FÍSICA da MATÉRIA CONDENSADA

Mestrado em Engenharia Física Tecnológica

Série 3b

1. Masses, Lagrangian, Hamiltonian and Legéndre transformation.

a) Starting from the Lagrangian $\mathcal{L}(\vec{x},\vec{v}) = -mc^2\sqrt{1-(\frac{\vec{v}}{c})^2} - V(\vec{x})$, for a point particle, show that the equation of motion of the particle $\frac{d\vec{p}}{dt} = -\nabla V$, with $\vec{p} = \frac{m\vec{v}}{\sqrt{1-(\frac{\vec{v}}{c})^2}}$ can be writen as $m_\perp \vec{a}_\perp + m_\parallel \vec{a}_\parallel = -\nabla V$, where $(\vec{a}_\perp)^i = \sum_j P_\perp^{ij}\frac{dv^j}{dt}$ and $\left(\vec{a}_\parallel\right)^i = \sum_j P_\parallel^{ij}\frac{dv^j}{dt}$, with $P_\parallel^{ij} = \frac{v^i v^j}{v^2}$ and $P_\perp = I - P_\parallel$. Determine the (transversal and longitudinal) masses $m_\perp$ and $m_\parallel$.

b) Using for the energy the expession $E = mc^2\sqrt{1+\left(\frac{\vec{p}}{mc}\right)^2} + V(\vec{x})$, obtain $\frac{\partial E}{\partial \vec{p}} = \vec{v}$ and $\frac{\partial^2 E}{\partial p^i \partial p^j} = \frac{1}{m_\perp}P_\perp^{ij} + \frac{1}{m_\parallel}P_\parallel^{ij}$, where $P_\parallel^{ij} = \frac{p^i p^j}{p^2}$ and $P_\perp = I - P_\parallel$. What are $m_\perp$ and $m_\parallel$, according to this definition? Verify that the masses and the projectors are the same as obtained above.

c) Explain this fact, using that the Hamiltonian is given by a Legéndre transformation of the Lagrangian.

Hint: $\frac{p}{mv} = \frac{1}{\sqrt{1-(\frac{v}{c})^2}} = \sqrt{1+\left(\frac{p}{mc}\right)^2}$.

2. Tight binding interaction and effective mass.

Consider a free electron system, in a d-dimensional lattice, with Hamiltonian given by

$$\mathcal{H} = \sum_{\alpha=1}^{d}\sum_{\vec{x}} a^\dagger(\vec{x}) t_\alpha a(\vec{x}+a\vec{e}_\alpha) + h.c. = \sum_{\vec{k}} a_{\vec{k}}^\dagger \epsilon(\vec{k}) a_{\vec{k}}$$

where $a(\vec{x}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} a_{\vec{k}}$ and $a^\dagger(\vec{x}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{x}}$, and t_α is real and negative.

a) Obtain the band energy

$$\epsilon(\vec{k}) = \sum_{\alpha=1}^{d} 2t_\alpha \cos(k_\alpha a).$$

b) Define the effective masses $m_{\alpha\beta}^{-1} = \frac{\partial^2\epsilon(\vec{k})}{\partial k_\alpha \partial k_\beta}$, for $k_\alpha = 0$ and $k_\alpha = \pm\pi/a$. Interpret physically the results.

3. Density of states in a d-dimensional isotropic system.

a) In a d-dimensional system, in the thermodynamic limit, we can write

$$\frac{1}{V}\sum_{\vec{k}_n} \to \int \frac{d^dk}{(2\pi)^d} f(k) = \int_0^\infty S_d k^{d-1} f(k) \frac{d^dk}{(2\pi)^d}$$

where $|k| = |\vec{k}|$ and S_d is the area of the sphere in a d-dimensional space.

Choosing $f(k) = e^{-\frac{\vec{k}^2}{2}}$, show that

$$S_d = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})}$$

giving $S_1 = 2$, $S_2 = 2\pi$ and $S_3 = 4\pi$, for $d = 1, 2, 3$.

b) Considering a system of free particles with energy given by $\epsilon(k) = \frac{(\hbar\vec{k})^2}{2m}$ (parabolic band), show that $\mathcal{D}_d(\epsilon(k)) =$, defined by

$$\int \frac{d^dk}{(2\pi)^d} f(\epsilon(k)) = \int_0^\infty \mathcal{D}_d(\epsilon) f(\epsilon) d\epsilon$$

is given by

$$\mathcal{D}_d(\epsilon) = \frac{S_d}{(2\pi)^d} k^{d-1} \frac{dk}{d\epsilon} = \frac{1}{2}\frac{S_d}{(2\pi)^d} k^{d-2} \frac{1}{\frac{d\epsilon}{dk^2}} = \frac{S_d}{(2\pi)^d}\frac{m}{\hbar^2}\left(\frac{2m\epsilon}{\hbar^2}\right)^{\frac{d-2}{2}}$$

c) Plot $\mathcal{D}_d(\epsilon)$, as a function of ϵ, for $d = 1, 2, 3$.

4. Quantum gas in two dimensions.

Consider a free Bosonic or Fermionic system, in 2 dimensions, in thermal equilibrium at temperature T.

a) Write down the equations for $N = < \hat{N} >$ and $E = < \mathcal{H} >$.

b) Solve the equation $N = < \hat{N} >$ for μ.

c) Show that the specific heat of the Bosonic and Fermionic systems is the same.

References:

Quantum Statistics of Ideal Gases in Two Dimensions, R. M. May, Phys. Rev. **153**, A1515 (1964).

Specific Heat of Two-Dimensional Ideal quantum Gases, V. V. Ul'yanov and S. S. Sokolov, Soviet Physics Journal **18**, 138-139 (1975).

5. Itinerant magnetism at $T = 0$.

Consider a system with a fixed number N of electrons, described by the Hubbard model with Hamiltonian given by

$$\mathcal{H} = \sum_{ij} \sum_{\sigma} c_{i\sigma}^{\dagger} t_{ij} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

without external magnetic field, at temperature $T = 0$.

a) Use the product of two Slater determinants, one for each value of the spin, or, equivalently, modify the usual Fermi sea, according to

$$|\Phi_{Stoner} >= \prod_{k<k_{F\uparrow}} c_{\vec{k}\uparrow}^{\dagger} \prod_{k<k_{F\downarrow}} c_{\vec{k}\downarrow}^{\dagger} |0>$$

for the ferromagnetic state with a uniform magnetization $M = \frac{1}{2}(N_{\uparrow} - N_{\downarrow})$, minimize the energy $E =< \mathcal{H} >$, subject to the constraint $N = N_{\uparrow} + N_{\downarrow}$, introducing a Lagrange multiplier μ, leading to the equations

$$\begin{aligned} \epsilon(k_{F\uparrow}) - \mu + U n_{\downarrow} &= 0 \\ \epsilon(k_{F\downarrow}) - \mu + U n_{\uparrow} &= 0 \end{aligned}$$

where $n_{\uparrow} = \frac{N_{\uparrow}}{V}$, $n_{\downarrow} = \frac{N_{\downarrow}}{V}$, giving

$$\epsilon(k_{F\uparrow}) + U n_{\downarrow} = \epsilon(k_{F\downarrow}) + U n_{\uparrow}$$

together with

$$N = N_{\uparrow} + N_{\downarrow}.$$

Interpret physically.

b) Considering free electrons with energy given by $\epsilon(k) = \frac{(\hbar k)^2}{2m}$ show that

$$\frac{2\mathcal{D}\frac{E}{V}}{n^2} = \frac{9}{20}\left[(1 + \frac{2m}{n})^{5/3} + (1 - \frac{2m}{n})^{5/3}\right] + \frac{1}{2}\mathcal{D}U(1 - (\frac{2m}{n})^2)$$

where $n = \frac{N}{V}$, $m = \frac{M}{V}$ and $\mathcal{D}$ is the density of states at k_F, in the absence of interactions i.e. for $U = 0$.

Minimizing the energy, verify that there is a trivial solution $m = 0$ and, using the nontrivial solution, find the Stoner condition $\mathcal{D}U > 1$ for the existence of the phase transition at $T = 0$.

c) Show that the magnetic phase is energetically more stable, when the Stoner criterion is satisfied.