Electron Gases of Many Flavours

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INTRODUCTION

1. OVERALL AIM

Analyse many flavour electron gases.

SPECIFIC AIMS OF THIS PROJECT

- Derive new analytical results for the system.
- Apply the formalism to electron-hole droplets.
- Verify the analytical results computationally.

2. BACKGROUND

Some semiconductors such as Si, Ge, and GaP have conduction band minima near the Brillouin zone boundary, Si has six degenerate valleys (Fig. 1).

We introduce a new quantum number, the *flavour*, which denotes an electron's valley. The total number of flavours is the number of valleys, ν. The Fermi momentum falls with number of flavours as

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

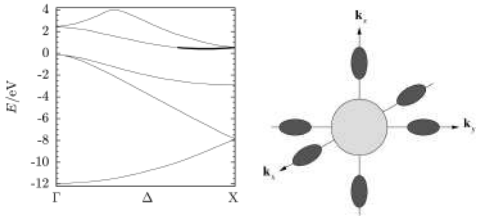

Fig. 1. *Left*: A conduction band minimum (bold curve) in the Si band structure. *Right*: The Fermi surface in Si (dark grey), and the surface of a single conduction band valley at Γ (light grey).

ANALYTICAL

3. LOCAL ENERGY

The polarisability was found to be

$$\Pi_0(\mathbf{q},\omega) = \frac{-n}{(\omega/q)^2 - q^2/4}$$

The uniform energy density was found with a functional integral analysis. A gradient expansion was derived using the polarisability giving

$$E = \frac{3}{10}\left(\frac{3\pi^2}{\nu}\right)^2 n^{5/3} - A_{3\mathrm{D}} n^{5/4} + \frac{|\nabla n|^2}{8n}.$$

The uniform density corresponding to the minimum in energy is expected to be seen in physical systems.

Typical length-scales of the many flavour electron gas are short so the functional is suitable for DFT.

4. ELECTRON-HOLE DROPLET

An approximation to the outer drop density profile is

$$n(r) = n_0\left(\frac{1}{r} - \frac{1}{r_0}\right)^2, r < r_0.$$

This is equivalent to solving Schrödinger's equation at low energy. The outside of the drop has a parabolic density profile with a definite cut-off. A possible analytical fitting function for the density profile is

$$n(r) = 1\Big/\left(\frac{1}{n_0(1/r - 1/r_0)} + \frac{1}{\bar{n}}\right).$$

Solutions for the density were also obtained numerically. The drop density profile is shown in Fig. 2.

The drop surface tension and surface thickness approach constant values as dot size increases. Their scaling relations $S\mu\nu^{9/5}$ and $D\mu\nu^{1/5}$ are consistent with numerical results.

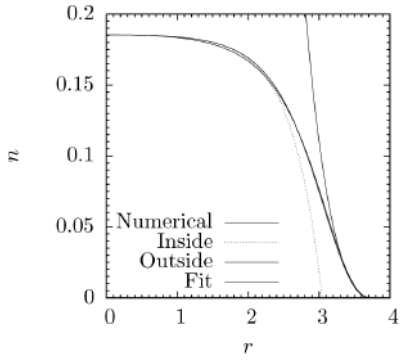

Fig. 2. An electron-hole drop density profile. Numerical results (solid line) are compared with analytical approximations (dotted lines). An analytical fitting function that approximates the entire density profile is shown by the dashed line.

COMPUTATIONAL

5. POLARISABILITY

A perturbative external potential $U=U_0\cos(qr)$ was applied to a uniform electron gas. This allowed us to probe the density response $1/\varepsilon$ at wave vector $\mathbf{q}$.

The two sets of results (Fig. 3), measured using VMC, consistently underestimate the density response. The DMC results agree with the analytic density response function and we are able to distinguish between the exact and approximate form for the response.

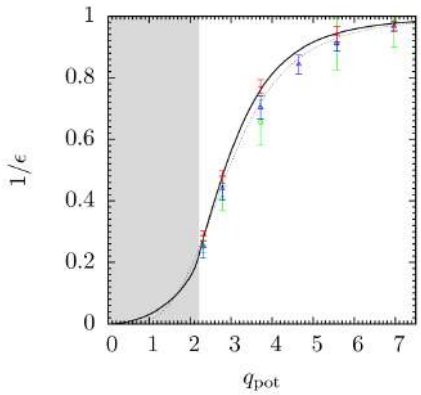

Fig. 3. The density response with external wave vector. Green points are found by directly measuring density following a VMC calculation, and blue by the change in energy. The red points were estimated from change in energy following a DMC simulation.

6. UNIFORM BACKGROUND

We ran DMC [2] simulations on a uniform electron gas and compared the calculated and analytic energy (Fig. 4).

The theory applies to ±1% over an order of magnitude in density. The lower critical density scales as $n\mu\nu$, the upper as $n\mu\nu^4$ (on going to 24 flavours). The range of applicability coincided with the total energy minimum.

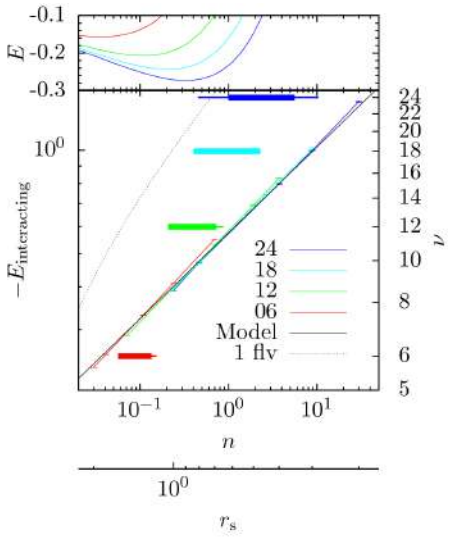

Fig. 4. The lower panel shows interacting energy versus density found using DMC for 6, 12, 18 and 24 flavours. The black line is the model, the dotted the single flavour result. The upper panel shows the analytic total energy density.

7. GRADIENT EXPANSION

We ran DFT calculations based on our functional to predict the ground-state in a quantum dot with parabolic potential $U=kr^2$. We checked our results by calculating the DMC energy.

Results (Fig. 5) show the DFT functional breaks down at low density as the uniform energy density no longer applies. The functional fails at high potential strength k as the gradient approximation breaks down.

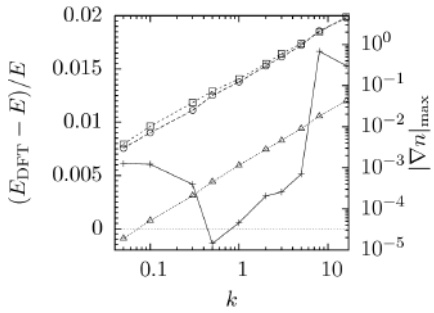

Fig. 5. The fractional deviation of DFT predicted energy from DMC energy versus strength of external potential k is shown by the crosses, the horizontal dashed line shows exact agreement. The dashed lines show the maximum allowed gradient (squares), maximum dot gradient (circles), and minimum allowed gradient (triangles) based on the secondary y-axis.

CONCLUSIONS

We developed new formalism for an electron gas of many flavours; a system that could be found in a multivalley semiconductor.

We found an exact expression for the energy density in a uniform system and a gradient expansion. The functional is suited to DFT.

The density profile of electron-hole drops was derived; and the surface tension and thickness investigated.

Analytical results for total energy, polarisability and the gradient expansion were computationally verified using QMC simulations.

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