## Homework 1
## Due Tuesday, September 29

1. Calculate the total internal energy per electron at zero temperature of a free noninteracting gas of electrons of density $n$, in the following two cases.

   (a) First assume that states with both spin directions are populated equally.

   (b) Now assume that the gas is *fully polarized*: only states corresponding to one spin direction, say "up", are populated.

   Compare the two energies.

2. Consider a system of $N$ free noninteracting electrons in a box of volume $V$. For simplicity, assume the electrons are spinless. Pair distribution function $g(\mathbf{r}-\mathbf{r}')$ measures the probability of finding an electron at location $\mathbf{r}$ and another electron at $\mathbf{r}'$. It can be calculated as:

$$\begin{aligned} g(\mathbf{r}-\mathbf{r}') &= N(N-1)\int d\mathbf{r}_1 \ldots d\mathbf{r}_N \\ &\times\ \delta(\mathbf{r}_1-\mathbf{r})\delta(\mathbf{r}_2-\mathbf{r}')|\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2. \end{aligned}$$

   Here $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the Slater determinant ground state wavefunction of this system. Express the result as a function of the Fermi momentum $k_F$ and $|\mathbf{r}-\mathbf{r}'|$. Plot $g$ as a function of $k_F|\mathbf{r}-\mathbf{r}'|$. Observe that it vanishes when $\mathbf{r}$ and $\mathbf{r}'$ approach each other—this reduction of $g$ when two electrons approach each other is called *exchange-correlation hole*. What is the characteristic size of the hole?
   Hint: Use *Leibnitz formula* for the determinant of a matrix to write the Slater determinant in a form, convenient for this calculation.

## Problem 1

a) Total internal energy:

$$E = \sum_{k\sigma} \varepsilon_k \, n_{k\sigma}$$

$$n_{k\sigma} = \begin{cases} 1, & k < k_F \\ 0, & k > k_F \end{cases}$$

$$E = 2V \int_{k<k_F} \frac{d k^3}{(2\pi)^3} \, \varepsilon_k =$$

$$= 2\cdot \frac{V}{8\pi^3} \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \int_0^{k_F} dk \cdot k^2 \cdot \frac{\hbar^2 k^2}{2m} =$$

$$= 2\cdot \frac{V}{8\pi^3} \cdot 4\pi \, \frac{\hbar^2}{2m} \int_0^{k_F} dk \cdot k^4 = V \, \frac{\hbar^2}{4\pi^2 m} \, \frac{k_F^5}{5}$$

$$k_F = \left(3\pi^2 n\right)^{1/3}$$

$$k_F^5 = \left(3\pi^2 n\right)^{5/3} = n \left(3\pi^2\right)^{5/3} n^{2/3}$$

$$E = V n \, \frac{\hbar^2}{2\pi^2 m} \cdot \left(3\pi^2\right)^{5/3} n^{2/3} \, \frac{1}{5} =$$

$$= N \, \frac{\left(3\pi^2\right)^{5/3} \hbar^2}{10\pi^2 m} \, n^{2/3}$$

Energy per electron:

$$\varepsilon = \frac{E}{N} = \frac{\left(3\pi^2\right)^{5/3} \hbar^2}{10\pi^2 m} \, n^{2/3}$$

(b) The ~~extra~~ difference in this case is a different value of $k_F$:

$$\frac{4\pi k_F^3}{3} \cdot \frac{V}{(2\pi)^3} = N$$

$$k_F^3 = 2\left(3\pi^2 n\right)$$

$$k_F = 2^{1/3} \cdot \left(3\pi^2 n\right)^{1/3}$$

$$E = V \int \frac{d\vec{k}}{(2\pi)^3} \varepsilon_k$$

also no factor of 2 for spin degeneracy here.

The ~~■~~ result is:

$$\varepsilon = \frac{1}{2} \frac{(3\pi^2)^{5/3} \hbar^2}{10\pi^2 m} n^{2/3} \cdot 2^{5/3} = 2^{2/3} \frac{(3\pi^2)^{5/3} \hbar^2}{10\pi^2 m} n^{2/3}$$

Thus the energy is a factor of $2^{2/3}$ higher than in the unpolarized case.

Problem 2

$$\Psi(\vec{r}_1, \dots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{k_1}(\vec{r}_1) & \cdots & \psi_{k_1}(\vec{r}_N) \\ \vdots & & \vdots \\ \psi_{k_N}(\vec{r}_1) & \cdots & \psi_{k_N}(\vec{r}_N) \end{vmatrix} =$$

$$= \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi_{k_{P_1}}(\vec{r}_1) \cdots \psi_{k_{P_N}}(\vec{r}_N)$$

Here $\sum_P$ is sum over all permutations of $1, 2, 3, \dots, N$ and $(-1)^P$ is the parity of permutation $P$.

$$g(\vec{r}-\vec{r}\,') = N(N-1) \cdot \frac{1}{N!} \int d\vec{r}_1 \dots d\vec{r}_N \; \delta(\vec{r}_1 - \vec{r}) \cdot$$

$$\cdot \delta(\vec{r}_2 - \vec{r}\,') \sum_{PP'} (-1)^P (-1)^{P'} \psi^*_{k_{P_1}}(\vec{r}_1) \dots \psi^*_{k_{P_N}}(\vec{r}_N) \cdot$$

$$\cdot \psi_{k_{P'_1}}(\vec{r}_1) \dots \psi_{k_{P'_N}}(\vec{r}_N)$$

Using $\int d\vec{r} \, \psi^*_{k_i}(\vec{r}) \psi_{k_j}(\vec{r}) = \delta_{ij}$, we obtain:

$$g(\vec{r}-\vec{r}\,') = \frac{1}{(N-2)!}\,(N-2)!\sum_{k\,k'}\Big[\psi^*_k(\vec{r})\,\psi_k(\vec{r})\cdot$$

$$\cdot\,\psi^*_{k'}(\vec{r}\,')\,\psi_{k'}(\vec{r}\,') - \psi^*_k(\vec{r})\,\psi_k(\vec{r}\,')\,\psi^*_{k'}(\vec{r}\,')\,\psi_{k'}(\vec{r})\Big]$$

$$= \frac{1}{V^2}\sum_{k\,k'}\left[1-e^{-i(\vec{k}-\vec{k}')\cdot(\vec{r}-\vec{r}\,')}\right]$$

Using $\displaystyle \frac{1}{V}\sum_{k} = \int \frac{d\vec{k}}{(2\pi)^3}$ we get:

$$g(\vec{r}-\vec{r}\,') = \int_{k<k_F}\frac{d\vec{k}}{(2\pi)^3}\,\frac{d\vec{k}'}{(2\pi)^3}\left[1-e^{-i(\vec{k}-\vec{k}')\cdot(\vec{r}-\vec{r}\,')}\right]$$

$$\int_{k<k_F}\frac{d\vec{k}\,d\vec{k}'}{(2\pi)^6} = \frac{1}{(2\pi)^6}\left(\frac{4\pi k_F^3}{3}\right)^2$$

~~In order to evaluate the second term change integration variables from $\vec{k}$ to~~

The second term is given by:

$$\int\frac{d\vec{k}}{(2\pi)^3}\,\frac{d\vec{k}'}{(2\pi)^3}\,e^{-i(\vec{k}-\vec{k}')\cdot(\vec{r}-\vec{r}\,')} =$$

$$= \int\frac{d\vec{k}}{(2\pi)^3}\,e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')}\int\frac{d\vec{k}'}{(2\pi)^3}\,e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}$$

$$\int \frac{d\vec{k}}{(2\pi)^3}\, e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')} = \frac{1}{8\pi^3}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \int_0^{k_F} dk\cdot k^2 \cdot$$

$$\cdot\, e^{-ik|\vec{r}-\vec{r}'|\cos\theta} =$$

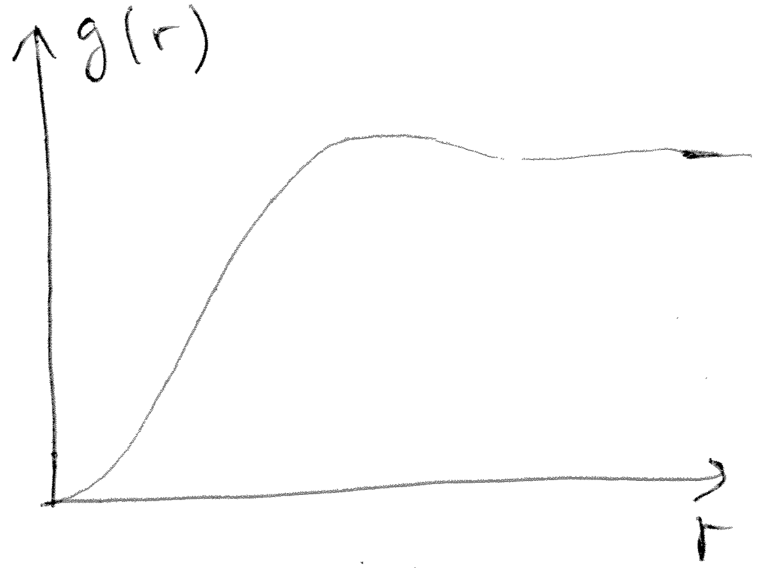
$$= \frac{1}{4\pi^2}\int_0^{k_F} dk\cdot k^2 \frac{1}{-ik|\vec{r}-\vec{r}'|}\left[e^{-ik|\vec{r}-\vec{r}'|} - e^{ik|\vec{r}-\vec{r}'|}\right] = \frac{1}{2\pi^2|\vec{r}-\vec{r}'|}\int_0^{k_F} dk\cdot k\cdot \sin\left(k|\vec{r}-\vec{r}'|\right) =$$

$$= \frac{1}{2\pi^2|\vec{r}-\vec{r}'|^3}\left[\sin\left(k_F|\vec{r}-\vec{r}'|\right) - k_F|\vec{r}-\vec{r}'|\cos\left(k_F|\vec{r}-\vec{r}'|\right)\right]$$

Thus we obtain:

$$g\left(|\vec{r}-\vec{r}'|\right) = \frac{1}{(2\pi)^6}\left(\frac{4\pi k_F^3}{3}\right)^2 - \frac{1}{4\pi^4|\vec{r}-\vec{r}'|^6}\left[\sin\left(k_F|\vec{r}-\vec{r}'|\right) - k_F|\vec{r}-\vec{r}'|\cos\left(k_F|\vec{r}-\vec{r}'|\right)\right]^2 =$$

$$= \frac{k_F^6}{36\pi^4}\left\{1 - \frac{9}{k_F^6|\vec{r}-\vec{r}'|^6}\left[\sin\left(k_F|\vec{r}-\vec{r}'|\right) - k_F|\vec{r}-\vec{r}'|\cos\left(k_F|\vec{r}-\vec{r}'|\right)\right]^2\right\}$$




The characteristic size of the hole is $\frac{1}{k_F}$.