

PHYSICS 320: Problem Set No. 2

Due: Fri. Sep. 17 2010

1. The exchange interaction for a general two body potential $V(\mathbf{r})$ is of the form

$$J = - \int \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_B^*(\mathbf{r}_1) \phi_A^*(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \phi_A(\mathbf{r}_1) \phi_B(\mathbf{r}_2),$$

for two electrons of like spin in single electron states with spatial wavefunctions $\phi_A(\mathbf{r})$ and $\phi_B(\mathbf{r})$. If there exists a complete orthonormal family of functions $\{u_m(\mathbf{r})\}$ such that

$$\int \int d\mathbf{r}_1 d\mathbf{r}_2 u_m^*(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) u_n(\mathbf{r}_1) = A_{mn} \delta_{mn}, \quad (1)$$

with $A_{mn} \geq 0$, show that $J \leq 0$ for any $\phi_A(\mathbf{r})$ and $\phi_B(\mathbf{r})$. Using this result or by an other means show that $J < 0$ for the following potential in 2 and 3 dimensions.

(a) $V(\mathbf{r}) = \delta(\mathbf{r})$

(b) $V(\mathbf{r}) = e^{-\alpha|\mathbf{r}|}/|\mathbf{r}|$

(c) $V(\mathbf{r})$ is the Coulomb potential, which means it is the solution of the Poisson equation

$$\nabla^2 V(\mathbf{r}) = -\delta(\mathbf{r}).$$

Note: In case the family of functions $\{u_m(\mathbf{r})\}$ in Eqn. 1 forms a continuous orthonormal set, δ_{mn} should be thought of as a Dirac delta function and not a Kronecker delta.

2. The expression for the single particle energy in the Jellium model

$$\epsilon(\mathbf{p}) = \frac{p^2}{2m} - \frac{e^2 p_F}{\pi \hbar} \left(1 + \frac{p_F^2 - p^2}{2pp_F} \log \left| \frac{p + p_F}{p - p_F} \right| \right),$$

where $p = |\mathbf{p}|$.

(a) Calculate the density of states and effective mass as functions of energy in the vicinity of the Fermi energy. What are their values at the Fermi energy?

(b) Now assume that the interaction between the electrons in the Jellium model is the screened Coulomb interaction of the form $e^{-\kappa r}/r$. Calculate the single particle energy $\epsilon(\mathbf{p})$ by putting this interaction into the exchange term. What are the values of the density of states and effective mass at the Fermi energy now?

3. For small values of r_s , the electron system in the Jellium model can be treated perturbatively in the interaction.

(a) Calculate the energy per electron as a function of r_s for the Jellium model in the HF approximation. Express your answer in Rydbergs. $1 \text{ Ry} = me^4/2\hbar^2 = 13.6 \text{ eV}$. Remember that an electron has two possible spin states \uparrow and \downarrow .

(b) The energy calculated above is the first order correction to the energy of the free electron gas. It can be shown that the second order correction requires the calculation of terms which look like

$$\epsilon_{\alpha_1, \alpha_2}^{(2)} = -\frac{2m}{\hbar^2} \sum_{\alpha_3, \alpha_4} \frac{|\langle \alpha_1, \alpha_2 | V | \alpha_3, \alpha_4 \rangle|^2}{k_4^2 + k_3^2 - k_2^2 - k_1^2},$$

where α_1 and α_2 are short for the set of momentum and spin labels (\mathbf{k}_1, s_1) and (\mathbf{k}_2, s_2) . The form of this term comes from second order perturbation theory in V and corresponds to the scattering of two electrons in state α_1 and α_2 into virtual states α_3 and α_4 and back. Show that for $s_1 = s_2 = \uparrow$, $\epsilon_{\alpha_1, \alpha_2}^{(2)}$ is infinite in the following way:

i. First calculate

$$\langle \alpha_1, \alpha_2 | V | \alpha_3, \alpha_4 \rangle = \frac{1}{\Omega^2} \int \int d\mathbf{r} d\mathbf{r}' e^{i(\mathbf{k}_3 - \mathbf{k}_1) \cdot \mathbf{r}} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} e^{i(\mathbf{k}_4 - \mathbf{k}_2) \cdot \mathbf{r}'}$$

Ω is the total volume of the system. (*Hint: It will help to use the Fourier transform of the Coulomb potential.*)

- ii. Now, put the expression you obtain into the one for $\epsilon_{\alpha_1, \alpha_2}^{(2)}$ and show that the result is infinite. Convert the sums over momenta into integrals and use the identity

$$\int d\mathbf{k} f(\mathbf{k}) \delta(\mathbf{k} - \mathbf{k}_0) \delta(\mathbf{k} - \mathbf{k}_0) = f(\mathbf{k}_0) \Omega.$$

It might also help to define the variable $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_3$.

Remark: The Brueckner-Gellmann theory removes divergences like the one above by going to infinite order in perturbation theory. This involves summing a series of infinite terms with alternating signs to obtain a finite answer.

4. In class, we considered the HF ground state for the jellium model with equal numbers of up and down spin electrons. Now consider a more general HF ground state in which a fraction f of the electrons have one spin and the other fraction $1 - f$ have the opposite spin. The order parameter for ferromagnetism is defined as $m = 2f - 1$. When there are equal numbers of up and down spin electrons, $m = 0$ and the system is paramagnetic. On the other hand if $m \neq 0$, the system is ferromagnetic.
- (a) Calculate the HF ground state energy per electron in Rydbergs as a function of m and r_s .
- (b) Show that there is a critical value r_c of r_s below which the ground state is ferromagnetic. What is the value of r_c ?
- (c) Does m change continuously at r_c ?
5. In this problem you will calculate the energy of a two dimensional Wigner crystal of in a system where the electrons and ions are interacting through the regular $1/r$ electrostatic potential. Assume that the ions form a uniform positively charged background of density n_p and the electrons organize themselves into a rhombic lattice (i.e. a lattice whose unit cell is a rhombus) with unit cell of side length a and angle θ (see Fig. 1). The energy of an electron (taken to be at the origin of coordinates for convenience) of a such a configuration is given by

$$E = \frac{e^2}{2} \sum_{\mathbf{l} \neq 0} \frac{1}{|\mathbf{l}|} - en_p \int \frac{1}{|\mathbf{r}|} d\mathbf{r}, \quad (2)$$

where the lattice points are labeled by \mathbf{l} . Here we ignore the kinetic energy of the electrons so that the problem is completely classical. For a 2D rhombic lattice

$$E(a, \theta) = -\frac{e^2}{a} f(\theta).$$

- (a) For the above system of electrons and ions show that

$$E(\theta) = -\frac{p(\theta)}{r_s} \text{ Ry.}$$

What is the relation between $p(\theta)$ and $f(\theta)$? Remember that the density of electrons $n_e = n_p = 1/(\pi r_s^2 a_0^2)$, where a_0 is the Bohr radius.

Sums such as the one in Eqn. 2 involving long range potentials typically converge very slowly and give inaccurate numerical results unless a lot of terms are considered. To improve convergence, one uses the Ewald summation technique. Operationally, this involves adding and subtracting a short range potential over a length scale α and then performing the sum by splitting it into real and Fourier space parts. It can be shown that this improves convergence greatly and

$$f(\theta) = \frac{2}{A(\theta)} (\pi\alpha^2)^{1/2} - \frac{1}{A(\theta)} (\pi\alpha^2)^{1/2} \sum_{\mathbf{k} \neq 0} U\left(\frac{|\mathbf{k}|^2 \alpha^2}{4}\right) + 2 \left(\frac{1}{\pi\alpha^2}\right)^{1/2} - \left(\frac{1}{\pi\alpha^2}\right)^{1/2} \sum_{\mathbf{l} \neq 0} U\left(\frac{|\mathbf{l}|^2}{\alpha^2}\right), \quad (3)$$

where $U(x) = \left(\frac{\pi}{x}\right)^{1/2} [1 - \text{erf}(x^{1/2})]$ and $\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du$, is the error function. Here, \mathbf{l} labels the points of a lattice, whose unit cell is a rhombus of unit side length, angle θ and area $A(\theta)$. \mathbf{k} labels the points of its reciprocal lattice.

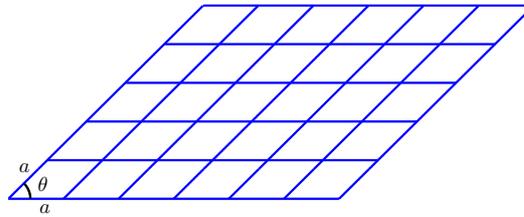


FIG. 1: Rhombic lattice

- (b) Calculate $A(\theta)$, the primitive translation vectors of the above lattice ($\mathbf{a}_1, \mathbf{a}_2$) and the primitive translation vectors of the reciprocal lattice ($\mathbf{g}_1, \mathbf{g}_2$). The vector $\mathbf{l} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, where n_1 and n_2 take all possible integer values. Similarly $\mathbf{k} = m_1\mathbf{g}_1 + m_2\mathbf{g}_2$, where m_1 and m_2 take all possible integer values.
- (c) Now, use the values from (b) to calculate $p(\theta)$ for all allowed values of $\theta \in (0, \pi/2]$ by numerically performing the sum for $f(\theta)$ in Eqn. 3 and then using the relation between $p(\theta)$ and $f(\theta)$ from (a). Plot $p(\theta)$ as a function of θ . α is just a parameter to make the sum converge quickly, so $f(\theta)$ should be independent of its value. Choose α accordingly. Also, keep only as many terms in the sums $\sum_{\mathbf{l} \neq 0}$ and $\sum_{\mathbf{k} \neq 0}$ as required to make the sum converge.
- (d) The calculated $p(\theta)$ should have a maximum at a particular value of θ so that the energy has a minimum. What is this value of θ and what kind of lattice does it correspond to? Is it a Bravais lattice? What is the value of $p(\theta)$ at this value of θ ?

(You do not need to know anything about the details of the Ewald summation technique for this problem. Simply perform the sum in Eqn. 3 numerically and the subsequent steps in parts (c) and (d). However, if you are interested in learning more about this technique, a good reference is chapter 12 of the book Understanding molecular simulation by Daan Frenkel and Berend Smith.)