Physics 502 - Solutions for assignment #1

(Dated: October 10, 2023)

1. Second quantization

a. From the definition of a second quantized operator, we can write the total spin operator as

$$\boldsymbol{S}_{\text{tot}} = \int d^3 r \, d^3 r' \sum_{\alpha,\beta} \langle \boldsymbol{r}, \alpha | \boldsymbol{S} | \boldsymbol{r}', \beta \rangle \hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r}) \hat{\psi}_{\beta}(\boldsymbol{r}') \tag{1}$$

where $\langle \boldsymbol{r}, \alpha | \boldsymbol{S} | \boldsymbol{r}', \beta \rangle = (\hbar/2) \boldsymbol{\sigma}_{\alpha\beta} \delta^{(3)}(\boldsymbol{r} - \boldsymbol{r}')$ is the "first quantized" total spin operator in the position, spin basis and $\hat{\psi}_{\alpha}(\boldsymbol{r})$ is the field operator that creates an electron with spin α at position \boldsymbol{r} . Hence, we can simplify the second quantized expression to

$$\boldsymbol{S}_{\text{tot}} = \frac{\hbar}{2} \int d^3 r \, \hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r}) \boldsymbol{\sigma}_{\alpha\beta} \hat{\psi}_{\beta}(\boldsymbol{r}) \tag{2}$$

where repeated indices are assumed to be summed over herein. The total spin can be written in terms of the spin density $\mathbf{S}(\mathbf{r})$ as $\mathbf{S}_{\text{tot}} = \int d^3r \, \mathbf{S}(\mathbf{r})$ and so we recognize the spin density as

$$\boldsymbol{S}(\boldsymbol{r}) = \frac{\hbar}{2} \psi^{\dagger}_{\alpha}(\boldsymbol{r}) \boldsymbol{\sigma}_{\alpha\beta} \hat{\psi}_{\beta}(\boldsymbol{r}).$$
(3)

We can expand the operator in terms of the annihilation operator $c_{k\alpha}$ for an electron plane wave of momentum k and spin α as

$$\hat{\psi}_{\alpha}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{k}\alpha} \tag{4}$$

and hence

$$\boldsymbol{S}(\boldsymbol{r}) = \frac{\hbar}{2V} \sum_{\boldsymbol{k},\boldsymbol{k}'} e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} c^{\dagger}_{\boldsymbol{k}\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{\boldsymbol{k}'\beta}.$$
(5)

b. We can write the Hamiltonian as

$$H = T + V \tag{6}$$

where

$$T = -\int d^3r \,\hat{\psi}^{\dagger}_{\alpha}(\mathbf{r}) \frac{\hbar \nabla_r^2}{2m} \hat{\psi}_{\alpha}(\mathbf{r}) \tag{7}$$

$$V = \frac{1}{2} \int d^3 r \, d^3 r' \, \hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r}) \hat{\psi}^{\dagger}_{\beta}(\boldsymbol{r}') \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}'|} \hat{\psi}_{\beta}(\boldsymbol{r}') \hat{\psi}_{\alpha}(\boldsymbol{r}). \tag{8}$$

To compute $[H, \mathbf{S}_{tot}]$, we will make liberal use of the following easily proven identities for arbitrary operators A, B, and C:

$$[A, BC] = [A, B]C + B[A, C]$$
(9)

$$[A, BC] = \{A, B\} C - B\{A, C\}$$
(10)

Using these and

$$\left\{\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r}), \hat{\psi}_{\beta}(\boldsymbol{r}')\right\} = \delta_{\alpha\beta}\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')$$
(11)

$$\left\{\hat{\psi}_{\alpha}(\boldsymbol{r}), \hat{\psi}_{\beta}(\boldsymbol{r}')\right\} = 0 \tag{12}$$

we can compute the commutator with each of the two terms of the Hamiltonian in turn.

$$\begin{aligned} [T, \mathbf{S}_{\text{tot}}] &= -\frac{\hbar^2}{2m} \frac{\hbar}{2} \boldsymbol{\sigma}_{\mu\nu} \int d^3 r \, d^3 r' \left[\hat{\psi}^{\dagger}_{\alpha}(\mathbf{r}) \nabla^2_r \hat{\psi}_{\alpha}(\mathbf{r}), \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}') \hat{\psi}_{\nu}(\mathbf{r}') \right] \\ &= -\frac{\hbar^3}{4m} \boldsymbol{\sigma}_{\mu\nu} \int d^3 r \, d^3 r' \left\{ \left[\hat{\psi}^{\dagger}_{\alpha}(\mathbf{r}) \nabla^2_r \hat{\psi}_{\alpha}(\mathbf{r}), \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}') \right] \hat{\psi}_{\nu}(\mathbf{r}') + \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}') \left[\hat{\psi}^{\dagger}_{\alpha}(\mathbf{r}) \nabla^2_r \hat{\psi}_{\alpha}(\mathbf{r}), \hat{\psi}_{\nu}(\mathbf{r}') \right] \right\} \\ &= -\frac{\hbar^3}{4m} \boldsymbol{\sigma}_{\mu\nu} \int d^3 r \, d^3 r' \left\{ \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}) \nabla^2_r \delta^{(3)}(\mathbf{r} - \mathbf{r}') \hat{\psi}_{\nu}(\mathbf{r}') - \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}') \delta^{(3)}(\mathbf{r} - \mathbf{r}') \nabla^2_r \hat{\psi}_{\nu}(\mathbf{r}) \right\} \\ &= -\frac{\hbar^3}{4m} \boldsymbol{\sigma}_{\mu\nu} \int d^3 r \left\{ \left(\nabla^2_r \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}) \right) \hat{\psi}_{\nu}(\mathbf{r}) - \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}) \nabla^2_r \hat{\psi}_{\nu}(\mathbf{r}) \right\} \\ &= -\frac{\hbar^3}{4m} \boldsymbol{\sigma}_{\mu\nu} \int d^3 r \left\{ \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}) \nabla^2_r \hat{\psi}_{\nu}(\mathbf{r}) - \hat{\psi}^{\dagger}_{\mu}(\mathbf{r}) \nabla^2_r \hat{\psi}_{\nu}(\mathbf{r}) \right\} \\ &= 0 \end{aligned}$$

where, in the fourth and fifth equalities, we have integrated by parts. The boundary terms vanish due to the periodic boundary conditions of the field operators. A similar calculation can be performed to show that $[V, S_{tot}] = 0$ which is more straightforward since there is no derivative operator.

Equivalently, the calculation can be done in terms c^{\dagger} , c operators. This is slightly more messy because of many k-summations involved but on the positive side there are no gradient terms to worry about so the evaluation of the kinetic term is easier.

2. Polarized electron gas

Most of this question was done in class – we just have to adapt the results to the situation with unequal population of spin-up and -down electrons.

a. The energy of an electron gas to first order in the Hartree-Fock expansion is given by:

$$E = R_y N \left[\frac{3}{5} (k_F a_0)^2 - \frac{3}{2\pi} (k_F a_0) \right]$$

where $R_y = \frac{e^2}{2a_0}$ is the Rydberg constant. The first term is the kinetic energy while the second is the exchange energy.

For the polarized gas $E = E_{\uparrow} + E_{\downarrow}$, N is replaced by N_{\pm} and k_F is replaced by $k_{F\pm}$. The separation of the potential energy term is non-trivial and follows from the fact that only the $\sigma = \sigma'$



FIG. 1: a. $r_s < 5.45, 6.03$ The second derivative of the energy at M = 0 is positive - minimum. In addition, the non-polarized state has lower energy. b. $5.45 < r_s < 6.03 \ E(M = 0)$ is still a local minimum but the non-polarized state has higher energy then the maximally polarized one. c. $r_s > 6.03 \ E(M = 0)$ is a maximum and the non-polarized state has higher energy then the maximally polarized one.

term contributes to the exchange energy. We can express everything in terms of M and N using

$$\frac{k_{F\pm}^3}{6\pi^2} = \frac{N_{\pm}}{V}$$
 and $N_{\pm} = \frac{N}{2}(1\pm M)$

and with the definition of r_s in terms of $\frac{N}{V}$ $(r_s = \left(\frac{3V}{4\pi N}\right)^{1/3} \frac{1}{a_0})$ we find:

$$E = R_y N \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{2r_s} \left[\frac{3}{5} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{r_s} \left((1+M)^{\frac{5}{3}} + (1-M)^{\frac{5}{3}}\right) - \frac{3}{2\pi} \left((1+M)^{\frac{4}{3}} + (1-M)^{\frac{4}{3}}\right)\right]$$

$$= R_y N \frac{1}{2} \left[\frac{2.21}{r_s^2} \left((1+M)^{\frac{5}{3}} + (1-M)^{\frac{5}{3}}\right) - \frac{0.916}{r_s} \left((1+M)^{\frac{4}{3}} + (1-M)^{\frac{4}{3}}\right)\right]$$

The factor of 1/2 in front comes from the fact that the initial expression for the energy assumed equal number of spin up and spin down electrons so, when we add each contribution explicitly, we must divide by two to avoid over counting.

b. The energy difference between the maximally polarized state and the non-polarized state is:

$$\Delta E = R_y N \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{2r_s} \left[\frac{3}{5} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{r_s} (2^{\frac{5}{3}} - 2) - \frac{3}{2\pi} (2^{\frac{4}{3}} - 2)\right]$$

which becomes negative for

$$r_s > r_s^c = \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{2\pi}{5} \frac{(2^{\frac{5}{3}} - 2)}{(2^{\frac{4}{3}} - 2)} \approx 5.45$$

Below a critical electron density the exchange energy dominates and the system minimizes its total energy by ferromagnetic alignments of spins.

c. We investigate the magnetization dependence of the energy near M = 0. The first derivative is always zero at M = 0 due to the relative sign between the $(1 + M)^y$ and the $(1 - M)^y$ terms. This point is an extremum. We can determine whether it represents a maximum or a minimum by taking the second derivative:

$$\frac{d^2 E}{dM^2} = R_y N \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{2r_s} \left[\frac{2}{3} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{r_s} \left((1+M)^{-\frac{1}{3}} + (1-M)^{-\frac{1}{3}}\right) - \frac{4}{6\pi} \left((1+M)^{-\frac{2}{3}} + (1-M)^{-\frac{2}{3}}\right)\right]$$

At M = 0 this expression changes sign when

$$r_s = \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \approx 6.03$$

Hence we conclude that E has a minimum at M = 0 when $r_s < 6.03$ and a maximum otherwise. The behaviour of E(M) is summarized in the figure.

3. The Hartree-Fock correction

As you have seen in class, in the Hartree-fock approximation the spectrum is given by: $H = \sum_{k\sigma} (\epsilon_k + \delta \epsilon_k) c^{\dagger}_{k\sigma} c_{k\sigma}$. The correction $\delta \epsilon_k$ is found by summing over the potential (we can do this at T = 0 with a step function at k_F). With the Coulomb potential this leads to

$$\delta \epsilon_k = -\frac{1}{\pi} 2e^2 k_F F(\frac{k}{k_F}),$$
$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|$$

a. To find the Fermi velocity we need to take a derivative at $k = k_F$,

$$v_F = \frac{\partial E_k}{\partial k}\Big|_{k_F} = \frac{\hbar^2 k}{m} - \frac{2e^2}{\pi} \left[\frac{1}{2x} - \frac{1+x^2}{4x^2} \ln \left|\frac{1+x}{1-x}\right|\right],$$

where $x = k/k_F$. From the above expression one can see that when $k \to k_F$ $(x \to 1)$ v_F diverges logarithmically.

b. Recall that the density of states can be calculated by integrating over a surface of constant energy (in our case the Fermi energy):

$$g(E) = \int \frac{1}{|\nabla_k E_k|} \cdot d\vec{S}.$$

This means that if v_F diverges (at k_F , regardless of orientation) then the density of states must vanish. The Sommerfeld expansion follows from expanding $K(\epsilon) = \int_{-\infty}^{\epsilon} H(\epsilon')d\epsilon'$ near $\epsilon = \mu$ in the expression

$$\int_{-\infty}^{\infty} H(\epsilon) f(\epsilon) d\epsilon = \int_{-\infty}^{\infty} K(\epsilon) \left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) d\epsilon$$

However, for the case at hand, the function $H(\epsilon)$ is non-analytic at the Fermi surface and the expansion is not justified. In general, a vanishing density of states will lead to difficulties calculating thermodynamic properties such as the specific heat. Consider the expression

$$C_V = \int_0^\infty (\epsilon - \epsilon_F) \frac{\partial f}{\partial T} g(\epsilon) d\epsilon \approx g(\epsilon_F) \int_0^\infty (\epsilon - \epsilon_F) \frac{\partial f}{\partial T} d\epsilon, \tag{14}$$

where we have pulled $g(\epsilon_F)$ outside the integral since $(\epsilon - \epsilon_F)\frac{\partial f}{\partial T}$ is sharply peaked around the Fermi energy. If $g(\epsilon_F)$ vanishes, this is no longer valid. The problem is you can't "heat up" the system if no energy eigenstates are available.

c. The Fourier transform of the screened Coulomb potential is

$$V(k) = \frac{4\pi e^2}{k^2 + \mu^2}.$$

Performing the sum $\delta \epsilon_{\mathbf{k}} = \sum_{k' < k_F} V(\mathbf{k} - \mathbf{k}')$ gives:

$$\delta\epsilon_{k} = \frac{e^{2}}{\pi} \left\{ -k_{F} + \mu \left[\tan^{-1} \left(\frac{k+k_{F}}{\mu} \right) + \tan^{-1} \left(\frac{k-k_{F}}{\mu} \right) \right] + \frac{k^{2} - k_{F}^{2} - \mu^{2}}{k} \ln \left| \frac{(k-k_{F})^{2} - \mu^{2}}{(k+k_{F})^{2} - \mu^{2}} \right| \right\}.$$

Clearly, there is no divergence at $k \to k_F$ and therefore v_F as well as the density of states at the Fermi energy are finite.