1. Coulomb Interaction in second Quantization

The total (Coulomb) interaction operator of an eletron gas in second Quantization is given by

$$\hat{V}_c = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int dr_1 dr_2 \frac{1}{4\pi\epsilon_0}\frac{e^2}{|r_1 - r_2|}\psi^\dagger_{\sigma_1}(r_1)\psi^\dagger_{\sigma_2}(r_2)\psi_{\sigma_2}(r_2)\psi_{\sigma_1}(r_1) \tag{1}$$

where $\psi^\dagger_{\sigma_1}(r_1)$ is a fermionic quantum field, which creates an electron on position r_1, and $\sigma = \pm\frac{1}{2}$.

(a) Why is the factor $\frac{1}{2}$ neccessary to correctly define the Coulomb interaction in this language?

Sonst würden wir die Wechselwirkung doppelt zählen (r1, r2) und (r2, r1)

(b) Apply the following Fourier transform

$$\psi^\dagger_\sigma(r) = \frac{1}{\sqrt{V}}\sum_k e^{-ikr} f^\dagger_\sigma(k) \qquad \psi_\sigma(r) = \frac{1}{\sqrt{V}}\sum_k e^{ikr} f_\sigma(k) \tag{2}$$

where V, is the volume of the crystal to obtain the Coulomb-Interaction in momentum space.
Hint: Apply the substitution $r = r_2 - r_1$ and a similar substitution for two momentum variables.

$$\hat{V}_c = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}\frac{1}{V^2}\left[\sum_{k_1} e^{-ik_1 r_1} f^\dagger_{\sigma_1}(k_1)\right]\left[\sum_{k_2} e^{-ik_2 r_2} f^\dagger_{\sigma_2}(k_2)\right]$$
$$\left[\sum_{k_3} e^{ik_3 r_2} f_{\sigma_2}(k_3)\right]\left[\sum_{k_4} e^{ik_4 r_1} f_{\sigma_1}(k_4)\right] dr_1 dr_2$$

$$= \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 V^2}\sum_{\sigma_1\sigma_2 k_1 k_2 k_3 k_4} f^\dagger_{\sigma_1}(k_1) f^\dagger_{\sigma_2}(k_2) f_{\sigma_2}(k_3) f_{\sigma_1}(k_4)$$
$$\int \frac{1}{|\vec{r}_1 - \vec{r}_2|} e^{i(k_4 - k_1) r_1} e^{i(k_3 - k_2) r_2} dr_1 dr_2$$

Variablenwechsel:
$$k_3 \to k_2 + q$$
$$k_4 \to k_1 - q'$$
$$r_1 \to r_2 + r$$

$$\hat{V}_c = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 V^2}\sum_{\sigma_1\sigma_2 k_1 k_2 q q'} f^\dagger_{\sigma_1}(k_1) f^\dagger_{\sigma_2}(k_2) f_{\sigma_2}(k_2 + q) f_{\sigma_1}(k_1 - q')$$
$$\int \frac{1}{|\vec{r}|} e^{-iq'(r_2 + r)} e^{iq r_2} dr\, dr_2$$

$$= \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 V^2}\sum_{\sigma_1\sigma_2 k_1 k_2 q q'} f^\dagger_{\sigma_1}(k_1) f^\dagger_{\sigma_2}(k_2) f_{\sigma_2}(k_2 + q) f_{\sigma_1}(k_1 - q')$$
$$\int \frac{1}{|\vec{r}|} e^{i(q - q') r_2} e^{iq' r} dr_2\, dr$$

$$= \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 V}\sum_{\sigma_1\sigma_2 k_1 k_2 q} f^\dagger_{\sigma_1}(k_1)\, f^\dagger_{\sigma_2}(k_2)\, f_{\sigma_2}(k_2+q)\, f_{\sigma_1}(k_1-q) \int \frac{e^{iqr}}{|\vec r|}\, dr$$

(c) Solve the remaining integral $V(\boldsymbol{q})$ in 3 spatial dimensions.
<u>Hint:</u> You will need to multiply a convergence factor $e^{-\kappa|\boldsymbol{r}|}$ with $\kappa > 0$ to the integral and evaluate $\kappa \to 0$ afterwards in order to make the integral converge. Give a physical argument to justify this procedure.

$$\int \frac{e^{iqr}}{|\vec r|}\, dr = \lim_{\kappa\to 0} \int \frac{e^{iqr}}{|\vec r|}\, e^{-\kappa|\vec r|}\, dr$$

$$= \lim_{\kappa\to 0} \int \frac{e^{iq|\vec r|\cos\theta}}{|\vec r|}\, e^{-\kappa|\vec r|}\, dr$$

$$= \lim_{\kappa\to 0} \int_0^\infty\int_0^\pi\int_0^{2\pi} r\, e^{iqr\cos\theta}\, e^{-\kappa r} \sin\theta\, d\varphi\, d\theta\, dr$$

$$= \lim_{\kappa\to 0} 2\pi \int_0^\infty r\, e^{-\kappa r}\, \frac{2\sin(qr)}{qr}\, dr$$

$$= \lim_{\kappa\to 0} 2\pi \int_0^\infty \frac{e^{-\kappa r}}{iq}\left[e^{iqr} - e^{-iqr}\right] dr$$

$$= \lim_{\kappa\to 0} \frac{2\pi}{iq}\left[-\frac{1}{-\kappa+iq} + \frac{1}{-\kappa-iq}\right]$$

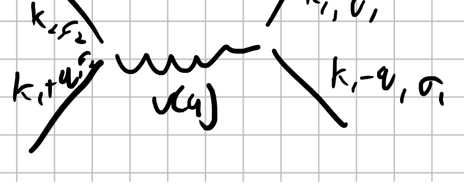
$$= \lim_{\kappa\to 0} -\frac{2\pi}{iq}\left[\frac{1}{-\kappa+iq} + \frac{1}{\kappa+iq}\right]$$

$$= \lim_{\kappa\to 0} -\frac{2\pi}{iq}\left[\frac{2iq}{-q^2-\kappa^2}\right]$$

$$= \lim_{\kappa\to 0} \frac{4\pi}{q^2+\kappa^2}$$

$$\to \frac{4\pi}{q^2}$$

(d) The result you just calculated will be required in order to do perturbation theory for the Coulomb interaction. How can the result be written as a Feynman-Diagram?



2. Bose-Einstein Distribution

From thermodynamics, the grand canonical partition function Z is known to be

$$Z = \mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right], \tag{5}$$

where μ denotes the chemical potential and the trace over the Hamilton operator $\hat{H}$ and total number operator $\hat{N}$ is taken over the whole many-particle Hilbert space (also known as Fock space) $\mathcal{F}$, i.e.

$$\mathrm{tr}\left[\hat{O}\right] = \sum_i \langle\psi_i|\hat{O}|\psi_i\rangle \tag{6}$$

for any base $\{|\psi_i\rangle\}$ of $\mathcal{F}$.

We can compute thermal averages of any operator $\hat{O}$ as

$$\left\langle\hat{O}\right\rangle = \frac{1}{Z}\,\mathrm{tr}\left[\hat{O}e^{-\beta(\hat{H}-\mu\hat{N})}\right]. \tag{7}$$

Suppose, that we can find a basis, labeled by the quantum number λ, in which the Hamiltonian is diagonal, i.e.

$$\hat{H} = \sum_\lambda \epsilon_\lambda \hat{n}_\lambda, \tag{8}$$

where $\hat{n}_\lambda$ is a *bosonic* number operator.

(a) Write $\hat{H}$ and $\hat{N}$ in terms of (bosonic) creation and annihilation operators.

$$\hat{H} = \sum_\lambda \varepsilon_\lambda a^\dagger_\lambda a_\lambda$$

$$\hat{N} = \sum_\lambda a^\dagger_\lambda a_\lambda$$

(b) Show, that one can write $Z = \prod_\lambda Z_\lambda$ and calculate Z_λ.
Hint: Geometric series

$$Z_\lambda = \mathrm{tr}\left[e^{-\beta(\varepsilon_\lambda-\mu)a^\dagger_\lambda a_\lambda}\right]$$

$$\mathrm{tr}\left[e^{\sum_\lambda -\beta(\varepsilon_\lambda-\mu)a^\dagger_\lambda a_\lambda}\right] = Z = \prod_\lambda Z_\lambda = \prod_\lambda \mathrm{tr}\left[e^{-\beta(\varepsilon_\lambda-\mu)a^\dagger_\lambda a_\lambda}\right]$$

$$Z = \mathrm{tr}\left[e^{\sum_\lambda -\beta(\varepsilon_\lambda-\mu)a^\dagger_\lambda a_\lambda}\right]$$

$$= \sum_\lambda \langle\psi_\lambda|e^{\sum_\lambda -\beta(\varepsilon_\lambda-\mu)a^\dagger_\lambda a_\lambda}|\psi_\lambda\rangle$$