PHYSICS 211B : CONDENSED MATTER PHYSICS HW ASSIGNMENT #3

(1) Define the operator

$$\Pi_N = \frac{1}{N!} \int_{\mathbb{R}^{dN}} d^d x_1 \cdots d^d x_N \, | \, \boldsymbol{x}_1 \cdots \boldsymbol{x}_N \, \rangle \langle \, \boldsymbol{x}_1 \cdots \boldsymbol{x}_N \, | \quad ,$$

where

$$|\,oldsymbol{x}_1\cdotsoldsymbol{x}_N\,
angle=\psi^\dagger(oldsymbol{x}_1)\cdots\psi^\dagger(oldsymbol{x}_N)\,|\,0\,
angle$$

where $\left[\psi(\boldsymbol{x}), \psi^{\dagger}(\boldsymbol{x}')\right]_{\mp} = \delta(\boldsymbol{x} - \boldsymbol{x}')$ for bosons (–) and fermions (+). Here each $\boldsymbol{x}_j \in \mathbb{R}^d$.

(a) Show that Π_N is a projector onto the totally symmetric and totally antisymmetric parts of the *N*-body Hilbert space for bosons and fermions, respectively.

(b) Show that one can also write

$$\Pi_N \equiv \int_{\Delta_N} d^d x_1 \cdots d^d x_N \, | \, \boldsymbol{x}_1 \cdots \boldsymbol{x}_N \, \rangle \langle \, \boldsymbol{x}_1 \cdots \boldsymbol{x}_N \, | \quad ,$$

where Δ_N is defined to be the subset of \mathbb{R}^{dN} for which

$$\Delta_N = \left\{ (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) \mid x_1^{(1)} < x_2^{(1)} < \dots < x_N^{(1)} \right\} \quad .$$

(2) Consider a one-dimensional electron gas with spin-independent interactions

$$u(x - x') = \frac{u_0}{\pi} \frac{\lambda}{(x - x')^2 + \lambda^2}$$

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Find the Hartree-Fock energies $\varepsilon(k)$.

(3) For *spinless* electrons interacting via a potential u(x), find the Hartree-Fock energies $\varepsilon(k)$. Show that when $\hat{u}(k) = \text{const.}$ that there is no interaction contribution to $\varepsilon(k)$. Interpret this physically.

(4) Consider a polarized electron gas (three dimensions, Coulomb interactions) in which N_{σ} denotes the number of electrons with spin polarization σ .

(a) Begin with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{\sigma} \int d^3x \ c^{\dagger}(\boldsymbol{x}) \ \nabla^2 \ c(\boldsymbol{x}) + \frac{1}{2} \sum_{\sigma,\sigma'} \int d^3x \int d^3x' \ c^{\dagger}_{\sigma}(\boldsymbol{x}) \ c^{\dagger}_{\sigma'}(\boldsymbol{x}') \ u(\boldsymbol{x} - \boldsymbol{x}') \ c_{\sigma'}(\boldsymbol{x}') \ c_{\sigma}(\boldsymbol{x}) \\ - \sum_{\sigma} \int d^3x \ c^{\dagger}_{\sigma}(\boldsymbol{x}) \ c_{\sigma}(\boldsymbol{x}) \int d^3x' \ u(\boldsymbol{x} - \boldsymbol{x}') \ n_0 + \frac{1}{2} \int d^3x \int d^3x' \ n_0 \ u(\boldsymbol{x} - \boldsymbol{x}') \ n_0$$

where $n_0 = N_0/V$ is the background number density and where $u(\mathbf{r}) = (e^2/r) e^{-Qr}$. is the Yukawa potential. At the appropriate time, you may take the $Q \to 0$ limit in order to recover the *jellium system*. Using the relation

$$c_{\sigma}(\boldsymbol{x}) = V^{-1/2} \sum_{\boldsymbol{k}} e^{i \boldsymbol{k} \cdot \boldsymbol{x}} c_{\boldsymbol{k},\sigma}$$

show that one may write

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} \varepsilon(\boldsymbol{k}) c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma} - n_0 \,\hat{u}(0) \sum_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma} + \frac{1}{2V} \sum_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}} \sum_{\sigma,\sigma'} \hat{u}(\boldsymbol{q}) c_{\boldsymbol{k}+\boldsymbol{q},\sigma}^{\dagger} c_{\boldsymbol{p}-\boldsymbol{q},\sigma'}^{\dagger} c_{\boldsymbol{p},\sigma'} c_{\boldsymbol{k},\sigma} + E_{\text{bg}}$$

with

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m}$$
, $\hat{u}(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2 + Q^2}$, $E_{\text{bg}} = \frac{2\pi e^2}{Q^2} \frac{N_0^2}{V}$

You may assume periodic boundary conditions in a $L \times L \times L$ box of volume $V = L^3$ in the limit $L \to \infty$. The allowed k values are then quantized according to $k = \frac{2\pi}{L} (n_x, n_y, n_z)$ where $n_{x,y,z} \in \mathbb{Z}$.

(b) Find the ground state energy to first order in the interaction potential as a function of $N = N_{\uparrow} + N_{\downarrow}$ and the magnetization $M = N_{\uparrow} - N_{\downarrow}$. You should assume a wavefunction

$$|\Psi\rangle = \prod_{|\mathbf{k}| < k_{\rm F\uparrow}} c^{\dagger}_{\mathbf{k},\uparrow} \prod_{|\mathbf{k}'| < k_{\rm F\downarrow}} c^{\dagger}_{\mathbf{k}',\downarrow} |0\rangle \quad .$$

where $n_{\sigma} = k_{F,\sigma}^3/6\pi^2 = N_{\sigma}/V$ is the number density of electrons of spin polarization σ . Along the way, show that

$$\langle \Psi \,|\, c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} \,c^{\dagger}_{\boldsymbol{p}-\boldsymbol{q},\sigma'} \,c_{\boldsymbol{p},\sigma'} \,c_{\boldsymbol{k},\sigma} \,|\, \Psi \,\rangle = n_{\boldsymbol{k},\sigma} \,n_{\boldsymbol{p},\sigma'} \,\delta_{\boldsymbol{q},0} - n_{\boldsymbol{p},\sigma} \,n_{\boldsymbol{k},\sigma} \,\delta_{\boldsymbol{q},\boldsymbol{p}-\boldsymbol{k}} \,\delta_{\sigma,\sigma'} \quad,$$

where $n_{\mathbf{k},\sigma} = \langle \Psi | c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} | \Psi \rangle$. Express your result for the energy as $E(n,\zeta,V)$, where $\zeta \equiv (n_{\uparrow} - n_{\downarrow})/(n_{\uparrow} + n_{\downarrow})$ is the dimensionless magnetization and $n = N/V = n_{\uparrow} + n_{\downarrow}$.

(c) Prove, to this order in the interaction, that the ferromagnetic state (M = N) has a lower energy than the unmagnetized state (M = 0) provided r_s exceeds a critical value $r_{s,1}$. Find that critical value $r_{s,1}$.

(d) Define $\varepsilon(\zeta) = E/N$ with $\zeta = M/N$. Show that $\varepsilon''(0) < 0$ when r_s exceeds a critical value $r_{s,2}$. Find $r_{s,2}$. You should find $r_{s,1} < r_{s,2}$. What happens for $r_s \in [r_{s,1}, r_{s,2}]$?