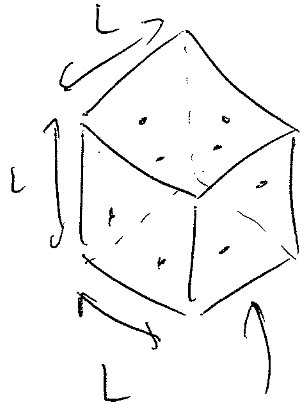
Phys 726 - Lecture 5

Ongoing example: Degenerate electron gas / Jellium model



N electrons confined to a volume $V = L^3$

region of compensating background charge

$$\rho(\vec{r}) = +\frac{eN}{V} = \text{const}$$

→ Interaction potential $\frac{e^{-\mu r}}{r}$ $\left(\frac{4\pi}{q^2+\mu^2} \text{ in Fourier space}\right)$

with regularization parameter $\mu \sim \frac{1}{L} \to 0$ at the end of the calculation

→ electronic hamiltonian is the sum of one- and two-body terms

$$\hat{H}_{el}^{(1)} = \sum_{\vec{k},\alpha} \frac{\hbar^2 k^2}{2m} c^\dagger_{\vec{k},\alpha} c_{\vec{k},\alpha}$$

all momenta

spin projections ↑, ↓

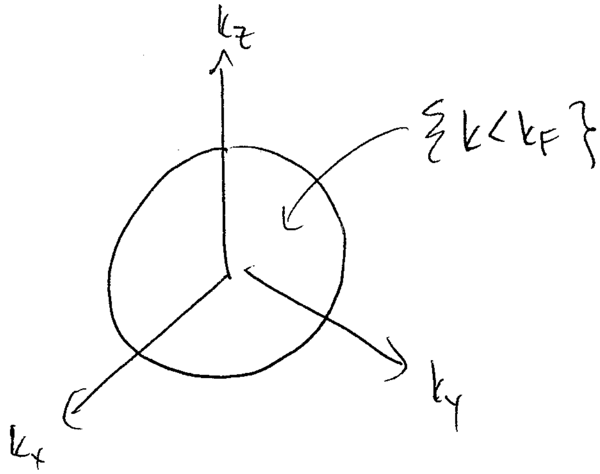
neglected uniform ($\vec{q}=0$) component exactly cancels the positive background contribution

$$\hat{H}_{el}^{(2)} = \frac{e^2}{2V} \sum_{\alpha,\beta} \sum_{\vec{k},\vec{k}',\vec{q}\neq 0} \frac{4\pi}{q^2} c^\dagger_{\vec{k}+\vec{q},\alpha} c^\dagger_{\vec{k}',\beta} c_{\vec{k}'+\vec{q},\beta} c_{\vec{k},\alpha}$$

$\varepsilon_k = \dfrac{\hbar^2 k^2}{2m}$ is the "bare" electronic dispersion,
here just the kinetic energy of a
free particle with momentum $\hbar\vec{k}$

$\hat{n}_{\vec{k},\alpha} = c^{\dagger}_{\vec{k},\alpha} c_{\vec{k},\alpha}$ is the operator that counts the
occupancy of each single-particle
mode $\vec{k},\alpha$

→ The noninteracting Hamiltonian $\hat{H} = \hat{H}^{(1)}_{el}$ has
a Fermi Sea ground state



$$|F\rangle = \left(\prod_{k<k_F} c^{\dagger}_{k\uparrow} c^{\dagger}_{k\downarrow} \right) |vac\rangle$$

↑ $N/2$ enclosed k vectors
produces a state with
N particles (definite
particle number)

with energy

$$\sum_{k,\alpha} \frac{\hbar^2 k^2}{2m} \langle F | \hat{n}_{k\alpha} | F \rangle = V \cdot \overset{\text{spin}}{2} \cdot \int \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \theta(k_F - k) = \frac{2V}{8\pi^3} \int_0^{k_F} 4\pi k^2 dk \cdot \frac{\hbar^2 k^2}{2m}$$

$$= \frac{V\hbar^2}{2\pi^2 m} \int_0^{k_F} k^4 dk = \frac{V\hbar^2}{2\pi^2 m} \cdot \frac{1}{5} k_F^5$$

and particle number

$$N = \sum_{\vec{k},\alpha} \langle F | \hat{n}_{\vec{k},\alpha} | F \rangle = 2 \cdot V \int \frac{d^3k}{(2\pi)^3} \theta(k_F - k)$$

$$= \frac{V}{\pi^2} \int_0^{k_F} k^2 dk = \frac{V}{3\pi^2} k_F^3$$

→ Energy per particle is

$$\frac{E_0}{N} = \frac{V\hbar^2}{2\pi^2 m} \cdot \frac{1}{5} k_F^5 \cdot \frac{3\pi^2}{V k_F^3} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$$

$\frac{3}{5}$ energy of a particle on the Fermi surface

* No obvious way to solve for the fully interacting Hamiltonian $\hat{H} = \hat{H}_{el}^{(1)} + \hat{H}_{el}^{(2)}$

→ we'll eventually consider mean field theory, trial wave functions (variational), and diagrammatic expansions

→ for now, <u>perturbation theory</u> : requires that $\hat{H}_{el}^{(2)}$ is in some sense "weak"

→ more formally, we assume that the ground states $|\psi_\lambda\rangle$ of the one-parameter Hamiltonian $\hat{H}_\lambda = \hat{H}_{el}^{(1)} + \lambda \hat{H}_{el}^{(2)}$ are smoothly connected along a path ~~from~~ $\lambda = 0$ to $\lambda = 1$; i.e. the noninteracting and fully interacting ground states are adiabatically connected

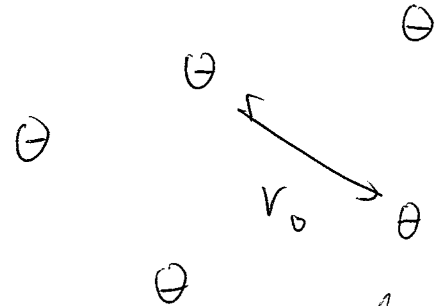
* We argued previously that perturbation theory is under good control in the high electronic density regime

→ make the replacements

$$\text{momentum} \quad k \rightarrow \frac{1}{r_0}\bar{k}$$
$$\text{volume} \quad V \rightarrow r_0^3 \bar{V}$$

where the bar quantities are dimensionless and r_0 is the ~~interatomic~~ inter-electronic spacing defined by $V = \frac{4}{3}\pi r_0^3 N$

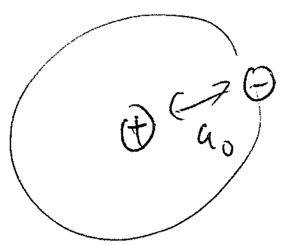
→ identify the two relevant length scales



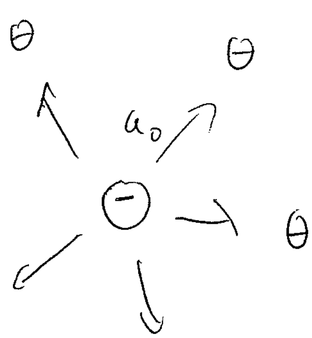
$$r_0 = \left(\frac{3V}{4\pi N}\right)^{1/3}$$

typical separation in the gas

Bohr radius $a_0 = \frac{\hbar^2}{me^2}$



radius of the bound state for a pair of attractive charges



radius of exclusion for like charges

→ the density regime is determined by the dimensionless ratio $r_s = r_0 / a_0$

$r_s \gg 1$ low density

$r_s \ll 1$ high density

→ attempt a perturbative expansion around $r_s = 0$

$$\hat{H} = \sum_{\bar{k},\alpha} \frac{\hbar^2 \bar{k}^2}{2 m r_0^2} c^\dagger_{\bar{k}\alpha} c_{\bar{k}\alpha} + \frac{e^2}{2 \bar{V} r_0^3} \sum_{\substack{\bar{k},\bar{k}' \\ \bar{q} \neq 0}} \frac{4\pi r_0^2}{\bar{q}^2} c^\dagger_{\bar{k}+\bar{q},\alpha} c^\dagger_{\bar{k}'\beta} c_{\bar{k}'+\bar{q}\beta} c_{\bar{k}\alpha}$$

$$= \frac{1}{2} \left(\frac{\hbar^2}{m r_0^2} \right) \hat{A} + \frac{2\pi}{\bar{V}} \left(\frac{e^2}{r_0} \right) \hat{B}$$

$$e^2 \left(\frac{\hbar^2}{m e^2} \right) \frac{1}{r_0^2}$$

$$\frac{e^2}{r_s a_0} = \frac{e^2}{a_0} \cdot \frac{1}{r_s}$$

$$= e^2 a_0 \cdot \frac{1}{r_s^2 a_0^2}$$

$$= \frac{e^2}{a_0} \cdot \frac{1}{r_s^2}$$

→ kinetic energy (Rydberg $\times \frac{1}{r_s^2}$) dominates the Coulomb energy (Rydberg $\times \frac{1}{r_s}$) when the electronic density is large ($r_s \to 0$)

$$\hat{H} = \frac{e^2}{a_0} \cdot \frac{1}{r_s^2} \left(\frac{1}{2} \hat{A} + \frac{2\pi}{V} \cdot r_s \cdot \hat{B} \right)$$

Result dating back to Bloch (1929) and Wigner (1934):

Ground state energy expansion:

$$E = \frac{Ne^2}{2a_0} \cdot \frac{1}{r_s^2} \left(C_0 + C_1 r_s + \underbrace{C_2 r_s^2 + \tilde{C}_2 r_s^2 \log r_s + \dots}_{\text{"correlation energy" contributions}} \right)$$

$\langle F | \hat{A} | F \rangle$ expectation ~~the~~ value of $\hat{A}$ in its own ground state

$\frac{4\pi}{V} \langle F | \hat{B} | F \rangle$ expectation value of $\hat{B}$ in the <u>unperturbed</u> ground state of $\hat{A}$

* We have already computed the noninteracting ground state energy

$$E_0 = \langle F | \hat{H}_{el}^{(1)} | F \rangle = N \cdot \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} = N \cdot \frac{3}{5} \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

$$= N \cdot \frac{3}{5} \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{\frac{4}{3}\pi r_0^3} \right)^{2/3} = \frac{3N}{5} \frac{\hbar^2}{2m} \left(\frac{9\pi}{4} \right)^{2/3} \frac{1}{r_0^2}$$

$$= \frac{3N}{5} \cdot \frac{1}{2} \underbrace{\frac{\hbar^2}{me^2} \frac{1}{a_0}}_{a_0/a_0 = 1} \frac{e^2}{a_0} \left(\frac{9\pi}{4} \right)^{2/3} \frac{1}{r_s^2}$$

$$= N \cdot \frac{e^2}{2a_0} \cdot \frac{3}{5} \left(\frac{9\pi}{4} \right)^{2/3} \cdot \frac{1}{r_s^2} = N \cdot \frac{e^2}{2a_0} \cdot \frac{2.21}{r_s^2}$$

So $$\frac{E}{N} = \frac{e^2}{2a_0 r_s^2} \left[2.21 + O(r_s) \right]$$

* First-order energy shift

$$\Delta E = \langle F | \hat{H}_{el}^{(2)} | F \rangle$$

$$= \frac{e^2}{2V} \sum_{\alpha\beta} \sum_{\substack{\vec{k},\vec{k}' \\ \vec{q}\neq 0}} \frac{4\pi}{q^2} \langle F | c^\dagger_{\vec{k}+\vec{q},\alpha} \, c^\dagger_{\vec{k}',\beta} \, c_{\vec{k}'+\vec{q},\beta} \, c_{\vec{k},\alpha} | F \rangle$$

"direct contribution" $\quad \underbrace{\delta_{k+q,k} \, \delta_{k',k'+q}}_{\delta_{q,0}} \, \theta(k_F - k)\, \theta(k_F - k')$

"exchange contribution" $\quad - \underbrace{\delta_{k+q,k'+q} \, \delta_{\alpha\beta} \, \delta_{k',k} \, \delta_{\alpha\beta}}_{\delta_{k,k'} \, \delta_{\alpha\beta}} \, \theta(k_F - |\vec{k}+\vec{q}|) \cdot \theta(k_F - k)$

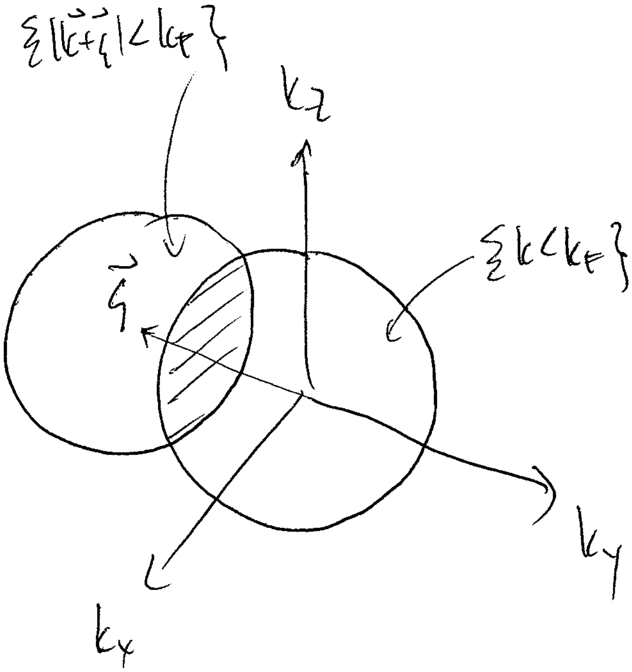
$$= -\frac{e^2}{2V} \sum_{\alpha} \sum_{\vec{k},\vec{q}\neq 0} \frac{4\pi}{q^2} \, \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$

* As system size $L \to \infty$, wave vector sums pass over to integrals $\sum_k \to V \int \frac{d^3k}{(2\pi)^3}$

$$\Delta E = -e^2 4\pi V \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \frac{1}{q^2} \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$

all points in a Fermi sphere centered on $\vec{q}$

all points in a Fermi sphere centered at zero momentum



→ monotonically decreasing as q increases from zero

→ vanishes when $q > 2k_F$

Overlap volume

$$\int d^3k\, \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$

$$= \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x) \quad \text{with } x = \frac{q}{2k_F}$$

* First-order energy shift

$$\Delta E = -e^2 4\pi V \cdot \frac{1}{(2\pi)^6} \int \underbrace{d^3q \cdot \frac{1}{q^2}}_{\substack{4\pi q^2 dq \\ = 4\pi dq \; = \; 8\pi k_F dx}} \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x)$$

spherical shells

enforce $q < 2k_F$

$$= -4\pi e^2 V (2\pi)^{-6} \frac{4}{3}\pi k_F^3 \cdot 8\pi k_F \int_0^1 dx \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right)$$

$$= -\frac{e^2}{2a_0} \frac{N}{r_s} \left(\frac{9\pi}{4}\right)^{1/3} \frac{3}{2\pi} = -\frac{e^2}{2a_0} N \frac{0.916}{r_s}$$

Ground state energy per particle in the high-density limit

$$\frac{E}{N} \xrightarrow{r_s \to 0} \frac{e^2}{2a_0} \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots \right)$$

Note that

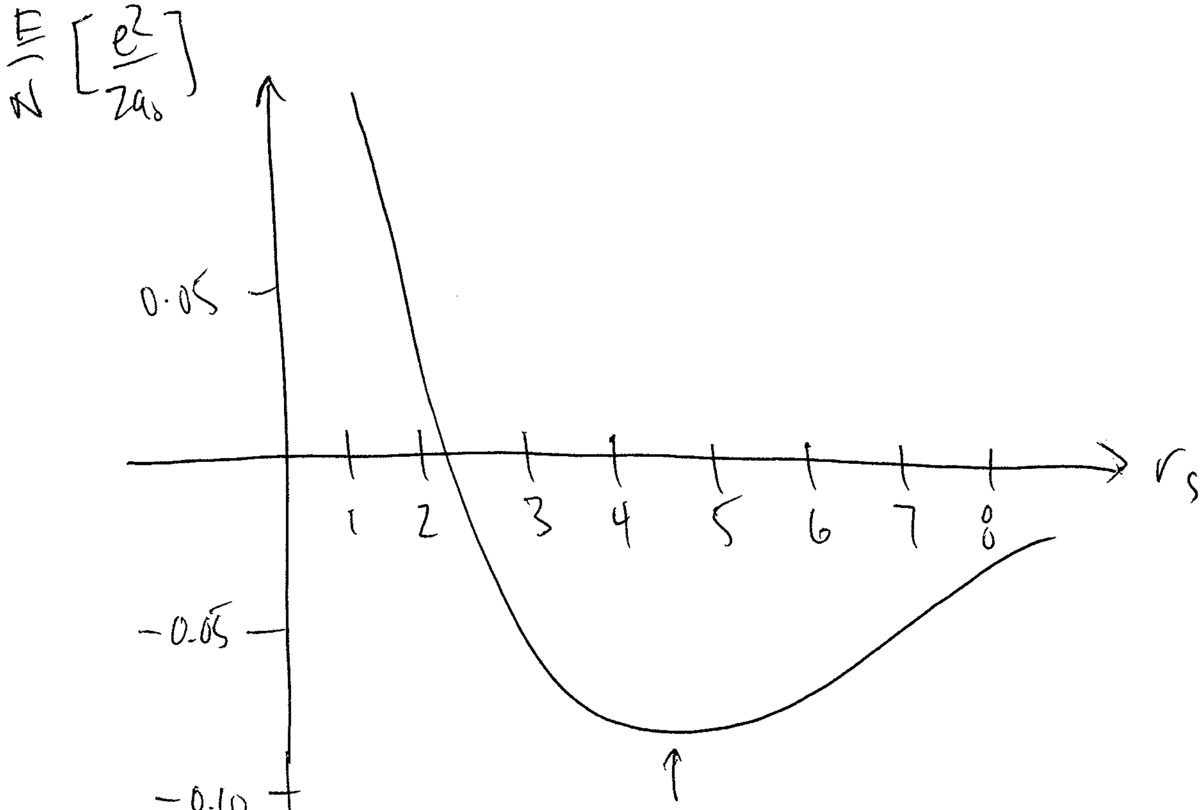
① the energy per particle is a constant, so the total energy is extensive (overall charge neutrality is important here, since the Coulomb interaction is long-ranged)

② the leading order term $\frac{e^2}{2a_0}\frac{2.21}{r_s^2}$ is just the kinetic energy of the electron gas

QUESTION: Would this be different if the particles were bosons rather than fermions?

③ the first-order correction is <u>negative</u> because it arises from a particle exchange process (the direct term is excluded by $q \neq 0$)

(4) Opposite signs of the competing terms ensure an energy minimum



minimum energy

$$\frac{E}{N} = -0.095\,\frac{e^2}{2a_0} = -1.29\,eV$$

at $r_s = 4.83$

QUESTION: What does the existence of a minimum tell us

(5) Comparison with real systems: e.g. metallic Na

$r_s = 3.96$ (measured density) $\quad E/N = -1.13\,eV$ (heat of vaporization)

* When does the expansion around $r_s = 0$ break down

→ is there a formal radius of convergence?

→ can other kinds of states intervene, so that abiabatic continuity with the noninteracting ground state breaks down?

* Consider the opposite limit $r_s \to \infty$ in which the Coulomb contribution ($\sim \frac{1}{r_s}$) swamps the kinetic energy ($\sim \frac{1}{r_s^2}$)

→ in that case, the motion of the electrons is quenched (up to zero-point motion)

→ have to consider the configuration (static) that minimizes the Coulomb interactions

→ so-called Wigner crystal
3D bcc $r_s \gtrsim 106$
2D triangular $r_s \gtrsim 31$