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Gareth Conduit

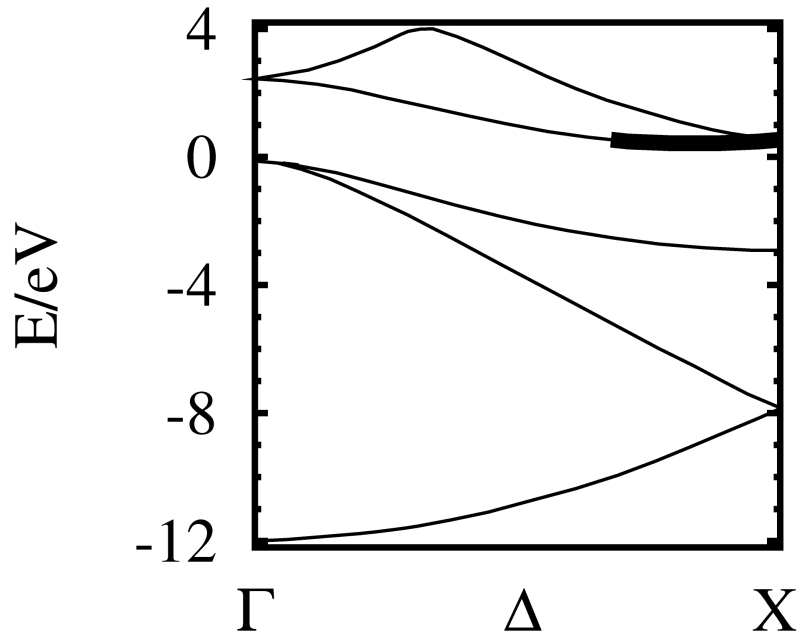
Electron gas of many flavours – Talk outline

- What is an electron gas of many flavours?
- Analytical results
- Computational verification
- Summary and further work

Work carried out in collaboration with Peter Haynes and David Khmelnitskii.

Electron gas of many flavours

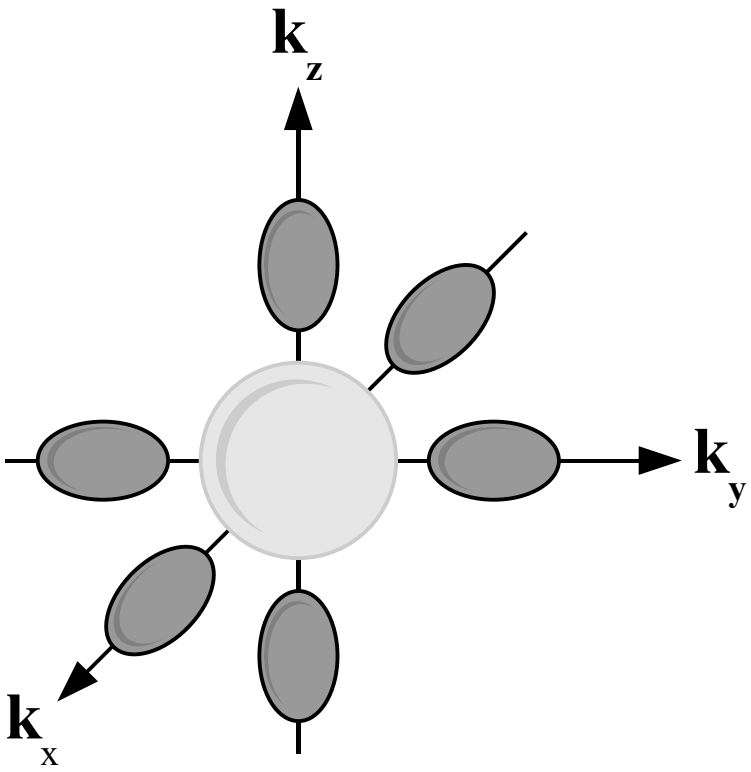
- Some semiconductors and semimetals have conduction band minima away from Γ point; these are degenerate by symmetry.
- Germanium has four minima, Silicon six. A Ge-Si alloy has 4+6=10 minima.



Electron gas of many flavours

- Electrons in different valleys do not obey Pauli exclusion principle with respect to each other, so there is a new quantum number, flavour ν.
- For given electron density n the Fermi momentum p_F is reduced

$$p_F = \sqrt[3]{\frac{3\pi^2 n}{\nu}}.$$



Analytical treatment

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

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

- The negative interacting term means there is a minimum in the energy as a function of density.

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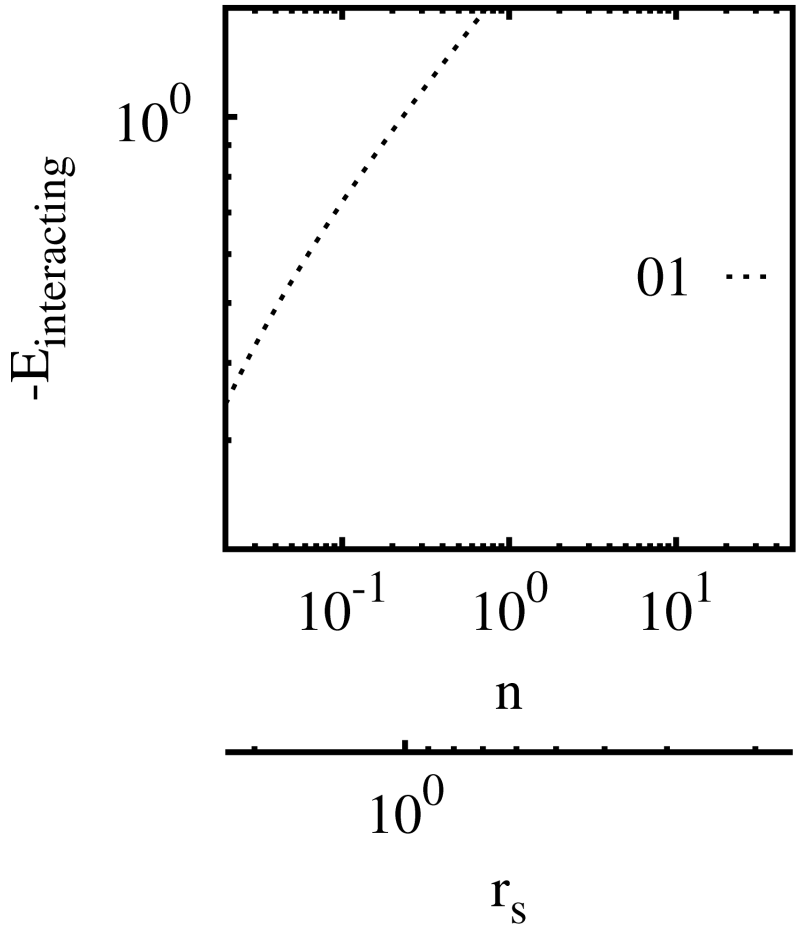
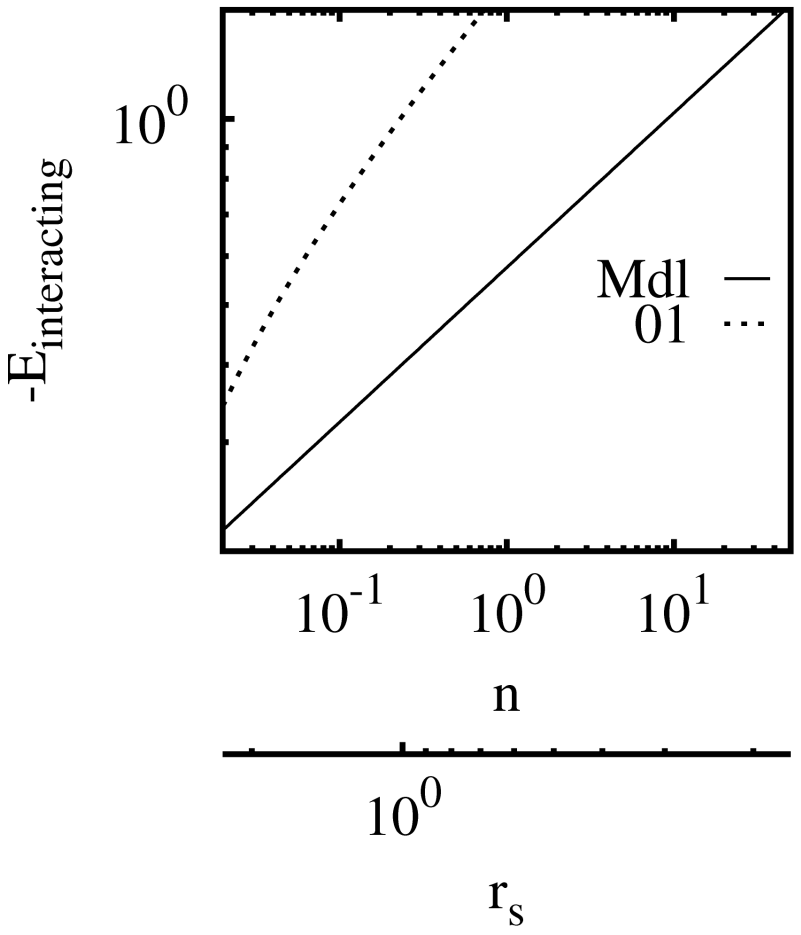
Uniform electron gas

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



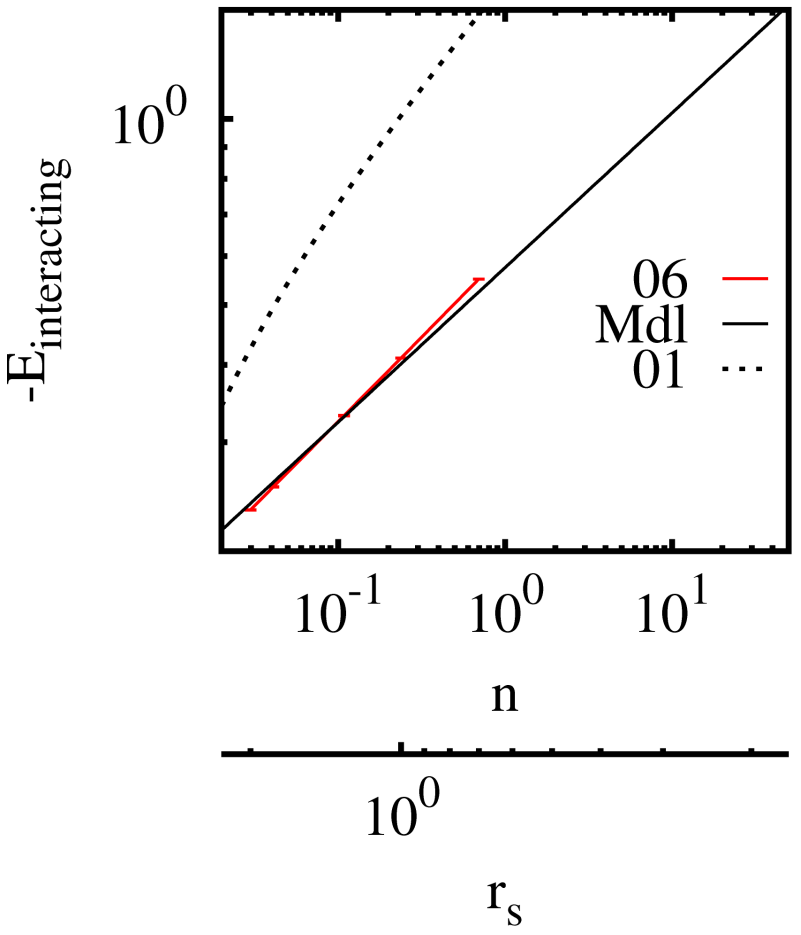
Uniform electron gas

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



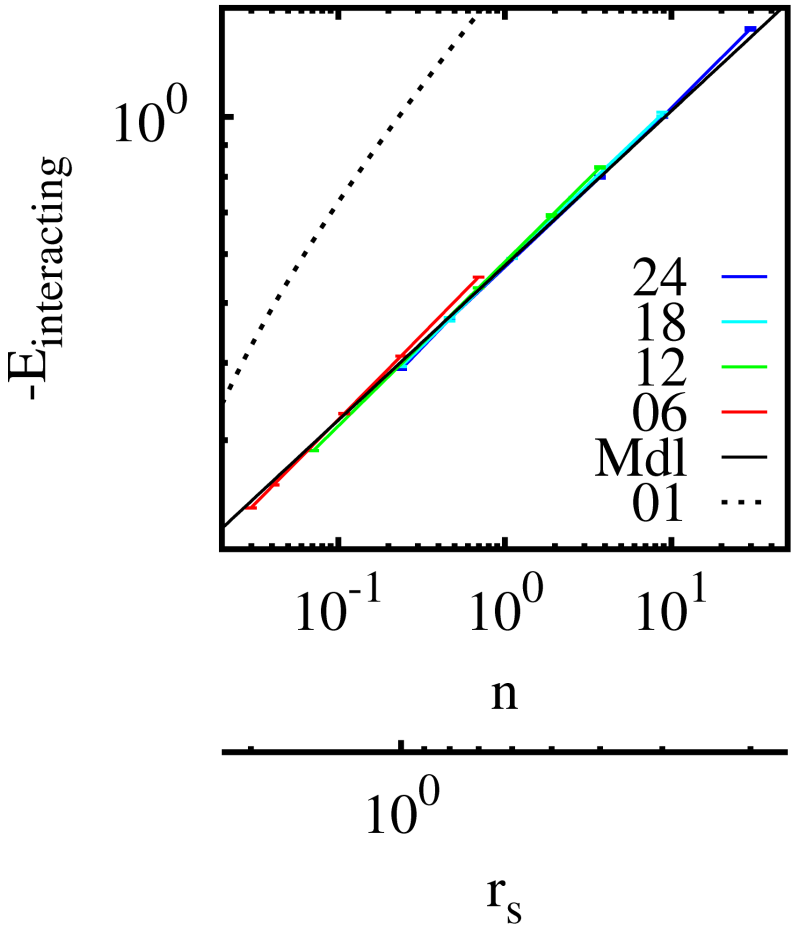
Uniform electron gas

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



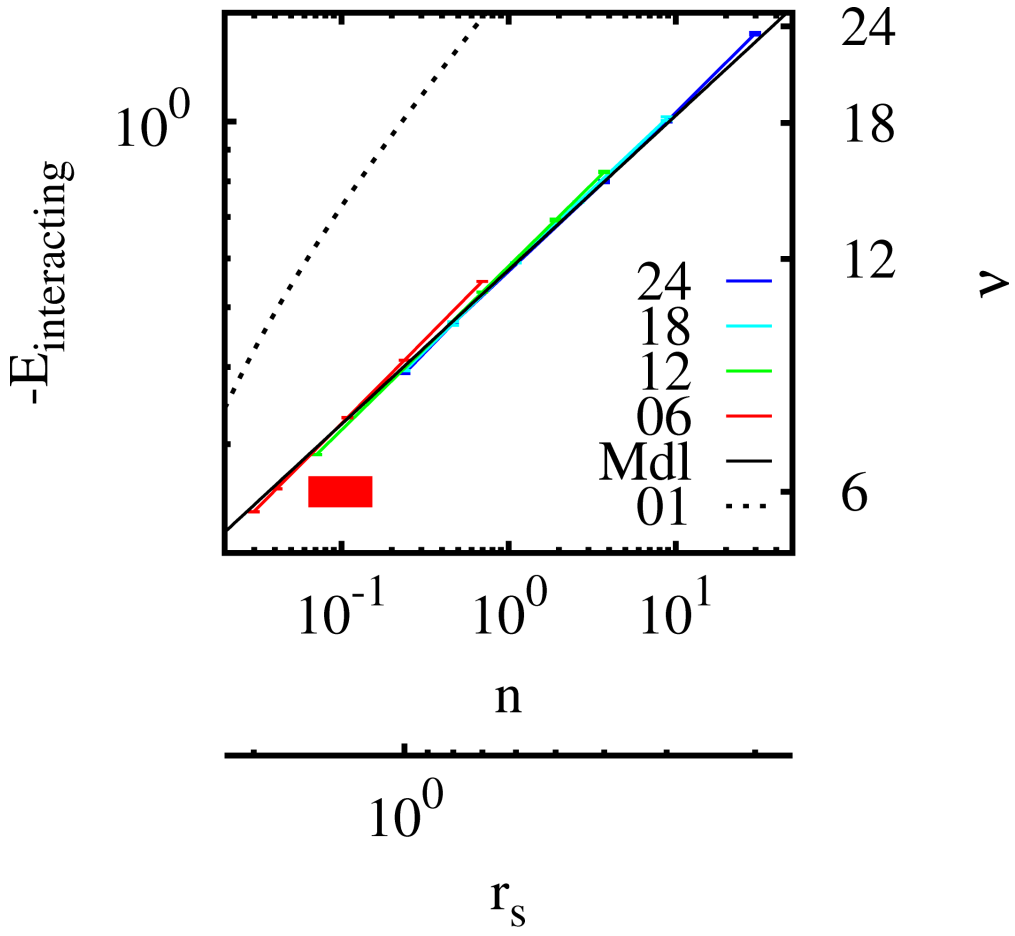
Uniform electron gas

- 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.



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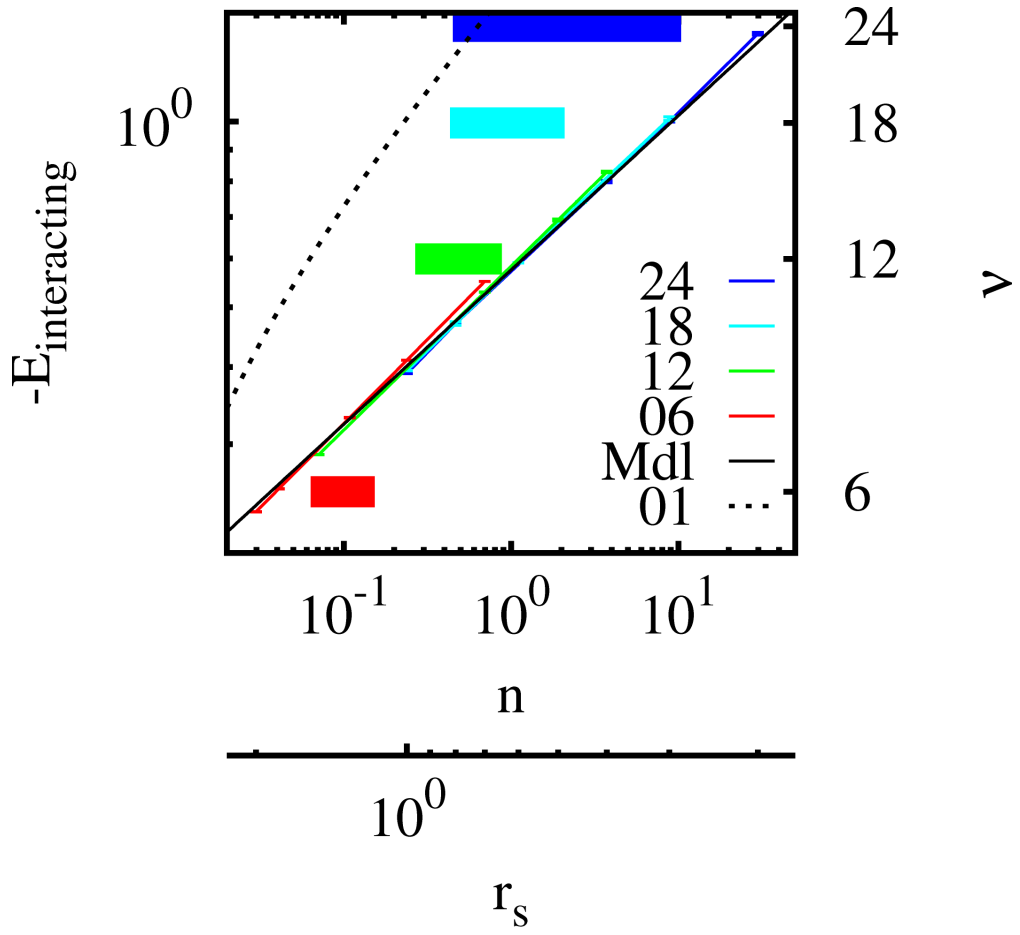
Uniform electron gas

- 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

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



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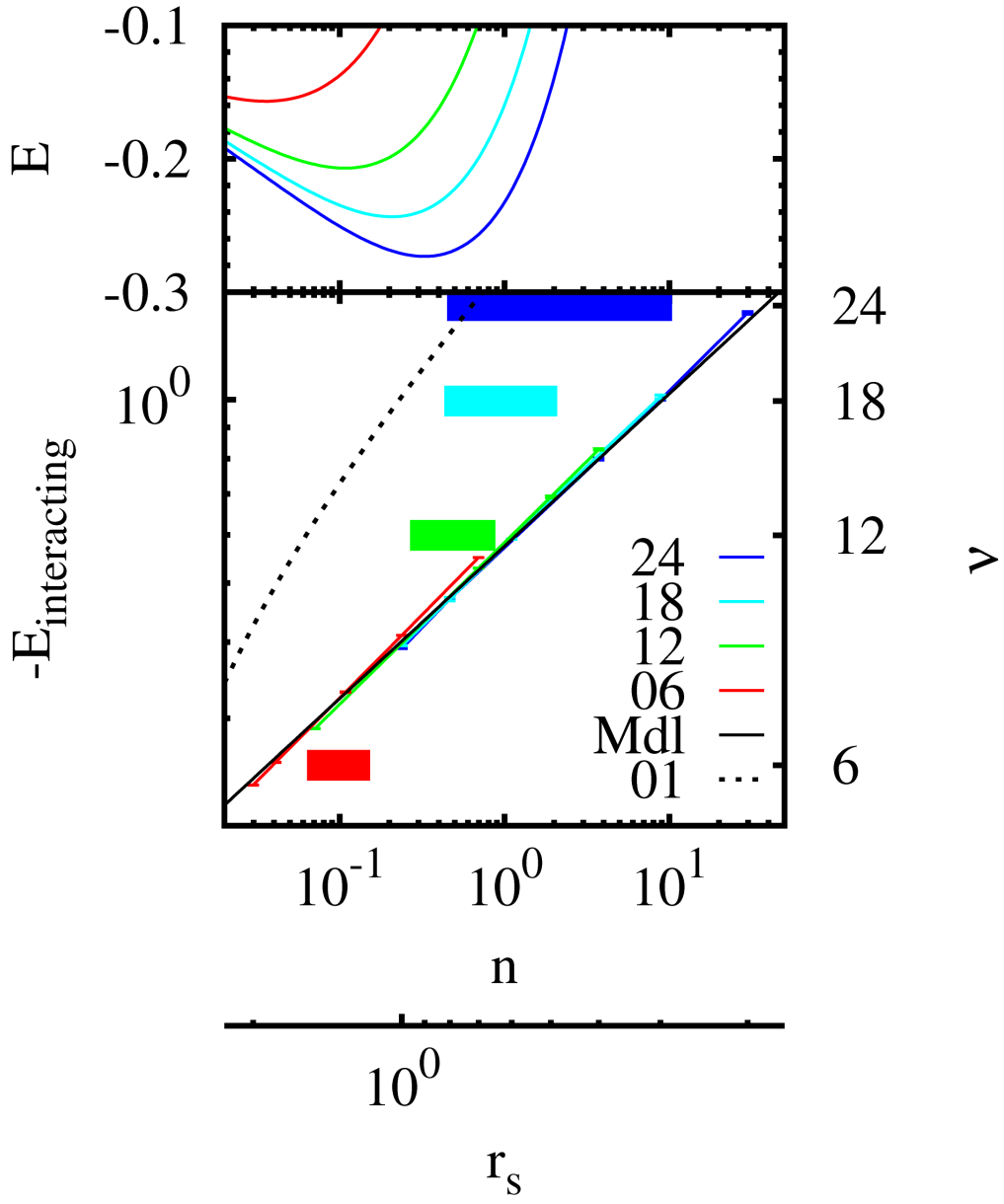
Uniform electron gas

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



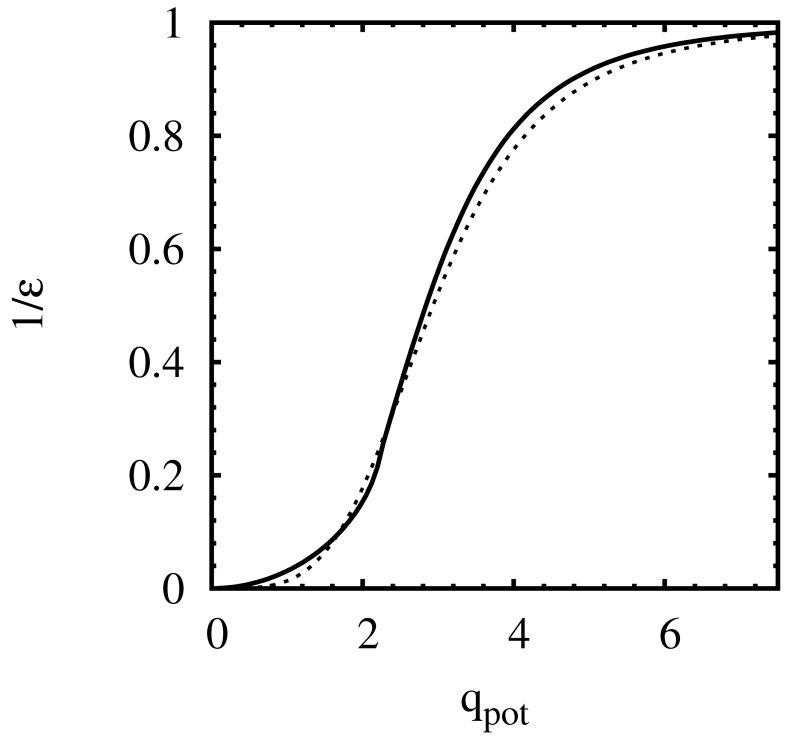
Density response function

- The density response to an external potential is

$$\Delta n(\mathbf{q}) = \frac{q^2}{4\pi}\left(\frac{1}{\epsilon(\mathbf{q})} - 1\right) U(\mathbf{q}).$$

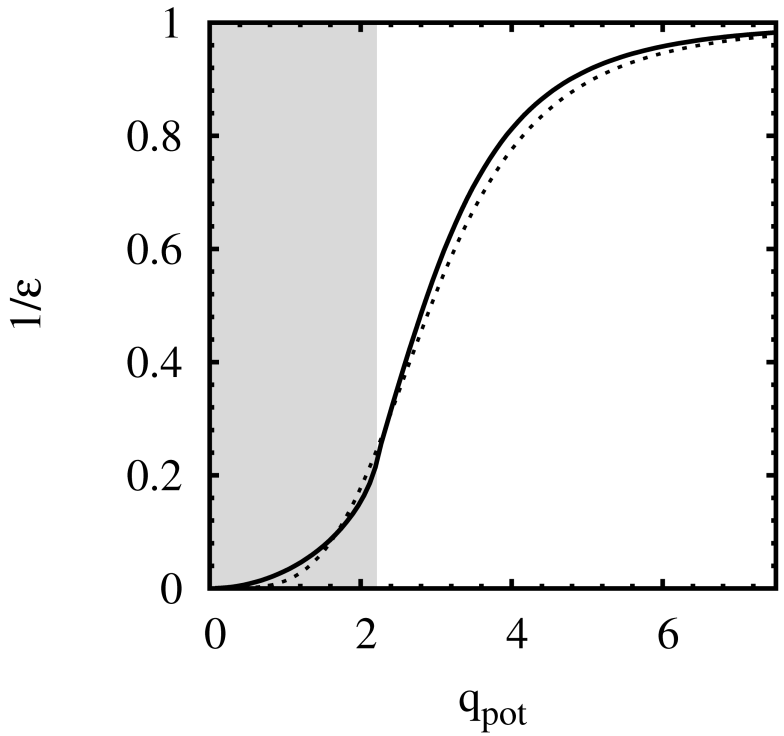
- Solid line shows the exact expression for $1/\epsilon(\mathbf{q})$.
- The dotted line shows an approximate expression

$$\frac{1}{\epsilon(\mathbf{q})} = \frac{1}{1 + 16\pi n/q^4}.$$



Density response function

- The shaded region shows where the theory is not expected to apply, $q < 2p_F$.
- A perturbing potential $U(q)\cos(qz)$ was applied to the uniform electron gas, and the ground state found with CASINO at different external potential strengths.
- From this we can estimate $1/\epsilon$ at the perturbing potential wave vector.



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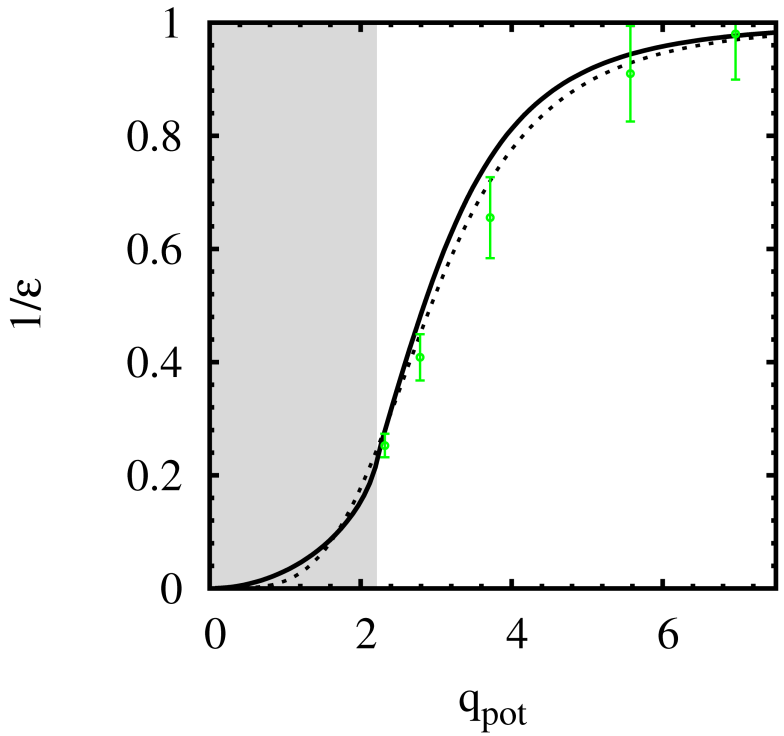
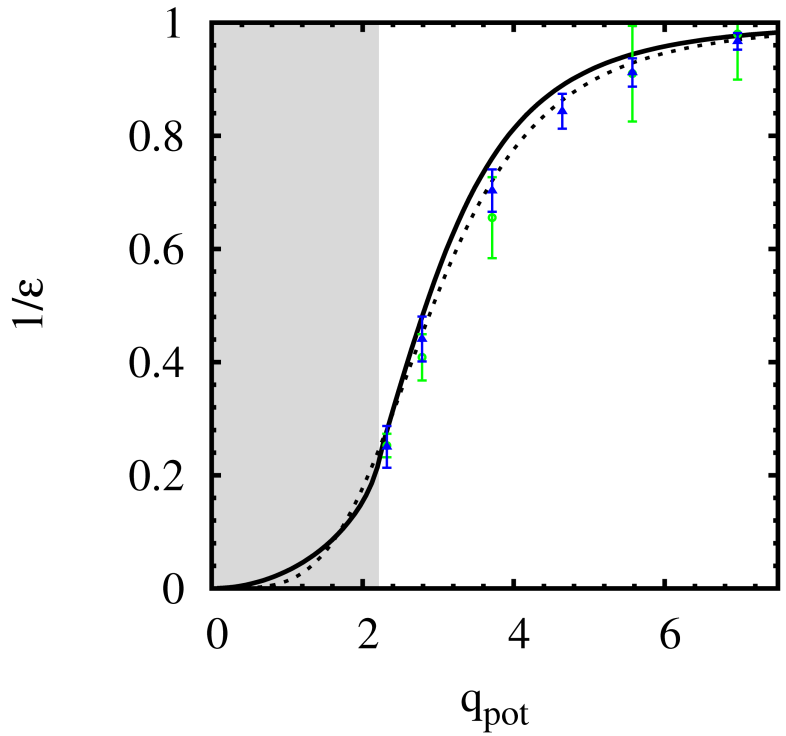
Density response function

- Simulations were run for a system with 24 flavours with density r_s=0.6.
- Green points shows results found by examining change in electron density in VMC.
- There are large errors as density does not commute with the Hamiltonian.



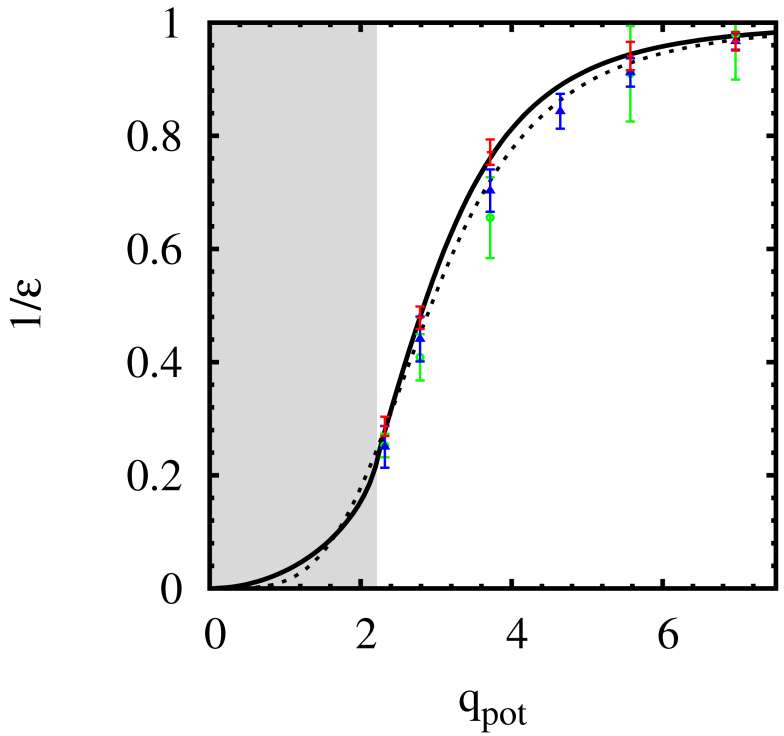
Density response function

- Blue points were estimated by VMC energy.
- These have smaller errors as they were estimated from the energy eigenstates.
- The function is again underestimated, but results are consistent with the VMC density results.



Density response function

- Red points found be looking at DMC energy.
- These more accurately predict the density response and agree better with the exact function.
- The DMC results can distinguish between the exact and approximate functions.



Summary and further work

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