

Part III Advanced Quantum Condensed Matter Physics

Question sheet II

1. Spin-polarized HF electron gas

Investigate under which conditions a fully spin-polarized HF electron gas with all electrons in a spin-up state has a lower energy than a normal HF electron gas, in which each HF single-electron orbital is doubly occupied by a spin-up and a spin-down electron.

Ground state energy of the normal HF electron gas without spin polarization:

$$E_0^{norm} = N \left(\frac{3 \hbar^2 k_F^2}{5 \cdot 2m} - \frac{3 e^2 k_F}{16 \pi^2 \epsilon_0} \right)$$

Ground state energy of the fully spin-polarized HF electron gas obtained from the above expression by replacing k_F by $2^{1/3} k_F$:

$$E_0^{pol} = N \left(\frac{3 \hbar^2 (2^{1/3} k_F)^2}{5 \cdot 2m} - \frac{3 e^2 (2^{1/3} k_F)}{16 \pi^2 \epsilon_0} \right)$$

Condition for spin-polarized ground state:

$$\frac{3 \hbar^2 (2^{1/3} k_F)^2}{5 \cdot 2m} - \frac{3 e^2 (2^{1/3} k_F)}{16 \pi^2 \epsilon_0} < \frac{3 \hbar^2 k_F^2}{5 \cdot 2m} - \frac{3 e^2 k_F}{16 \pi^2 \epsilon_0}$$

$$k_F < \frac{5}{2\pi} \frac{1}{2^{1/3} + 1} \frac{m e^2}{4\pi \epsilon_0 \hbar^2} = \frac{5}{2\pi} \frac{1}{2^{1/3} + 1} \frac{1}{a_B}$$

$$\Rightarrow r_s > 5.45$$

Prediction of a normal to ferromagnetic transition at low densities. However, the value of $r_s = 5.45$ is not realistic since this is in the range of common metal carrier densities, and ordinary metals are not spin-polarized. By taking into account correlations of the jellium model, the value of r_s at which the transition is expected is shifted to $r_s = 75$.

2. Density functional theory

Write an essay about density functional theory (DFT). For which problems is DFT particularly powerful, for which problems is DFT less suitable?

- Hohenberg-Kohn theorem, determination of ground state density from Kohn-Sham equations; local density approximation
- Order N scaling to obtain exact ground state energy and density

- Very accurate (1%) determination of binding energies, bond lengths, vibrational frequencies etc.
- Can be coupled to molecular dynamics for atomistic simulations (surface diffusion, protein folding, etc.)
- No justification for interpretation of ε_i in Kohn-Sham equations as quasiparticle energies, therefore application to band structure calculation not straightforward.
- Size limitation to $N = 1000-10000$, picosecond timescales.

3. Ground state energy in Density Functional theory

Show that the ground state energy in Density-Functional Theory is given by:

$$E_0 = \sum_i \varepsilon_i - \frac{1}{2} \sum_{i,j} \langle \phi_i \phi_j | \frac{e^2}{4\pi\epsilon_0 r_{12}} | \phi_i \phi_j \rangle + E_{xc}[n] - \int d^3r V_{xc}(r) n(r)$$

- Multiply Kohn-Sham equations with $\phi_i^*(\vec{r})$, and integrate over r :

$$\sum_i \int \phi_i^*(\vec{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{nucl}(\vec{r}) + V_{coul}(\vec{r}) + V_{xc}(\vec{r}) \right] \phi_i(\vec{r}) = \sum_i \varepsilon_i$$

- Compare terms with:

$$E[n(\vec{r}); v_{ext}(\vec{r})] = \sum_i \langle \phi_i | -\frac{\hbar^2 \nabla^2}{2m} + v_{ext} | \phi_i \rangle + \frac{1}{2} \sum_{i,j} \langle \phi_i \phi_j | \frac{e^2}{4\pi\epsilon_0 r_{12}} | \phi_i \phi_j \rangle + E_{xc}[n]$$

4. Local Density approximation (see below)

LDA - DFT

- LDA: - a assumption that locally, in a sufficiently small volume the exchange correlation energy density can be represented as that of a homogeneous electron gas with that local density
- exchange - correlation energy of homogeneous electron gas is known exactly
 - LDA provides explicit form of density dependence of $E_{xc}[n]$

$$\rightarrow E_{xc}[n] = -\frac{A}{r_s} + B \ln r_s + \text{const } C$$

$$\frac{4}{3}\pi (r_s a_B)^3 = \frac{V}{N} = \frac{1}{n} \quad r_s = \frac{1}{a_B} \left(\frac{3}{4\pi}\right)^{1/3} n^{-1/3}$$

$$E_{xc}[n] = -A a_B \left(\frac{4\pi}{3}\right)^{1/3} n^{1/3} + B \ln \left(\frac{1}{a_B} \left(\frac{3}{4\pi}\right)^{1/3} n^{-1/3}\right) + \text{const } C$$

$$V_{xc}[n] = \frac{d}{dn} (n \cdot E_{xc}[n]) = -A a_B \left(\frac{4\pi}{3}\right)^{1/3} \frac{4}{3} n^{-2/3} + \frac{d}{dn} (B n \ln \left(\frac{1}{a_B} \left(\frac{3}{4\pi}\right)^{1/3} n^{-1/3}\right)) + C$$

$$= -A a_B \left(\frac{4\pi}{3}\right)^{1/3} \frac{4}{3} n^{-2/3} + B \ln \left(\frac{1}{a_B} \left(\frac{3}{4\pi}\right)^{1/3} n^{-1/3}\right) + B \cdot n \cdot \left(-\frac{1}{3}\right) n^{-4/3}$$

$$+ B \cdot n \cdot a_B \left(\frac{4\pi}{3}\right)^{1/3} - \frac{B}{3} + C$$

→ homogeneous electron jellium

$$- V_{xc}[r] = \text{const}$$

$$- p_i \propto \epsilon^{ik} \hat{k}$$

- Hartree term cancelled with ion-ion interaction

$$\Rightarrow \epsilon(k) = \frac{\hbar^2 k^2}{2m} - A a_B \left(\frac{4\pi}{3}\right)^{1/3} \frac{4}{3} n^{1/3} + B \ln \left(\frac{1}{a_B} \left(\frac{3}{4\pi}\right)^{1/3} n^{-1/3}\right)$$

$$- \frac{B}{3} + C = \frac{\hbar^2 k^2}{2m} - \frac{4A}{3 r_s} + B \ln r_s - \frac{B}{3} + C$$

→ dispersion relationship still quadratic, $m^* = m_e$, but shifted in energy to lower values; HF different energy shift, effective mass, deviation from quadratic dispersion

→ Total energy of HF/DFT is the same since kinetic energy

$T_e[n]$ is the same, Hartree term cancelled in both cases

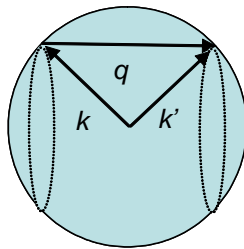
$$\text{and } E_{xc}^{\text{DFT}}/N = E_{xc} \text{ for } n \text{ const}$$

5. Provide an argument why the imaginary part of the dielectric function of a homogeneous electron gas is zero at $\omega = 0$: $\varepsilon_2(\vec{q}, \omega = 0) = 0$

Hint: Consider the condition on momentum conservation that is implied in the expression below for ε_2 , and determine the region in phase space which satisfies this condition.

$$\varepsilon_2(\vec{q}, \omega) = \frac{2\pi e^2}{\varepsilon_0 |\vec{q}|^2 V} \sum_{\alpha, \beta} \left| \langle \psi_\beta | e^{i\vec{q}\cdot\vec{r}} | \psi_\alpha \rangle \right|^2 \delta(E_\beta - E_\alpha - \hbar\omega) [f(E_\alpha) - f(E_\beta)]$$

Inserting plane waves for the wavefunctions one obtains $k' = k + q$. For $\omega = 0$ the energy conservation condition and the condition imposed by the occupation factor is only satisfied on a 1D ring perpendicular to q , the radius of which shrinks to zero as q approaches $2k_F$. For the 2D integration in k -space which is left to do after the delta function introduced by the momentum conservation, this is a surface of zero area.



6. **Weiss mean field theory of magnetism**

Show that for a system of independent paramagnetic moments of total spin S in an external magnetic field B the magnetisation is given by:

$$\frac{M}{M_s} = B_s(y) \quad y = \frac{g\mu_B SB}{k_B T} \quad M_s : \text{saturation magnetization}$$

$$B_s(y) = \frac{2S+1}{2S} \coth\left(\frac{2S+1}{2S} y\right) - \frac{1}{2S} \coth\frac{y}{2S} \quad : \text{Brillouin function}$$

Hint: Start with the expression below for the magnetisation in thermodynamic equilibrium, where n is the concentration of paramagnetic moments, and derive a system. Calculate the partition function, and then use the relationship between Z and M to calculate the magnetisation.

$$M = -n \frac{\sum_{S_z=-S}^S g\mu_B S_z e^{-\frac{g\mu_B S_z B}{k_B T}}}{\sum_{S_z=-S}^S e^{-\frac{g\mu_B S_z B}{k_B T}}}$$

The partition function is given by:

$$Z = \sum_{S_z=-S}^S e^{-\frac{g\mu_B S_z B}{k_B T}} \Rightarrow M = nk_B T \frac{\partial \ln Z}{\partial B}$$

$$x = \frac{g\mu_B B}{k_B T} \quad P = 2S + 1$$

$$Z = e^{-\frac{g\mu_B S B}{k_B T}} \left(1 + e^x + (e^x)^2 + (e^x)^3 + \dots + (e^x)^{P-1} \right) = e^{-\frac{g\mu_B S B}{k_B T}} \frac{1 - (e^x)^P}{1 - e^x}$$

$$= \frac{\sinh\left[(2S+1)\frac{x}{2}\right]}{\sinh\left[\frac{x}{2}\right]}$$

$$M = nk_B T \frac{g\mu_B}{k_B T} \frac{\sinh\left[\frac{x}{2}\right] \frac{(2S+1)}{2} \cosh\left[(2S+1)\frac{x}{2}\right] \sinh\left[\frac{x}{2}\right] - \sinh\left[(2S+1)\frac{x}{2}\right] \frac{1}{2} \cosh\left[\frac{x}{2}\right]}{\left(\sinh\left[\frac{x}{2}\right]\right)^2}$$

$$= ng\mu_B \left(\frac{(2S+1)}{2} \coth\left[(2S+1)\frac{x}{2}\right] - \frac{1}{2} \coth\left[\frac{x}{2}\right] \right)$$

$$= ng\mu_B S \left(\frac{(2S+1)}{2S} \coth\left[\frac{(2S+1)}{2S} y\right] - \frac{1}{2S} \coth\left[\frac{y}{2S}\right] \right) \quad y = xS$$

Explain how this result can be used to calculate the magnetisation as a function of temperature of a ferromagnet in mean field theory.

Introduce molecular field $B_{mf} = \lambda M$ which adds to the external field, and can then be treated formally in the same way as the paramagnet case. Equation involving Brillouin function can be solved graphically (see lecture notes).

7. Uniaxial ferromagnet

A uniaxial ferromagnet is described by the Hamiltonian:

$$H = -\sum_i 2J_0 \vec{S}_i \cdot \vec{S}_{i+1} - \sum_i 2K_0 S_i^z \cdot S_{i+1}^z$$

(a) *Discuss the physical origin of the second term in the Hamiltonian.*

Uniaxial magnetocrystalline anisotropy, z-axis is the easy axis of magnetization

(b) Show that the state with all spins fully aligned along the z-axis is an eigenstate of the Hamiltonian.

$$\begin{aligned} (S_i^x S_j^x + S_i^y S_j^y) |\uparrow\uparrow \dots \uparrow\rangle &= \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) |\uparrow\uparrow \dots \uparrow\rangle = 0 \\ H |\uparrow\uparrow \dots \uparrow\rangle &= \left(-2(J_0 + K_0) \frac{N}{4} \right) |\uparrow\uparrow \dots \uparrow\rangle \end{aligned}$$

(c) Obtain an expression for the spinwave spectrum as a function of wave vector q , if the ferromagnet is a one-dimensional chain.

$$\begin{aligned} |q\rangle &= \frac{1}{\sqrt{N}} \sum_j e^{i\bar{q}\cdot\bar{R}_j} S_j^- |0\rangle \\ H|q\rangle &= -\sum_i \left[2J_0 S_i^z S_{i+1}^z + J_0 (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + 2K_0 S_i^z S_{i+1}^z \right] \frac{1}{\sqrt{N}} \sum_j e^{iqR_j} |j\rangle \\ &= -\frac{1}{\sqrt{N}} \sum_j e^{iqR_j} \left[2J_0 \left(\frac{N-2}{4} - 2\frac{1}{4} \right) |j\rangle + J_0 |j+1\rangle + J_0 |j-1\rangle + 2K_0 \left(\frac{N-2}{4} - 2\frac{1}{4} \right) |j\rangle \right] \\ &= -\frac{1}{\sqrt{N}} \sum_j e^{iqR_j} \left[2J_0 \left(\frac{N}{4} - 1 \right) |j\rangle + J_0 |j+1\rangle + J_0 |j-1\rangle + 2K_0 \left(\frac{N}{4} - 1 \right) |j\rangle \right] \\ &= -2J_0 \left(\frac{N}{4} - 1 \right) |q\rangle - J_0 e^{-iqa} \frac{1}{\sqrt{N}} \sum_j e^{iq(R_j+a)} |j+1\rangle - J_0 e^{iqa} \frac{1}{\sqrt{N}} \sum_j e^{iq(R_j-a)} |j-1\rangle - 2K_0 \left(\frac{N}{4} - 1 \right) |q\rangle \\ &= -2J_0 \left(\frac{N}{4} - 1 \right) |q\rangle - J_0 e^{-iqa} |q\rangle - J_0 e^{+iqa} |q\rangle - 2K_0 \left(\frac{N}{4} - 1 \right) |q\rangle \\ &= -2J_0 \left(\left(\frac{N}{4} - 1 \right) + \cos qa \right) |q\rangle - 2K_0 \left(\frac{N}{4} - 1 \right) |q\rangle \\ \Rightarrow E(q) &= -2J_0 \left(\left(\frac{N}{4} - 1 \right) + \cos qa \right) - 2K_0 \left(\frac{N}{4} - 1 \right) \\ &= -2J_0 \left(\frac{N}{4} - (1 - \cos qa) \right) - 2K_0 \left(\frac{N}{4} - 1 \right) = E_0 + 2J_0(1 - \cos qa) + 2K_0 \end{aligned}$$

(d) Compare your results with the spin-wave spectrum obtained for the Heisenberg model without the second term.

Excitation gap proportional to $2K_0$ at low wavevector induced by the magnetocrystalline anisotropy, prevents divergence of number of magnons in 1D (and 2D)

- (e) Deduce the temperature dependence at low temperatures for the number of spin waves for the Heisenberg model ($K_0 = 0$) and the Ising model ($J_0 = 0$) for each of the three structures above. Show that there is no long range order above absolute zero for the Heisenberg model in one or two dimensions.

$$1D: \hbar\omega = (J_0 a^2 q^2 + 2K_0)$$

Isingmodel: $\hbar\omega = 2K_0 \equiv \Delta$ energy cost finite & independent of q

$$N_{magnon} \propto e^{-\Delta/k_B T}$$

$$\text{Specific heat: } c_v \propto \frac{\Delta^2}{k_B T^2} e^{-\Delta/k_B T}$$

Heisenbergmodel: $\hbar\omega = J_0 a^2 q^2 \equiv Dq^2$

$$N_{magnon} \propto \int \frac{d^d q}{e^{Dq^2/k_B T} - 1} \approx k_B T \int \frac{d^d q}{Dq^2}$$

$$1D: d^d q = dq$$

Integral diverges in both 1D and 2D, but converges in 3D

8. Heisenberg Hamiltonian in 2D

$$H = -J \sum_{ij} S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)$$

$$H |q\rangle = -\frac{1}{\sqrt{N}} \sum_i e^{iqR_i} J \left[(8N-8) \frac{1}{4} - 8 \frac{1}{4} \right] + J [|l-1\rangle_x + |l+1\rangle_x + |l-1\rangle_y + |l+1\rangle_y]$$

$$E = -2N - 4J - 2J(\cos q_x a + \cos q_y a)$$
$$= -2NJ + J(4 - 2(\cos q_x a + \cos q_y a))$$