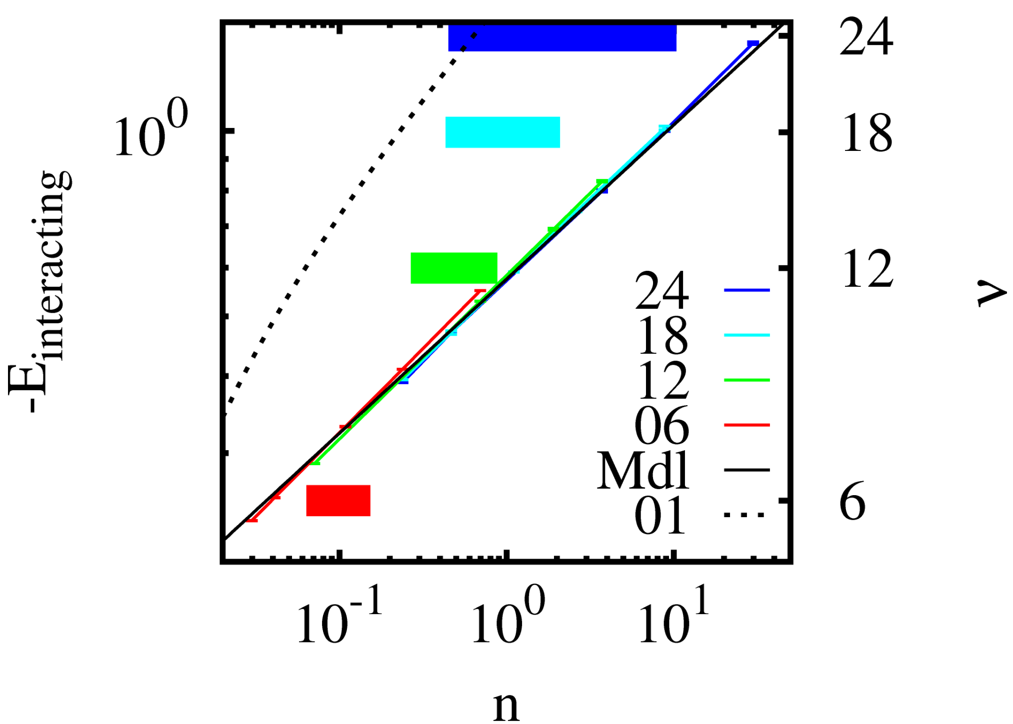
Uniform electron gas

- The thick red bar shows the range over which six flavour computational results and theory agree to ±1%
- Plotted against number of flavours on the secondary y-axis



Uniform electron gas

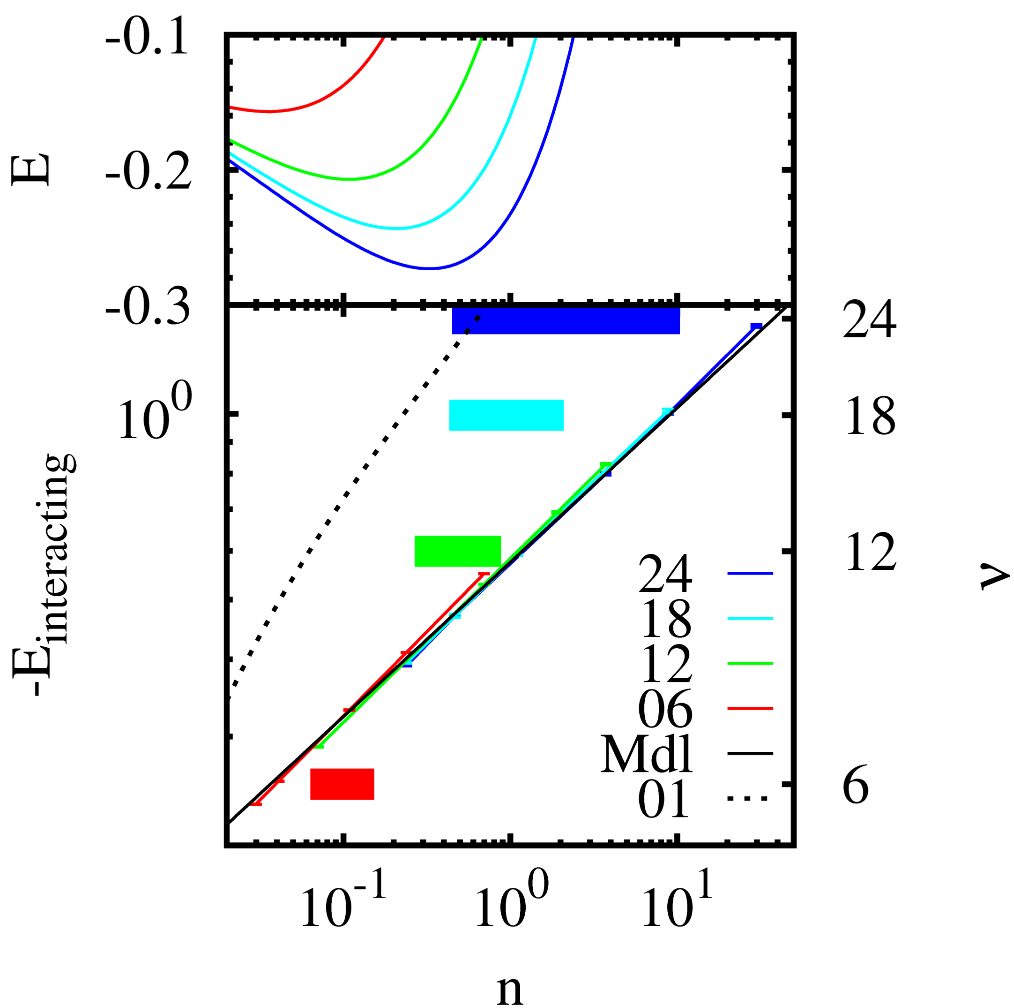
- Green, light and dark blue bars show where 12, 18, and 24 flavour results agree with theory to ±1%
- Range of applicability increases slowly up to 18 flavours
- The 24 flavour result applies over a broader range, consistent with



$$n_{lower} \propto \nu \qquad n_{upper} \propto \nu^4$$

Uniform electron gas

- Upper panel shows variation of total energy with number of flavours
- Range of applicability is typically at high density side of this minimum



Diffusion Monte Carlo study of a valley degenerate electron gas and application to quantum dots, GJC & PD Haynes, Phys. Rev. B **78**, 195310 (2008)

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Summary and further work

- We have derived analytical expressions for ground state energy of many flavour electron gas, and a local gradient expansion
- The theory has been applied to electron-hole droplets and quantum dots
- Using CASINO we have verified the ground state energy and the density response function