Lecture 38: Properties of Many-Body Systems

Monday, April 27, 2020

0.1 Coulomb Gas

In the last lecture we were discussing negatively charged Fermions in a positively charged background. We can write the classical Hamiltonian as

$$H = \sum_{i=1}^{\infty} \frac{p_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j} \frac{e^{-\mu|x_i - x_j|}}{|x_i - x_j|} + \frac{e^2}{2} \int \mathrm{d}^3 x, x' \, \frac{\rho(x)\rho(x')}{|x - x'|} e^{-\mu|x-x'|} - e^2 \sum_i \int \mathrm{d}^3 x \, \rho(x) \frac{e^{-\mu|x - x_i|}}{|x_i - x|}$$

The terms in order are the free particle kinetic energy, the pairwise interaction, the self-interaction of the background, and the interaction of the background with the electrons:

$$H = H_{\mathrm{KE}} + H_{\mathrm{Coulomb}} + H_{\mathrm{Background}} + H_{\mathrm{Background—Electrons}}$$

Since $\rho(x)$ is uniform, we can say $\rho(x) = \frac{N}{V}$ where N is both the number of electrons and the number of positive background charges, since we will assume the system is electrically neutral. In the end, we will take $\mu \to 0$ as we discussed in the last class.

$$\begin{aligned}
H_{\mathrm{bg}} &= \frac{e^2}{2} \int \mathrm{d}^3 x, x' \left(\frac{N}{V}\right)^2 \frac{e^{-\mu|x-x'|}}{|x - x'|} \\
&= \frac{e^2}{2} \left(\frac{N}{V}\right)^2 V \int \frac{e^{-\mu r}}{r} (4\pi) r^2 \, \mathrm{d}r \\
&= \frac{e^2}{2} \left(\frac{N^2}{V}\right) (4\pi) \int_0^\infty e^{-\mu r} r \, \mathrm{d}r \\
&= (\ldots)(-\partial_\mu \int_0^\infty e^{-\mu r} \, \mathrm{d}r) \\
&= \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2}
\end{aligned}$$

$$\begin{aligned}
H_{\mathrm{bg—e}} &= -e^2 \sum_i \int \mathrm{d}^3 x \, \frac{\rho(x) e^{-\mu|x - x_i|}}{|x - x_i|} \\
&= -e^2 \frac{N}{V} \sum_i \int \frac{e^{-\mu|x-x_i|}}{|x - x_i|} \, \mathrm{d}^3 x \\
&= -e^2 \frac{N}{V} \underbrace{\sum_i}_{N} \int_0^\infty 4\pi r e^{-\mu r} \\
&= -\frac{e^2 N^2}{V} \frac{4\pi}{\mu^2}
\end{aligned}$$

so

$$H = H_{\mathrm{KE}} + H_{\mathrm{C}} - \frac{e^2 N^2}{2V} \left(\frac{4\pi}{\mu^2}\right)$$

Now we will quantize in the Fock space. This is often called second-quantization. What basis should we quantize in (momentum, energy, position)? Obviously we want to choose the simplest one. We can treat the Coulomb interaction as a perturbation and treat H_{KE} as leading order (we will have to justify this later), so we can choose the momentum basis:

$$H_{\mathrm{KE}} = \sum_{k^2} a_k^\dagger a_k \frac{\hbar^2 k^2}{2m}$$

$$H_{\mathrm{C}} = \frac{e^2}{2}\sum_{i\neq j}\frac{e^{-\mu|x_i-x_j|}}{|x_i-x_j|}$$

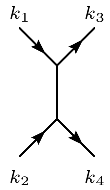
Last time we showed that we can write pairwise interactions as

$$V = \sum_{i\neq j} N_i N_j \frac{1}{2} V_{ij} + \sum_i \frac{1}{2} V_{ii} N_i (N_i - 1) = \frac{1}{2}\sum_{ij} a_i^\dagger a_j^\dagger a_i a_j$$

On the homework, we'll show that

$$V = \frac{1}{2}\sum_{k_1\lambda_1}\cdots\sum_{k_4\lambda_4}\langle k_1\lambda 1, k_2\lambda_2|\, V\, |k_3\lambda_3, k_4\lambda_4\rangle = \frac{e^2}{2V}\sum_{k_1\lambda_1\ldots k_4\lambda_4}\delta_{k_1+k_2,k_3+k_4}\frac{4\pi}{q^2+\mu^2} a_{k_1\lambda_1}^\dagger\cdots a_{k_4\lambda_4}^\dagger a_{k_1\lambda_1}\cdots a_{k_4\lambda_4}$$

where $q = k_1 - k_3$. This is just momentum conservation and represents a Feynman diagram:



Therefore

$$H = \sum_k a_k^\dagger a_k \frac{\hbar^2 k^2}{2m} + \frac{2^2}{2V}\sum_{k_i\lambda_i}(\cdots) - \frac{e^2 N^2}{2V}\left(\frac{4\pi}{\mu^2}\right)$$

Let's solve this when $q = 0$ (no momentum is exchanged) or $k_1 = k_3 = k$ and $k_2 = k_4 = q$: The interaction term is now

$$\begin{aligned}
H_{\mathrm{C}} &= \frac{e^2}{2V}\sum_{k,p}\sum_{\lambda_1,\lambda_2} a_{k,\lambda_1}^\dagger a_{p,\lambda_2}^\dagger a_{p,\lambda 3} a_{k,\lambda_4} \\
&= \frac{e^2}{2V}\sum\sum\left[N_{\lambda_1}(k)N_{\lambda_2}(p) - N_{\lambda_1}(k)\delta_{\lambda_1,\lambda_2}\right] \\
&= \frac{4\pi}{\mu^2}\frac{e^2}{2V}\left[N^2 - N\right]
\end{aligned}$$

Due to the $q = 0$ interaction, $\frac{E}{N} = \frac{4\pi e^2}{\mu^2(2V)}$, and this exactly cancels the other divergent μ term. We will then remove the forward scattering term:

$$H = \sum_\lambda\sum_k a_{\lambda k}^\dagger a_{\lambda k}\frac{\hbar^2 k^2}{2m} + 4\pi\frac{e^2}{2}\sum_{q\neq 0}\sum_{\lambda_i} a_{k_1,lambda_1}^\dagger a_{k_2,\lambda_2} a_{k_3,\lambda_3}^\dagger a_{k_4,\lambda_4}\frac{\delta_{k_1+k_2,k_3+k_4}}{q^2}$$

where the sum over $q = 0$ is the same as a sum over $k_1 \neq k_3$. Let's try to calculate the ground-state energy. We refer to the first term in this Hamiltonian as the one-particle operator or "free" operator and the second term the two-particle operator. It's easy to find the ground state for the first part, and then we can treat the Coulomb interaction as a perturbation. When can we do this? Counter-intuitively, the denser the gas is, the less important the Coulomb interaction becomes! Define r_0 as the typical inter-particle spacing. The potential energy will therefore go like PE $\sim \frac{e^2}{r_0}$. However, think about the kinetic energy: KE $\sim \frac{p^2}{2m}$. By the uncertainty principle, $px \sim \hbar$, so $p \sim \frac{\hbar}{x} \sim \frac{\hbar}{r_0}$. Then KE $\sim \frac{\hbar^2}{2mr_0^2}$! As we force particles into smaller and smaller regions, the uncertainty of p grows, which cases the kinetic energy to get smaller (much faster than the potential energy grows). If we want KE >> PE, we need $\frac{\hbar^2}{2mr_0^2} >> \frac{e^2}{r_0}$ or $r_0 << \frac{\hbar^2}{2me^2} = \frac{a_0}{2}$, so we expect our approximation to hold when

$$\frac{r_0}{a_0} \equiv r_s << 1$$

At leading order,

$$(H_0 = H_{\mathrm{KE}})\,|\Omega\rangle \equiv E_0\,|\Omega\rangle$$

the ground state is just filling up the Fermi sea, where we will call the highest energy state $E_F = \frac{\hbar^2 k_F^2}{2m}$. The leading-order result is

$$N = \sum_{k,\lambda} \Theta(k_F - k) = \sum_{\lambda} \frac{1}{(2\pi)^3} \int \mathrm{d}^3k\, V \Theta(k - k_F) = (2V)(4\pi) \frac{1}{(2\pi)^3} \int_0^{k_F} k^2 \,\mathrm{d}k = \frac{V}{3\pi^2} k_F^3$$

so

$$K_F = \left[\frac{3\pi N}{V} \right]^{1/3}$$

Therefore

$$E_0 = \underbrace{2}_{\text{spin}} \int^{k_F} \frac{V\,\mathrm{d}^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} = \frac{V\hbar^2}{2m\pi^2} \frac{k_F^5}{5}$$

or

$$E_0 = \frac{e^2}{2a_0} N \frac{3}{5} \left[\frac{a_0 \pi}{4} \right]^{2/3} \frac{1}{r_s^2}$$

This is divergent as $r_s \to 0$, which is true, since the momentum should diverge as we compress the system. We should hope that our first-order correction fixes this.