6 Energy of the electron gas

As the illustration of the usefulness of the formalism just developed we will calculate the energy of the gas of electrons. This example is interesting because it illustrates also some problems arising in higher orders of the perturbation calculus and specific methods of circumventing them. The technique of Feynman diagrams will be also presented although in a slightly nonstandard context.

6.1 The Hamiltonian

The model consists of N electrons and a uniform background of positive charges. Because of this simplification it can serve only as the first approximation to more complex situations encountered in metals or plasma where one has to take into account also localization (which is more important) and motion of the positively charged ions.

We consider the system of electrons and ions enclosed in a finite box of volume $V = L^3$. In order to maintain translational invariance the periodic boundary conditions are imposed. We will also consider only the volume effects by taking the thermodynamical limit $N \to \infty$, $V \to \infty$; the surface phenomena are then neglected.

The basis of 1-particle electron states can be taken in the form of plane waves

$$\psi_{\mathbf{k}\lambda}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \eta_\lambda \ , \tag{6.1}$$

where η_λ with $\lambda = \pm\frac{1}{2}$ is the spin function

$$\eta_{+\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \qquad \eta_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ ,$$

and $\mathbf{k} = (k_x, k_y, k_z)$ with $k_i = (2\pi/L)n_i$, $n_i = 0, 1, 2, \ldots$ The formula (6.1) can be also written as

$$\langle \mathbf{r}, \lambda' | \mathbf{k}, \lambda \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \delta_{\lambda,\lambda'} \ .$$

In the standard formulation the Hamiltonian describing the system of N electrons and a (non-dynamical) distribution $n(\mathbf{r})$ of positive charges consists of three terms $H = H_{\rm el} + H_{\rm b} + H_{\rm el-b}$:

$$H_{\rm el} = \sum_{i=1}^{N} \frac{\hat{\mathbf{P}}_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j}^{N} \frac{1}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} e^{-\mu|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} \equiv H_{\rm el}^0 + H_{\rm el}' \ , \tag{6.2}$$

$$H_{\rm b} = \frac{e^2}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} e^{-\mu|\mathbf{r} - \mathbf{r}'|} \ , \tag{6.3}$$

$$H_{\rm el-b} = -e^2 \sum_{i=1}^{N} \int d^3\mathbf{r}' \frac{n(\mathbf{r}')}{|\hat{\mathbf{r}}_i - \mathbf{r}'|} e^{-\mu|\hat{\mathbf{r}}_i - \mathbf{r}'|} \ , \tag{6.4}$$

where we have introduced some regularization μ of the long range Coulomb forces. In the following we will consider only the uniform distribution of the positive charges $n(\mathbf{r}) = N/V$ and will take the thermodynamical limit $N \to \infty$, $V \to \infty$, keeping N/V =const. Each term of the Hamiltonian is separately divergent in the limit $\mu \to 0$. However, the energy (per particle) given by the sum of the three terms is finite provided the thermodynamical limit is taken in such a way that

$$\mu L \gg 1 \ , \tag{6.5}$$

which physically corresponds to keeping the long range forces regularized at each stage of the limiting procedure.

From the quantum mechanics point of view, $H_{\rm b}$ is not an operator, but a c-number. It can be computed by shifting the integration variable:

$$\begin{aligned} H_{\rm b} &= \frac{e^2}{2} \frac{N^2}{V^2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{e^{-\mu|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} = \frac{e^2}{2} \frac{N^2}{V} \int d^3\mathbf{r} \frac{e^{-\mu|\mathbf{r}|}}{|\mathbf{r}|} \\ &= \frac{e^2}{2} \frac{N^2}{V} 4\pi \int_0^\infty dr r^2 \frac{e^{-\mu r}}{r} = \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2} \ . \end{aligned} \tag{6.6}$$

(due to the condition (6.5) we could extend the last integral to the whole space.)

$H_{\rm el-b}$ is a 1-particle operator acting in the many-electron Hilbert space. According to the prescription (5.42) we write it as

$$H_{\rm el-b} = -e^2 \int d^3\mathbf{r}' \ n(\mathbf{r}') \sum_{\mathbf{k}'\lambda'} \sum_{\mathbf{k},\lambda} \langle \mathbf{k}', \lambda' | \frac{e^{-\mu|\hat{\mathbf{r}} - \mathbf{r}'|}}{|\hat{\mathbf{r}} - \mathbf{r}'|} | \mathbf{k}, \lambda \rangle \ a^\dagger_{\mathbf{k}'\lambda'} a_{\mathbf{k}\lambda}$$

$$= -e^2 \int d^3\mathbf{r}' n(\mathbf{r}') \sum_{\mathbf{k}'\lambda'} \sum_{\mathbf{k}\lambda} a^\dagger_{\mathbf{k}'\lambda'} a_{\mathbf{k}\lambda} \int d^3\mathbf{r} \frac{1}{\sqrt{V}} e^{-i\mathbf{k}'\cdot\mathbf{r}} \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

$$= -e^2 \frac{N}{V^2} \sum_{\lambda} \sum_{\mathbf{k},\mathbf{k}'} a^\dagger_{\mathbf{k}'\lambda} a_{\mathbf{k}\lambda} \int d^3\mathbf{r}\ e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} \int d^3\mathbf{r}'\ \frac{e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} .$$

Again, due to the condition (6.5) the last integration can be extended to the whole space. The integration variable can be then shifted, so that the integral becomes independent of $\mathbf{r}$ and yields $4\pi/\mu^2$, similarly as in (6.6). The remaining integral over $d^3\mathbf{r}$ gives then $V\delta_{\mathbf{k},\mathbf{k}'}$, and we obtain

$$H_{\mathrm{el-b}} = -e^2 \frac{N}{V} \frac{4\pi}{\mu^2} \sum_{\mathbf{k}\lambda} a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} = -e^2 \frac{N}{V} \frac{4\pi}{\mu^2} \mathcal{N} ,$$

where $\mathcal{N}$ is the total particle number operator (5.44). This operator gives the same number N on any state belonging to the subspace $\mathcal{H}^{(N)}$ (we are working in) of the big Hilbert space $\mathcal{H} = \oplus_{N=0}^{\infty} \mathcal{H}^{(N)}$, so we effectively get

$$H_{\mathrm{b}} + H_{\mathrm{el-b}} = -\frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2} . \tag{6.7}$$

The kinetic energy operator in H_{el} is easily rewritten in the second quantized form by applying the rule (5.42):

$$\frac{1}{2m} \sum_{i=1}^{N} \hat{\mathbf{P}}_i^2 \to \frac{1}{2m} \sum_{\mathbf{k}'\lambda'} \sum_{\mathbf{k},\lambda} a^\dagger_{\mathbf{k}'\lambda'} a_{\mathbf{k}\lambda} \langle \mathbf{k}', \lambda' | \hat{\mathbf{P}}^2 | \mathbf{k}, \lambda \rangle ,$$

where

$$\langle \mathbf{k}', \lambda' | \hat{\mathbf{P}}^2 | \mathbf{k}, \lambda \rangle = \frac{1}{V} \int d^3\mathbf{r} e^{-i\mathbf{k}'\cdot\mathbf{r}} \eta^\dagger_{\lambda'} \left(-\hbar^2 \boldsymbol{\nabla}^2 \right) e^{i\mathbf{k}\cdot\mathbf{r}} \eta_\lambda = \hbar^2 \mathbf{k}^2 \delta_{\lambda',\lambda} \delta_{\mathbf{k}'\mathbf{k}} ,$$

so that

$$H^0_{\mathrm{el}} \equiv H^{\mathrm{kin}}_{\mathrm{el}} = \sum_{\mathbf{k},\lambda} \frac{\hbar^2 \mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} \tag{6.8}$$

Finally we apply the general prescription (5.56) to the interaction part of the Hamiltonian H_{el}. Since the interaction does not depend on the spin variable, (5.56) takes the form

$$H'_{\mathrm{el}} = \frac{1}{2} \sum_{\lambda,\lambda'} \int d^3\mathbf{r} \int d^3\mathbf{r}' a^\dagger_\lambda(\mathbf{r}) a^\dagger_{\lambda'}(\mathbf{r}') V(\mathbf{r}-\mathbf{r}') a_{\lambda'}(\mathbf{r}') a_\lambda(\mathbf{r}) ,$$

where $V(\mathbf{r}-\mathbf{r}')$ is the (regularized) Coulomb interaction. We now use the rules (5.37) allowing to pass to the momentum representation

$$a_\lambda^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}\lambda}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}} \ , \qquad a_\lambda(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}\lambda} e^{i\mathbf{k}\cdot\mathbf{r}} \ ,$$

to get

$$H'_{\text{el}} = \frac{e^2}{2}\frac{1}{V^2}\sum_{\mathbf{k}_1\ldots\mathbf{k}_4}\sum_{\lambda,\lambda'} a_{\mathbf{k}_1\lambda}^\dagger a_{\mathbf{k}_2\lambda'}^\dagger a_{\mathbf{k}_3\lambda'} a_{\mathbf{k}_4\lambda}$$
$$\times \int d^3\mathbf{r}' \int d^3\mathbf{r} e^{-i\mathbf{k}_1\cdot\mathbf{r}} e^{-i\mathbf{k}_2\cdot\mathbf{r}'} \frac{e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} e^{i\mathbf{k}_3\cdot\mathbf{r}'} e^{-i\mathbf{k}_4\cdot\mathbf{r}} \ .$$

After the change of variables: $\mathbf{x} = \mathbf{r}-\mathbf{r}'$, $d^3\mathbf{r}d^3\mathbf{r}' = d^3\mathbf{x}d^3\mathbf{r}'$, the double integral becomes

$$\int d^3\mathbf{r}' \ e^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{r}'} \int d^3\mathbf{x} \ e^{i\mathbf{q}\cdot\mathbf{x}} \ \frac{e^{-\mu|\mathbf{x}|}}{|\mathbf{x}|}$$

where $\mathbf{q} = \mathbf{k}_4 - \mathbf{k}_1$. The first integration then gives $V\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}$, and the second can be performed by choosing the z-axis parallel to the vector $\mathbf{q}$ so that $\mathbf{q}\cdot\mathbf{x} = qx\cos\theta \equiv qx\xi$

$$2\pi\int_0^\infty dx \ x^2 \int_{-1}^{+1} d\xi \ e^{iqx\xi} \ \frac{e^{-\mu x}}{x} = \frac{2\pi}{iq}\int_0^\infty dx \left(e^{(iq-\mu)x} - e^{-(iq+\mu)x}\right)$$
$$= \frac{2\pi}{iq}\left(\frac{1}{\mu-iq} - \frac{1}{\mu+iq}\right) = \frac{4\pi}{\mathbf{q}^2+\mu^2} \ .$$

As a result we obtain

$$H'_{\text{el}} = \frac{e^2}{2V}\sum_{\lambda,\lambda'}\sum_{\mathbf{k}_1\ldots\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\frac{4\pi}{|\mathbf{k}_4-\mathbf{k}_1|^2+\mu^2} a_{\mathbf{k}_1\lambda}^\dagger a_{\mathbf{k}_2\lambda'}^\dagger a_{\mathbf{k}_3\lambda'} a_{\mathbf{k}_4\lambda}$$
$$= \frac{e^2}{2V}\sum_{\lambda_1,\lambda_2}\sum_{\mathbf{k}_1,\mathbf{k}_2}\sum_{\mathbf{q}} \frac{4\pi}{\mathbf{q}^2+\mu^2} a_{\mathbf{k}_1+\mathbf{q}\lambda_1}^\dagger a_{\mathbf{k}_2-\mathbf{q}\lambda_2}^\dagger a_{\mathbf{k}_2\lambda_2} a_{\mathbf{k}_1\lambda_1} \ ,$$

where we have introduced the unrestricted summation over $\mathbf{q}$.

Before we begin the quantum mechanical calculations it is convenient to extract from H'_{el} the contribution of the $\mathbf{q}=0$ term, which (on the

$\mathcal{H}^{(N)}$ subspace) is also not an operator, but a c-number:

$$(H'_{\rm el})_{\mathbf{q}=0} = \frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{\lambda_1,\lambda_2}\sum_{\mathbf{k}_1,\mathbf{k}_2} a^\dagger_{\mathbf{k}_1\lambda_1}a^\dagger_{\mathbf{k}_2\lambda_2}a_{\mathbf{k}_2\lambda_2}a_{\mathbf{k}_1\lambda_1}$$

$$= \frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{\lambda_1,\lambda_2}\sum_{\mathbf{k}_1,\mathbf{k}_2}\left(a^\dagger_{\mathbf{k}_1\lambda_1}a_{\mathbf{k}_1\lambda_1}a^\dagger_{\mathbf{k}_2\lambda_2}a_{\mathbf{k}_2\lambda_2} - a^\dagger_{\mathbf{k}_1\lambda_1}a_{\mathbf{k}_2\lambda_2}\delta_{\lambda_1,\lambda_2}\delta_{\mathbf{k}_1,\mathbf{k}_2}\right)$$

$$= \frac{e^2}{2V}\frac{4\pi}{\mu^2}\left(\mathcal{N}^2 - \mathcal{N}\right) ,$$

where we have applied successively the two anticommutation rules

$$a_{\mathbf{k}_2\lambda_2}a_{\mathbf{k}_1\lambda_1} = -a_{\mathbf{k}_1\lambda_1}a_{\mathbf{k}_2\lambda_2} , \qquad a^\dagger_{\mathbf{k}_2\lambda_2}a_{\mathbf{k}_1\lambda_1} = -a_{\mathbf{k}_1\lambda_1}a^\dagger_{\mathbf{k}_2\lambda_2} + \delta_{\lambda_1,\lambda_2}\delta_{\mathbf{k}_1,\mathbf{k}_2} .$$

Thus, the $\mathbf{q}=0$ term combines with $H_{\rm b} + H_{\rm el-b}$ (6.7) to give

$$H_{\rm b} + H_{\rm el-b} + (H'_{\rm el})_{\mathbf{q}=0} = -\frac{e^2}{2}\frac{N^2}{V}\frac{4\pi}{\mu^2} + \frac{e^2}{2V}\frac{4\pi}{\mu^2}(N^2 - N) = -\frac{e^2}{2V}\frac{4\pi}{\mu^2}N .$$

The N^2 terms have canceled each other as a result of the electrical neutrality of the system as the whole. The last term arises because of the unaccounted surface effects but it is unimportant in the thermodynamical limit: *per particle* this contribution to the energy is $\propto 1/V\mu^2 = (1/L)(1/(L\mu)^2) \to 0$ (in other words, this term is not an extensive quantity, we are interested in).

In the remaining part of $H'_{\rm el}$ (which we will continue to denote $H'_{\rm el}$ remembering however, that now $\mathbf{q} \neq 0$) we can set $\mu = 0$.

It is also useful to express the Hamiltonian in atomic units, in order to see in which circumstances the perturbation calculus can be used to compute the ground state energy of the system. To this end we define r_0 and r_s by

$$V = \frac{4}{3}\pi r_0^3 N , \qquad r_s = \frac{r_0}{a_0} = \frac{1}{a_0}\left(\frac{3}{4\pi}\frac{V}{N}\right)^{\frac{1}{3}} , \tag{6.9}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius. r_0 characterizes therefore the average length separating two electrons and r_s is the same length in units of a_0. We can then write

$$\frac{\hbar^2\mathbf{k}^2}{2m} = \frac{\hbar^2}{me^2}\,\frac{e^2}{2}\,\frac{\tilde{\mathbf{k}}^2}{r_0^2} = \frac{e^2}{2}\,\frac{a_0}{r_0^2}\,\tilde{\mathbf{k}}^2 = \frac{e^2}{2a_0}\,\frac{1}{r_s^2}\,\tilde{\mathbf{k}}^2 ,$$

$$\frac{e^2}{2V}\frac{1}{\mathbf{q}^2} = \frac{e^2}{2r_0\bar{V}}\ \frac{1}{\tilde{\mathbf{q}}^2} = \frac{e^2}{2a_0}\ \frac{1}{r_s^2}\ \frac{r_s}{\bar{V}}\ \frac{1}{\tilde{\mathbf{q}}^2}\ ,$$

where we have introduced dimensionless wave vectors $\tilde{\mathbf{k}} = r_0\mathbf{k}$ etc., and the reduced dimensionless volume $\bar{V} = V/r_0^3$. In these variables the Hamiltonian takes the form

$$H = \frac{e^2}{2a_0r_s^2}\left(\sum_{\tilde{\mathbf{k}},\lambda}\tilde{\mathbf{k}}^2 a^\dagger_{\tilde{\mathbf{k}},\lambda}a_{\tilde{\mathbf{k}},\lambda} + \frac{r_s}{\bar{V}}\sum_{\tilde{\mathbf{k}}_1,\tilde{\mathbf{k}}_2}\sum_{\lambda_1,\lambda_2}\sum_{\tilde{\mathbf{q}}\neq 0}\frac{4\pi}{\tilde{\mathbf{q}}^2}a^\dagger_{\tilde{\mathbf{k}}_1+\tilde{\mathbf{q}}\lambda_1}a^\dagger_{\tilde{\mathbf{k}}_2-\tilde{\mathbf{q}}\lambda_2}a_{\tilde{\mathbf{k}}_2\lambda_2}a_{\tilde{\mathbf{k}}_1\lambda_1}\right).$$

It becomes now clear, that the perturbation calculus can be reliable provided $r_s \to 0$ or, more precisely, provided $r_s/\bar{V} \ll 1$, that is, if $r_s/\bar{V} \propto V^{\frac{1}{3}}/a_0N \propto L/N$ is small. This is interesting as it has nothing to do with the weakness of the electrostatic force nor does it require a short range of the potential; instead the necessary condition is satisfied for a dense electron gas ($r_s \to 0$).

6.2 Ground state energy of the electron gas

We will now calculate the ground state energy by using the ordinary quantum mechanical perturbation calculus. Neglecting the Coulomb interaction of the electrons the ground state is a state described in subsection 5.4

$$|\text{ground}\rangle \equiv |\text{F}\rangle\ ,$$

i.e. the state in which all one particle states with momenta $\mathbf{k}$ such that $|\mathbf{k}| < k_F$ are occupied. k_F is called the Fermi momentum (more precisely, the Fermi wave number) and the states such that $|\mathbf{k}| = k_F$ form the so-called Fermi shell. For a given volume V the Fermi momentum can be related to the number of electrons N:

$$N = \langle\text{F}|\mathcal{N}|\text{F}\rangle = \sum_{\mathbf{k},\lambda}\theta(k_F - |\mathbf{k}|) = 2\sum_{\mathbf{k}}\theta(k_F - |\mathbf{k}|) \tag{6.10}$$

where $\theta(k)$ is the Heaviside step function. Replacing the sum by the integral according to the rule (5.29) we get

$$N = 2\frac{V}{(2\pi)^3}\int d^3\mathbf{k}\ \theta(k_F - |\mathbf{k}|) = \frac{V}{4\pi^3}4\pi\int_0^\infty dk\ k^2\theta(k_F - k) = \frac{Vk_F^3}{3\pi^2}\ .$$

Therefore,

$$k_F = \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}} = \left(3\pi^2 N \frac{3}{4\pi N r_0^3}\right)^{\frac{1}{3}} = \left(\frac{9}{4}\pi\right)^{\frac{1}{3}} \frac{1}{r_0} , \qquad (6.11)$$

where we have used the definition (6.9) of r_0.

The state $|\mathrm{F}\rangle$ is obviously the eigenstate of the unperturbed Hamiltonian H^0_{el} and the lowest order approximation to the ground state energy E is given by

$$\begin{aligned} E^{(0)} &= \langle \mathrm{F}|H^0_{\mathrm{el}}|\mathrm{F}\rangle = 2\sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m}\theta(k_F - |\mathbf{k}|) \\ &\to \frac{\hbar^2}{m}\frac{V}{(2\pi)^3}\int d^3\mathbf{k}\ \mathbf{k}^2\ \theta(k_F - |\mathbf{k}|) = \frac{\hbar^2}{m}\frac{V}{2\pi^2}\frac{k_F^5}{5} = N\frac{3}{5}\left(\frac{\hbar^2 k_F^2}{2m}\right) , \end{aligned}$$

that is, the average electron energy is 3/5 of the Fermi energy. This can be also rewritten as

$$E^{(0)} = \frac{3}{5}\frac{\hbar^2}{2m}\left(\frac{9}{4}\pi\right)^{\frac{2}{3}}\frac{N}{r_0^2} = \frac{3}{5}\left(\frac{9}{4}\pi\right)^{\frac{2}{3}}\frac{a_0 e^2}{2r_0^2}N = \frac{3}{5}\left(\frac{9}{4}\pi\right)^{\frac{2}{3}}\frac{e^2}{2a_0}\frac{N}{r_s^2} , \quad (6.12)$$

where $e^2/2a_0 = 13.6$ eV (1 Rydberg) and $(3/5)(9\pi/4)^{2/3} = 2.21$.

The first order correction $\Delta E^{(1)}$ to the above result is given as usually by

$$\Delta E^{(1)} = \langle \mathrm{F}|H'_{\mathrm{el}}|\mathrm{F}\rangle = \frac{e^2}{2V}\sum_{\mathbf{q}\neq 0}\frac{4\pi}{\mathbf{q}^2}\sum_{\lambda_1,\lambda_2}\sum_{\mathbf{k}_1,\mathbf{k}_2}\langle \mathrm{F}|a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2}a_{\mathbf{k}_2\lambda_2}a_{\mathbf{k}_1\lambda_1}|\mathrm{F}\rangle ,$$

It is clear that the matrix element is nonzero only if $|\mathbf{k}_1| < k_F$, $|\mathbf{k}_2| < k_F$, $|\mathbf{k}_1 + \mathbf{q}| < k_F$ and $|\mathbf{k}_2 - \mathbf{q}| < k_F$, i.e., if all momenta are below the Fermi shell. Therefore, there are only two possible terms contributing to the sums over $(\mathbf{k}_1, \lambda_1)$ and $(\mathbf{k}_2, \lambda_2)$:

$$\text{either} \quad \begin{cases} (\mathbf{k}_1 + \mathbf{q}, \lambda_1) = (\mathbf{k}_1, \lambda_1) \\ (\mathbf{k}_2 - \mathbf{q}, \lambda_2) = (\mathbf{k}_2, \lambda_2) \end{cases} \quad \text{or} \quad \begin{cases} (\mathbf{k}_1 + \mathbf{q}, \lambda_1) = (\mathbf{k}_2, \lambda_2) \\ (\mathbf{k}_2 - \mathbf{q}, \lambda_2) = (\mathbf{k}_1, \lambda_1) \end{cases} .$$

The first combination is however not possible because $\mathbf{q} \neq 0$. Thus,

$$\Delta E^{(1)} = \frac{e^2}{2V}\sum_{\mathbf{q}\neq 0}\frac{4\pi}{\mathbf{q}^2}\sum_{\lambda}\sum_{\mathbf{k}}\langle \mathrm{F}|a^\dagger_{\mathbf{k}+\mathbf{q}\lambda}a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}+\mathbf{q}\lambda}a_{\mathbf{k}\lambda}|\mathrm{F}\rangle$$

$$= -\frac{e^2}{2V}\sum_{\mathbf{q}\neq 0}\frac{4\pi}{\mathbf{q}^2}\sum_{\lambda}\sum_{\mathbf{k}}\langle \mathrm{F}|a^\dagger_{\mathbf{k}+\mathbf{q}\lambda}a_{\mathbf{k}+\mathbf{q}\lambda}a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}|\mathrm{F}\rangle$$
$$= -\frac{e^2}{2V}\sum_{\mathbf{q}\neq 0}\frac{4\pi}{\mathbf{q}^2}\sum_{\lambda}\sum_{\mathbf{k}}\langle \mathrm{F}|\mathcal{N}_{\mathbf{k}+\mathbf{q}\lambda}\mathcal{N}_{\mathbf{k}\lambda}|\mathrm{F}\rangle$$
$$= -\frac{e^2}{2V}\sum_{\mathbf{q}\neq 0}\frac{4\pi}{\mathbf{q}^2}\sum_{\lambda}\sum_{\mathbf{k}}\theta(k_F-|\mathbf{k}+\mathbf{q}|)\,\theta(k_F-|\mathbf{k}|)\ ,$$

where in the second line we have used $a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}+\mathbf{q}\lambda} = -a_{\mathbf{k}+\mathbf{q}\lambda}a^\dagger_{\mathbf{k}\lambda}$ valid for $\mathbf{q}\neq 0$. Replacing the sums by integrals according to the rule (5.29) and introducing the new integration variable $\mathbf{p} = \mathbf{k}+\frac{1}{2}\mathbf{q}$ (the Jacobian is 1) we get

$$\Delta E^{(1)} = -4\pi e^2\frac{V}{(2\pi)^6}\int\frac{d^3\mathbf{q}}{\mathbf{q}^2}\int d^3\mathbf{p}\ \theta(k_F-|\mathbf{p}+\frac{1}{2}\mathbf{q}|)\ \theta(k_F-|\mathbf{p}-\frac{1}{2}\mathbf{q}|)\ ,$$

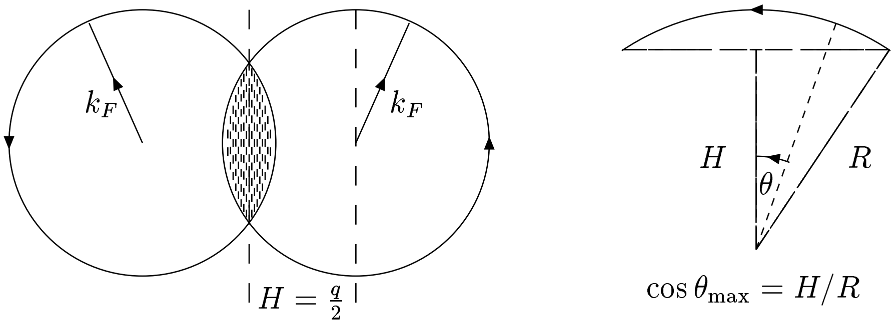


Figure 3: Geometrical meaning of the integral over $d^3\mathbf{p}$.

Geometrically the integration over $d^3\mathbf{p}$ gives simply the volume of the intersection of two balls each of radius k_F, the centers of which are separated by $|\mathbf{q}|$. It is easier to compute half of this volume (and multiply it later by 2). As follows from Figure 3 and denoting $|\mathbf{q}|/2 \equiv H$, $k_F \equiv R$, this (half of the) volume is given by the integral

$$\frac{1}{2}\text{volume} = \int_0^{2\pi}d\varphi\int_0^{\theta_{\max}}d\theta\sin\theta\int_{H/\cos\theta}^{R}dr\ r^2 = 2\pi\int_{H/R}^{1}d\xi\int_{H/\xi}^{R}dr\ r^2$$
$$= \frac{2\pi}{3}\int_{H/R}^{1}d\xi\left(R^3-\frac{H^3}{\xi^3}\right) = \frac{2\pi}{3}R^3\left(1-\frac{3}{2}\frac{H}{R}+\frac{1}{2}\frac{H^3}{R^3}\right)$$

$$= \frac{2\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) ,$$

where $x = |\mathbf{q}|/2k_F$. Obviously $0 \leq x \leq 1$, since the volume of the intersection is zero if $|\mathbf{q}| > 2k_F$. Therefore,

$$\begin{aligned}
\Delta E^{(1)} &= -4\pi e^2 \frac{V}{(2\pi)^6} \int \frac{d^3\mathbf{q}}{\mathbf{q}^2}\, 2\, \frac{2\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x) \\
&= -4\pi e^2 \frac{V}{(2\pi)^6} 4\pi \int_0^\infty dq\, \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x) \\
&= -4\pi e^2 \frac{V}{(2\pi)^6} \frac{4\pi}{3} k_F^3 8\pi k_F \frac{3}{8} = -\frac{3e^2}{4\pi} \left(\frac{V k_F^3}{3\pi^2}\right) k_F = -\frac{3e^2}{4\pi} N k_F \\
&= -\frac{3e^2}{4\pi} N \left(\frac{9}{4}\pi\right)^{\frac{1}{3}} \frac{1}{r_0} = -\frac{e^2}{2a_0} \frac{N}{r_s} \frac{3}{2\pi} \left(\frac{9}{4}\pi\right)^{\frac{1}{3}} .
\end{aligned}$$

Combining this result with the result (6.12) we get for the energy of the electron gas ground state

$$\begin{aligned}
E^{(0)} + \Delta E^{(1)} + \ldots &= \frac{e^2}{2a_0}\, N\, \left[\frac{3}{5}\left(\frac{9}{4}\pi\right)^{\frac{2}{3}} \frac{1}{r_s^2} - \frac{3}{2\pi}\left(\frac{9}{4}\pi\right)^{\frac{1}{3}} \frac{1}{r_s} + \ldots\right] \\
&= \frac{e^2}{2a_0}\, N\, \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \ldots\right] .
\end{aligned}$$

which, as we have discussed, should be a good approximation to the exact value for $r_s \to 0$, when the perturbative calculus is reliable. We note that the energy of the gas is an extensive quantity ($\propto N$) as it should be. The correction term just computed is called *the exchange energy* because, as we have seen, it originates from the exchange of two electrons below the Fermi shell. It is negative because of the Fermi statistics. The other terms indicated by dots are called *the correlation energy*.

Due to the attractive character of the exchange interactions, the energy has a minimum as a function of r_s for $r_s \approx 4.83$, where $E/N \approx -1.29$ eV. This indicates that the system of electrons is in a bound state. While this minimum is outside the expected range of validity of the perturbative expansion in powers of r_s one can argue, that we have in fact computed the expectation value of the total Hamiltonian in a trial state $|F\rangle$. Therefore, by the Ritz variational principle, the true energy of the ground state of the electron gas can only be lower, that is, necessarily negative (at the minimum). Moreover, the values of r_s and of E/N at the minimum are rather close to the values measured for metals like sodium, for which the experiment gives $r_s = 3.96$ and $E/N = -1.13$ eV. Thus, this simple model accounts for a dominant part of the binding energy of metals.

In the limit of small electron gas densities, $r_s \to \infty$, it can be shown (Wigner) that one can get a lower value of the energy by chosing a different trial state in which electrons are localized around ions (forming the so-called Wigner crystall). For such a state one gets

$$E = \frac{e^2}{2a_0}\,N\,\left[-\frac{1.79}{r_s} + \frac{2.66}{r_s^{3/2}} + \ldots\right] .$$

which for $r_s \to \infty$ gives a smaller value than our result. Therefore, by the Ritz principle, for large r_s this is closer to the true ground state energy.

6.3 Higher order corrections

We can try to go one step further and compute the correlation energy by using the second order perturbation calculus. According to our counting of powers of r_s this should give us the contribution of order $\Delta E \propto (e^2/a_0 r_s^2) \times r_s^2 = e^2/a_0$. However we will find that the second order contribution contains an infrared divergent term. To get around this difficulty we will have (following Gell-Mann & Brueckner) to sum an infinite subset of contributions from all orders of the perturbative expansion. As a result, we will obtain the contribution of order $(e^2/a_0)\ln r_s$.

Before we start the calculation it is convenient to pass to the electron-hole picture. In this picture the ground state of the system is

$$|F\rangle = a^\dagger_{\mathbf{k}_1\lambda_1}\ldots a^\dagger_{\mathbf{k}_N\lambda_N}|\Omega\rangle\ , \qquad \text{for}\quad |\mathbf{k}_i| \le k_F\ .$$

We also define the hole operators

$$b_{-\mathbf{p}-\lambda} \equiv a^\dagger_{\mathbf{p}\lambda}\ , \qquad b^\dagger_{-\mathbf{p}-\lambda} \equiv a_{\mathbf{p}\lambda}\ ,$$

so that the absence in the Fermi shell of the electron with momentum $\mathbf{p}$ and spin λ is perceived as a positive charge hole with momentum $-\mathbf{p}$ and spin $-\lambda$. We have then

$$b_{-\mathbf{p}-\lambda}|F\rangle = a_{\mathbf{p}\lambda}|F\rangle = 0$$

and since

$$H = E_F + \sum_{\lambda} \sum_{|\mathbf{k}|>k_F} \frac{\hbar^2\mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} - \sum_{\lambda} \sum_{|\mathbf{k}|<k_F} \frac{\hbar^2\mathbf{k}^2}{2m} b^\dagger_{\mathbf{k}\lambda} b_{\mathbf{k}\lambda} \ , \qquad (6.13)$$

the state $b^\dagger_{\mathbf{k}\lambda}|F\rangle$ has the energy $E_F - \hbar^2\mathbf{k}^2/2m$. In terms of the particle and hole creation operators the perturbation Hamiltonian

$$H'_{\rm el} = 2\pi\frac{e^2}{V} \sum_{\lambda_1,\lambda_2} \sum_{\mathbf{k}_1,\mathbf{k}_2} \sum_{\mathbf{q}\neq 0} \frac{1}{\mathbf{q}^2} a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1} a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2} a_{\mathbf{k}_2\lambda_2} a_{\mathbf{k}_1\lambda_1} \ , \qquad (6.14)$$

contains $2^4 = 16$ different terms (some of them are pairwise equivalent), which graphically can be represented as in figure 4. To compute higher orders corrections to the ground state energy we use the formula from the standard, time-independent perturbation calculus:

$$\Delta E^{(2)} = \sum_{n\neq F} \frac{\langle F|H'_{\rm el}|n\rangle\langle n|H'_{\rm el}|F\rangle}{E_F - E_n} \ , \qquad (6.15)$$

$$\Delta E^{(3)} = \sum_{n\neq F} \sum_{m\neq F} \frac{\langle F|H'_{\rm el}|m\rangle\langle m|H'_{\rm el}|n\rangle\langle n|H'_{\rm el}|F\rangle}{(E_F - E_n)(E_F - E_m)} \ , \qquad (6.16)$$

and so on. Let us consider the intermediate state $|n\rangle$ contributing to $\Delta E^{(2)}$. The Hamiltonian (6.14) has two annihilation operators on its right extreme, so in order to give a nonzero result they both have to have momenta below the Fermi shell ($|\mathbf{k}_1| < k_F$, $|\mathbf{k}_2| < k_F$), that is, they both have to be the hole creation operators. On the other hand, the two left creation operators in the Hamiltonian (6.14) cannot have $|\mathbf{k}_1 + \mathbf{q}| < k_F$, $|\mathbf{k}_2 - \mathbf{q}| < k_F$ because if they had, they would reproduce the state $|F\rangle$, which cannot occur as the intermediate state $|n\rangle$. They must therefore create electrons with momenta above the Fermi shell. In principle the factor $\langle F|H'_{\rm el}|n\rangle\langle n|H'_{\rm el}|F\rangle$ can be computed by constructing the state $|n\rangle$ as

$$|n\rangle = a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1} a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2} b^\dagger_{\mathbf{k}_2\lambda_2} b^\dagger_{\mathbf{k}_1\lambda_1}|F\rangle \ ,$$

with the proper ordering of operators (one should remember that the basis states should be ordered as in (5.11)!) and then evaluating directly the matrix elements. It is however more practical to note that if there

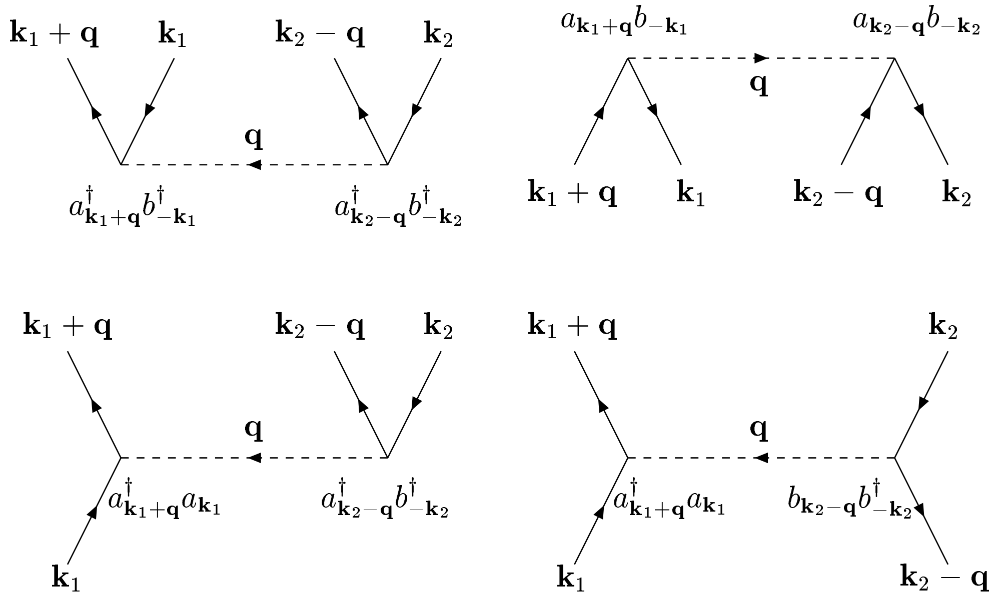


Figure 4: Graphical representation of four (of the 16) terms of the interaction Hamiltonian (6.14). Solid lines entering the vertex from below (leaving the vertex upwards) represent annihilation (creation) of an electron by the interaction. Solid lines entering the vertex from above (leaving the vertex downwards) represent creation (annihilation) of a hole by the interaction. The creation (annihilation) of the hole with momentum $-\mathbf{k}$ in the vertex is marked as the electron line entering (leaving) this vertex from above (downwards) with momentum $+\mathbf{k}$. Dashed line represent the momentum transfer between the annihilated/created pairs of particles.

was no denominator in (6.15) and if we could forget about the condition $n \neq F$ we could write

$$\sum_n \langle F|H'_{\mathrm{el}}|n\rangle\langle n|H'_{\mathrm{el}}|F\rangle = \langle F|H'_{\mathrm{el}}H'_{\mathrm{el}}|F\rangle$$

$$= \left(2\pi\frac{e^2}{V}\right)^2 \sum_{\mathbf{k}_1\lambda_1}\sum_{\mathbf{k}_2\lambda_2}\sum_{\mathbf{q}}\sum_{\mathbf{p}_1\chi_1}\sum_{\mathbf{p}_2\chi_2}\sum_{\mathbf{r}}\frac{1}{\mathbf{r}^2}\frac{1}{\mathbf{q}^2}$$

$$\times\langle F|b_{\mathbf{p}_1+\mathbf{r}\chi_1}b_{\mathbf{p}_2-\mathbf{r}\chi_2}a_{\mathbf{p}_2\chi_2}a_{\mathbf{p}_1\chi_1}a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2}b^\dagger_{\mathbf{k}_2\lambda_2}b^\dagger_{\mathbf{k}_1\lambda_1}|F\rangle$$

where we have taken into account only that term in the second Hamiltonian that annihilates two electrons above the fermi shell and two holes. (Extending the summation over intermediate states to $|F\rangle$ has in fact no consequences for this particular term of H'_{el} as acting on $|F\rangle$ this term gives always a state different from $|F\rangle$.) The computation is now simpler: it consists of moving succesively all annihilation operators to the right so that they eventually act on $|F\rangle$ giving zero. Consider for example the rightmost annihilation operator $a_{\mathbf{p}_1\chi_1}$. Anticommuting it with the leftmost creation operator $a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}$ we get two terms: $-a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}a_{\mathbf{p}_1\chi_1}+\delta_{\mathbf{p}_1,\mathbf{k}_1+\mathbf{q}}\delta_{\chi_1\lambda_1}$. In the second term we have finished with the operator $a_{\mathbf{p}_1\chi_1}$ and got instead a numerical factor. In the first term we still have $a_{\mathbf{p}_1\chi_1}$ and we must anticommute it with $a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2}$ getting again a delta term and a term in which this particular operator can be already anticommuted twice throught $b^\dagger_{\mathbf{k}_2\lambda_2}b^\dagger_{\mathbf{k}_1\lambda_1}$ (without getting any delta) to annihilate $|F\rangle$. We then do the same with $a_{\mathbf{p}_2\chi_2}$ and so on. The whole procedure is easily seen to be equivalent to applying the following mnemonic rules: Treat for a while all a's and $a^\dagger$'s (and also b's and $b^\dagger$'s) as fully anticommuting (that is, forget about the possible delta terms in their anticommutation rules). Anticommute them so that each a stands to the left of some $a^\dagger$ and each b to the left of some $b^\dagger$. There are of course several such possibilities. In the case at hand, since there are two a's and two b's, there are four different possibilities. One of them is

$$\langle F|b_{\mathbf{p}_1+\mathbf{r}\chi_1}b_{\mathbf{p}_2-\mathbf{r}\chi_2}a_{\mathbf{p}_2\chi_2}a_{\mathbf{p}_1\chi_1}a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2}b^\dagger_{\mathbf{k}_2\lambda_2}b^\dagger_{\mathbf{k}_1\lambda_1}|F\rangle$$

$$\to \langle F|a_{\mathbf{p}_2\chi_2}a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}a_{\mathbf{p}_1\chi_1}a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2}b_{\mathbf{p}_1+\mathbf{r}\chi_1}b^\dagger_{\mathbf{k}_2\lambda_2}b_{\mathbf{p}_2-\mathbf{r}\chi_2}b^\dagger_{\mathbf{k}_1\lambda_1}|F\rangle \tag{6.17}$$

where the overall sign is + because the number of anticommutations needed to reach this particular configuration of the operators was even. Another configuration which we can get applying this rule is

$$\to -\langle F|a_{\mathbf{p}_2\chi_2}a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1}a_{\mathbf{p}_1\chi_1}a^\dagger_{\mathbf{k}_2-\mathbf{q}\lambda_2}b_{\mathbf{p}_2-\mathbf{r}\chi_2}b^\dagger_{\mathbf{k}_2\lambda_2}b_{\mathbf{p}_1+\mathbf{r}\chi_1}b^\dagger_{\mathbf{k}_1\lambda_1}|F\rangle \tag{6.18}$$

where now there is a minus sign because the number of anticommutations needed was odd. In the next step we replace all pairs of adjacent annihilation and creation operators by the appropriate deltas (in other words we *contract* the relevant operators): $a_{\mathbf{p}_2\chi_2} a^\dagger_{\mathbf{k}_1+\mathbf{q}\lambda_1} \to \delta_{\mathbf{p}_2,\mathbf{k}_1+\mathbf{q}} \delta_{\chi_2,\lambda_1}$ etc. From the term (6.17) we get then the following contribution to the matrix element $\langle F|H'_{\rm el}H'_{\rm el}|F\rangle$:

$$\left(2\pi\frac{e^2}{V}\right)^2 \sum_{\mathbf{k}_1\lambda_1}\sum_{\mathbf{k}_2\lambda_2}\sum_{\mathbf{q}}\sum_{\mathbf{p}_1\chi_1}\sum_{\mathbf{p}_2\chi_2}\sum_{\mathbf{r}} \frac{1}{\mathbf{r}^2}\frac{1}{\mathbf{q}^2}\,\frac{1}{\text{denominator}}$$
$$\times\delta_{\mathbf{p}_2,\mathbf{k}_1+\mathbf{q}}\delta_{\chi_2,\lambda_1}\;\delta_{\mathbf{p}_1,\mathbf{k}_2-\mathbf{q}}\delta_{\chi_1,\lambda_2}\;\delta_{\mathbf{p}_1+\mathbf{r},\mathbf{k}_2}\delta_{\chi_1,\lambda_2}\;\delta_{\mathbf{p}_2-\mathbf{r},\mathbf{k}_1}\delta_{\chi_2,\lambda_1}\;, \tag{6.19}$$

(because $\langle F|F\rangle = 1$) whereas from (6.18) we get

$$-\left(2\pi\frac{e^2}{V}\right)^2 \sum_{\mathbf{k}_1\lambda_1}\sum_{\mathbf{k}_2\lambda_2}\sum_{\mathbf{q}}\sum_{\mathbf{p}_1\chi_1}\sum_{\mathbf{p}_2\chi_2}\sum_{\mathbf{r}} \frac{1}{\mathbf{r}^2}\frac{1}{\mathbf{q}^2}\,\frac{1}{\text{denominator}}$$
$$\times\delta_{\mathbf{p}_2,\mathbf{k}_1+\mathbf{q}}\delta_{\chi_2,\lambda_1}\;\delta_{\mathbf{p}_1,\mathbf{k}_2-\mathbf{q}}\delta_{\chi_1,\lambda_2}\;\delta_{\mathbf{p}_2-\mathbf{r},\mathbf{k}_2}\delta_{\chi_2,\lambda_2}\;\delta_{\mathbf{p}_1+\mathbf{r},\mathbf{k}_1}\delta_{\chi_1,\lambda_1}\;. \tag{6.20}$$

It can be checked that the two remaining configurations will give contributions equivalent to the two ones written down above. Hence, these two results have to be multiplied by the so-called *combinatoric factors* of 2 each. These combinatoric factors can be easily calculated as the number of possible ways in which the fermionic lines of the two vertices shown in the first line of fig. 4 can be joined (respecting the direction of arrows!) to obtain a given closed connected diagram. Two distinct Feynman diagrams that can be formed in this way, corresponding to the analytic expressions (6.19) and (6.20), are shown in figure 5.

Looking at the diagrams it is easy to restore the "energetic" denominators $E_F - E_n$. For both diagrams they are the same (provided we change the summation variable $\mathbf{p}_2 \to -\mathbf{p}_2$) and read:

$$\begin{aligned} E_n - E_F &= \frac{\hbar^2(\mathbf{p}_1+\mathbf{q})^2}{2m} - \frac{\hbar^2\mathbf{p}_1^2}{2m} + \frac{\hbar^2(-\mathbf{p}_2-\mathbf{q})^2}{2m} - \frac{\hbar^2(-\mathbf{p}_2)^2}{2m} \\ &= \frac{\hbar^2}{m}\left[\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)\right]\;. \end{aligned} \tag{6.21}$$

In agreement with (6.13) the energy of the holes is negative. The analytic expressions corresponding to these Feynman diagrams are easily deduced

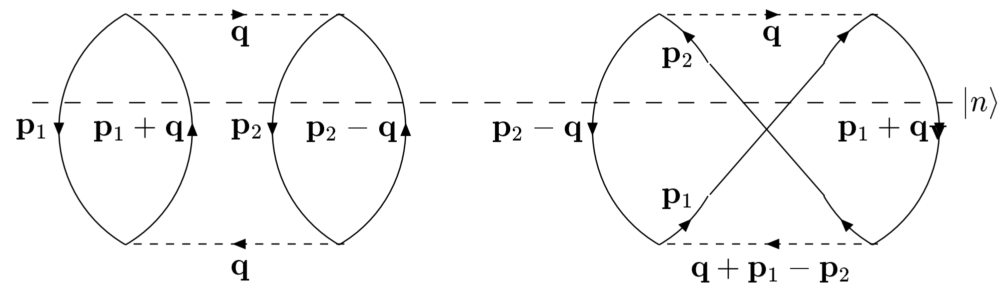


Figure 5: Feynman diagrams corresponding to the second order corrections to the energy of the electron gas. Dashed line crossing all the fermion lines shows the intermediate state $|n\rangle$.

from the established results:

$$\Delta E_a^{(2)} = 2 \cdot 4 \left(2\pi \frac{e^2}{V}\right)^2 \frac{V^3}{(2\pi)^9} \times \int_\Delta d^3\mathbf{q}\, d^3\mathbf{p}_1\, d^3\mathbf{p}_2\, \frac{1}{\mathbf{q}^4} \frac{-m/\hbar^2}{\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1 + \mathbf{p}_2)} \tag{6.22}$$

$$\Delta E_b^{(2)} = -2 \cdot 2 \left(2\pi \frac{e^2}{V}\right)^2 \frac{V^3}{(2\pi)^9} \times \int_\Delta d^3\mathbf{q}\, d^3\mathbf{p}_1\, d^3\mathbf{p}_2\, \frac{1}{\mathbf{q}^2} \frac{1}{(\mathbf{q} + \mathbf{p}_1 + \mathbf{p}_2)^2} \frac{-m/\hbar^2}{\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1 + \mathbf{p}_2)} \tag{6.23}$$

where we have replaced the independent summations over momenta by integrations applying the rule (5.29). In both cases the integration region Δ is defined by the conditions

$$\Delta = \begin{cases} |\mathbf{p}_1| < k_F\ , & |\mathbf{p}_1 + \mathbf{q}| > k_F \\ |\mathbf{p}_2| < k_F\ , & |\mathbf{p}_2 - \mathbf{q}| > k_F \end{cases} .$$

The factors of 2 in both, $\Delta E_a^{(2)}$ and $\Delta E_b^{(2)}$ are the combinatoric factors mentioned above. The origin of the relative minus sign in front of $\Delta E_b^{(2)}$ is the odd number of anticommutations of a's and b's needed to get this contribution. The minus signs associated with $m/\hbar^2$ come from the "energetic" denominators: $E_F - E_n$ is minus the quantity calculated in (6.21).[38] Different contractions of the spin deltas in (6.19) and (6.20) result in factors of 4 and 2 in (6.22) and (6.23), respectively (the difference is readily seen in Feynman diagrams in fig. 5: each closed fermionic loop corresponds to a sum over independent spin variable and brings in a factor of 2). Finally, the difference in the momentum denominators ($\mathbf{q}^4$ in (6.22) and $\mathbf{q}^2(\mathbf{q}+\mathbf{p}_1+\mathbf{p}_2)^2$ in (6.23)) resulting from the factor $(1/\mathbf{q}^2)(1/\mathbf{r}^2)$ in (6.17) and (6.18) reflects the differences (evident from diagrams) in the contraction of the momenta.

The diagramatic approach can be easily applied to visualize different contributions also in higher orders of the perturbative calculus. Some of the Feynman diagrams appearing in the third (6.16) and fourth orders are shown in figures 6 and 7. Each intermediate state (factors $|n\rangle\langle n|$ in formulae like (6.15) and (6.16)) is represented by a horizontal long-dashed line cutting the whole diagram. The interactions from the Hamiltonians H' in (6.15) and (6.16) etc. are represented by short-dashed lines connecting solid lines and are of the form shown in fig. 4. It is also easy to understand that the condition that the state $|F\rangle$ does not appear as an intermediate state means that any long-dashed line has to be crossed by at least one particle and one hole line.

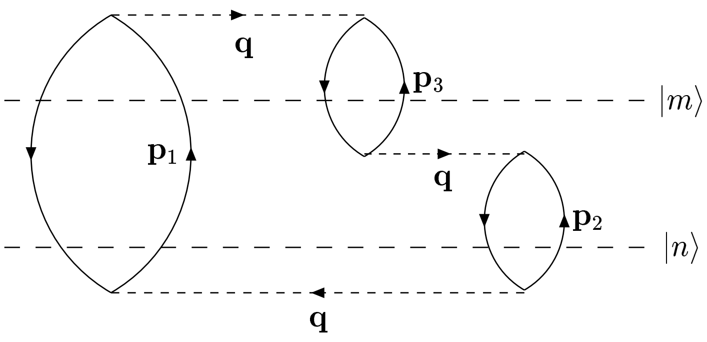


Figure 6: Most divergent Feynman diagram in the third order of perturbation calculus.

Returning to the two contributions (6.22) and (6.23) in the second

[38] If all these minuses are taken into account together, then the rule is that compared to contribution $\Delta E_a^{(2)}$ which has a minus sign, each closed fermion loop in the Feynman diagram brings in a factor of (-1) (and the energetic denominators should then be included with reversed sign i.e. as $E_n - E_F$).

order we note that the important difference between the two contributions is that the integration over $d^3\mathbf{q}$ in $\Delta E_a^{(2)}$ is divergent for $\mathbf{q} \to 0$ due to the factor of $\mathbf{q}^4$, while $\Delta E_b^{(2)}$ is perfectly finite. It is easy to identify the class of most divergent diagrams. These are the diagrams which in the n-th order of perturbation calculus have the maximal possible number of loops in the corresponding Feynman diagram. For example, the most divergent diagram in the third order is shown in figure 6. The corresponding contribution is

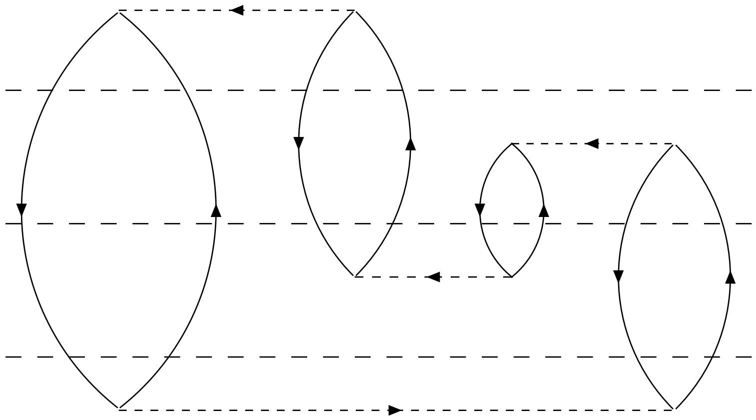
$$\Delta E_{\text{div}}^{(3)} \propto \int d^3\mathbf{p}_1\ d^3\mathbf{p}_2\ d^3\mathbf{p}_2\ d^3\mathbf{q}\ \frac{1}{\mathbf{q}^6}\ \frac{m/\hbar^2}{\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1 + \mathbf{p}_2)}\ \frac{m/\hbar^2}{\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1 + \mathbf{p}_3)}$$

The overall sign of this expression is positive in agreement with the rule formulated in the footnote on the previous page: compared to the diagram contributing to $\Delta E_a^{(2)}$ this diagram has one fermionic loop more. In the higher orders there are more divergent diagrams. The most divergent ones in the fourth order are shown in figure 7.

We will now resum the most divergent contribution from each order of the perturbation expansion. Let us first isolate the prefactor of the expressions corresponding to the most divergent contribution in the n-th order (that is corresponding to the Feynman diagram with n loops). It reads

$$-\kappa_n(-1)^n 2^n \left(2\pi\frac{e^2}{V}\right)^n \left(\frac{V}{8\pi^3}\right)^n \frac{V}{8\pi^3}\left(\frac{m}{\hbar^2}\right)^{n-1} \int \frac{d^3\mathbf{q}\ d^3\mathbf{p}_1 \ldots d^3\mathbf{p}_n}{\mathbf{q}^{2n}\ [\mathbf{p}_i^{2(n-1)}]} \tag{6.24}$$

In agreement with the rule, n loops give the factor $(-1)^n$. 2^n arises from sums over n independent spin variables (one for each loop). n Hamiltonians in the n-th order produce the factor $(2\pi e^2/V)^n$. Each of the $n+1$ integrations over momenta (including the one over $\mathbf{q}$) gives $(V/8\pi^3)$. $n-1$ "energetic denominators" in the n-th order bring $(m/\hbar^2)^{n-1}$ and the factor $[\ldots]$ (which depends on all $\mathbf{p}_i$ and $\mathbf{q}$) in the denominator of the integral; for the moment the only important thing is that $[\ldots]$ has dimension of momentum to the $2(n-1)$-th power. Finally, κ_n is the combinatoric factor telling how many different contractions of the annihilation and creation operators lead to the same analytical expression (the same Feynman diagram). For a given n-loop diagram in the n-th order one finds that $\kappa_n = 2^{n-1}$. Obviously, for $n = 2$ this reproduces the expression (6.22) for $\Delta E_a^{(2)}$.



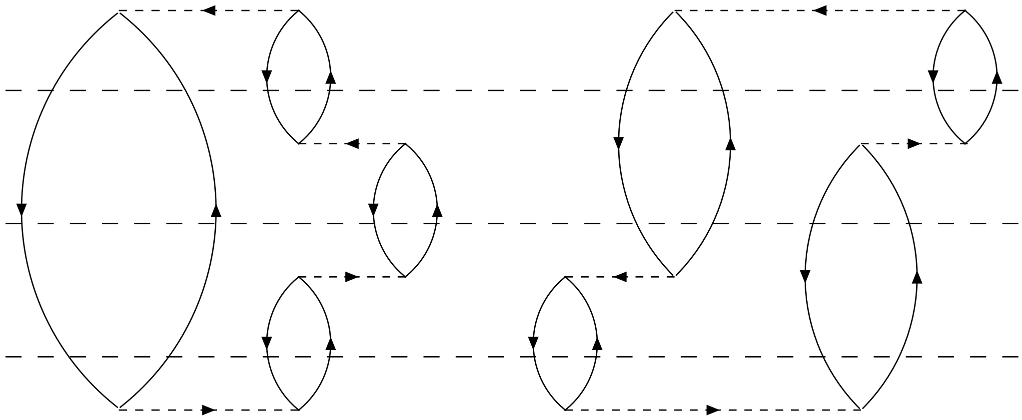


Figure 7: Different topologies of the most divergent Feynman diagrams in the fourth order of perturbation calculus. Intermediate states are marked by the long dashed lined.

It is now convenient to rescale all the momenta in the integrals, so that they are normalize to the Fermi momentum: $\mathbf{k} = k_F\tilde{\mathbf{k}}$ (where $\mathbf{k} = \mathbf{p}_i$ or $\mathbf{q}$). The integral becomes then a dimensionless factor times k_F^{5-n}. We can then write

$$k_F^{5-n} = \left(3\pi^2\frac{N}{V}\right)^{\frac{5-n}{3}} = 3\pi^2\frac{N}{V}\left(\frac{4}{9\pi}\frac{3}{4\pi}\frac{V}{N}\right)^{\frac{n-2}{3}} = 3\pi^2\frac{N}{V}\left(\frac{4}{9\pi}r_0^3\right)^{\frac{n-2}{3}}$$

and for the prefactor (6.24) times k_F^{5-n} we get

$$\begin{aligned}
&-\kappa_n\left(-\frac{me^2}{2\pi^2\hbar^2}\right)^n\frac{V}{8\pi^3}\frac{\hbar^2}{m}k_F^{5-n}\\
&= -\kappa_n\left(-\frac{me^2}{2\pi^2\hbar^2}\right)^n\frac{3}{8\pi}\frac{\hbar^2}{m}N\left[\left(\frac{4}{9\pi}\right)^{\frac{1}{3}}\left(\frac{3}{4\pi}\frac{V}{N}\right)^{\frac{1}{3}}\frac{me^2}{\hbar^2}\frac{\hbar^2}{me^2}\right]^{n-2}\\
&= -\kappa_n\left(\frac{1}{2\pi^2}\right)^n\frac{3}{8\pi}\frac{me^4}{\hbar^2}N\left[\left(\frac{4}{9\pi}\right)^{\frac{1}{3}}r_s\right]^{n-2}\\
&= -\kappa_n\left(\frac{3}{4\pi}\frac{e^2}{2a_0}N\right)\left(\frac{1}{2\pi^2}\right)^n\left[\left(\frac{4}{9\pi}\right)^{\frac{1}{3}}r_s\right]^{n-2} = -\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right)\left[-\frac{\beta r_s}{\pi^2}\right]^{n-2},
\end{aligned}$$

where $\beta = (4/9\pi)^{1/3}$. We have used the definition (6.9) of r_s in terms of N, V and a_0. For $n = 2$ this prefactors equals $-(3/5\pi^5)\ N\times$ (1 Ry). To resum the divergent contributions it remains to calculate the dimensionless integrals.

To this end we need to write in a compact form the integrands of the integrals over $d^3\mathbf{q}d^3\mathbf{p}_1\dots d^3\mathbf{p}_n$ in (6.24). A trick allowing to do that was invented by Gell-Mann and Brueckner and consists of introducing an auxiliary function

$$F_{\mathbf{q}}(t) \equiv \int_\Delta d^3\mathbf{p}\exp\left\{-|t|\left(\frac{1}{2}\mathbf{q}^2 + \mathbf{q}\cdot\mathbf{p}\right)\right\} \tag{6.25}$$

where the integration region Δ is such that $|\mathbf{p}| < 1$, $|\mathbf{p}+\mathbf{q}| > 1$ (in the rescaled momentum variables - we have omited the tildas). It can be then checked, that in the formula (6.24) the sum A_n of the integrands corresponding to topologically distinct Feynman diagrams arising in the n-th order can be written as

$$A_n = \frac{1}{n}\int_{-\infty}^{+\infty}dt_1\dots\int_{-\infty}^{+\infty}dt_n\ \delta(t_1+\dots+t_n)F_{\mathbf{q}}(t_1)\cdot\ldots\cdot F_{\mathbf{q}}(t_n)\ .$$

For example, for $n = 2$ we reproduce the denominator of (6.22):

$$
\begin{aligned}
A_2 &= \frac{1}{2}\int_{-\infty}^{+\infty} dt_1 \int_\Delta d^3\mathbf{p}_1\ d^3\mathbf{p}_2\ \exp\Big\{-|t_1|[\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)]\Big\} \\
&= \int_0^{+\infty} dt_1 \int_\Delta d^3\mathbf{p}_1\ d^3\mathbf{p}_2\ \exp\Big\{-|t_1|[\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)]\Big\} \\
&= \int_\Delta d^3\mathbf{p}_1\ d^3\mathbf{p}_2\ \frac{1}{\mathbf{q}^2 + \mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)} \ .
\end{aligned}
$$

To make use out of this trick we write

$$
\delta(t_1 + \ldots + t_n) = \int_{-\infty}^{+\infty} \frac{d\tilde{u}}{2\pi} e^{i\tilde{u}t_1} \cdot \ldots \cdot e^{i\tilde{u}t_n}
$$

so that

$$
A_n = \frac{1}{n}\int_{-\infty}^{+\infty} \frac{d\tilde{u}}{2\pi} \int_{-\infty}^{+\infty} dt_1\ e^{i\tilde{u}t_1} F_\mathbf{q}(t_1) \ldots \int_{-\infty}^{+\infty} dt_n\ e^{i\tilde{u}t_n} F_\mathbf{q}(t_n) \ .
$$

Thus, after the change of variables $\tilde{u} = |\mathbf{q}|u$, we have

$$
A_n = \frac{|\mathbf{q}|}{2\pi n}\int_{-\infty}^{+\infty} du\ \ [Q_\mathbf{q}(u)]^n \ \ , \tag{6.26}
$$

where

$$
Q_\mathbf{q}(u) = \int_\Delta d^3\mathbf{p} \int_{-\infty}^{+\infty} dt \exp\left\{iu|\mathbf{q}|t - \left(\frac{1}{2}\mathbf{q}^2 + \mathbf{q}\cdot\mathbf{p}\right)|t|\right\} \ , \tag{6.27}
$$

The sum of the most divergent contributions to the ground state energy then reads

$$
\Delta E_{\text{div}} = -\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right)\sum_{n=2}^{\infty}\left[-\frac{\beta r_s}{\pi^2}\right]^{n-2}\int \frac{d^3\mathbf{q}}{\mathbf{q}^{2n}}\ A_n
$$

$$
= -\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right)\int \frac{d^3\mathbf{q}}{|\mathbf{q}|^3}\frac{1}{2\pi}\int_{-\infty}^{+\infty} du \sum_{n=2}^{\infty}\frac{(-1)^n}{n}\,[Q_\mathbf{q}(u)]^n\left(\frac{\beta r_s}{\pi^2\mathbf{q}^2}\right)^{n-2} \ .
$$

We have interchanged here the order of the summation and the integration over $d^3\mathbf{q}$ in the hope that the sum of the integrands is then already free from divergence for $|\mathbf{q}| \to 0$.

In principle, to compute the complete $\mathcal{O}(r_s^0)$ contribution to the ground state energy we have to find the $n = 2$ term in the above sum exactly.

For the remaining terms it suffices to take into account only the contribution of the lower end of the integration over $|\mathbf{q}|$. Here we will not attempt to calculate the finite part of the $n = 2$ term as it can be done only numerically. We will compute instead only the contribution of the divergent parts of all terms which will give the contribution $\propto \ln(r_s)$. To do this we need to find $Q_{\mathbf{q}}(u)$ only for $|\mathbf{q}| \ll 1$, so we can neglect the $\mathbf{q}^2$ term in the exponent of the integrand of (6.27):

$$
\begin{aligned}
Q_{\mathbf{q}}(u) &\approx \int_{\Delta} d^3\mathbf{p} \int_{-\infty}^{+\infty} dt\ e^{iu|\mathbf{q}|t - \mathbf{q}\cdot\mathbf{p}|t|} \\
&\approx 2\pi \int_0^1 d\xi \int_{1-\xi|\mathbf{q}|}^{1} dp\ p^2 \int_{-\infty}^{+\infty} dt\ e^{iu|\mathbf{q}|t - |\mathbf{q}||\mathbf{p}||t|} \ .
\end{aligned}
$$

We have written the integral over $d^3\mathbf{p}$ in spherical coordinates chosing the p_z axis parallel to the vector $\mathbf{q}$ introducing $\xi \equiv \cos\theta$ and taking into account that the integration region is such that $|\mathbf{p}| < 1$, $|\mathbf{p}+\mathbf{q}| > 1$. Since for $|\mathbf{q}| \ll 1$

$$
|\mathbf{p}+\mathbf{q}| \approx |\mathbf{p}| + |\mathbf{q}|\cos\theta = |\mathbf{p}| + |\mathbf{q}|\xi \ ,
$$

the latter condition implies that $\cos\theta > 0$ and that $p \equiv |\mathbf{p}| > 1 - |\mathbf{q}|\cos\theta = 1 - |\mathbf{q}|\xi$. Moreover, for $|\mathbf{q}| \ll 1$ the integral over dp can be approximated as

$$
\int_{1-\xi|\mathbf{q}|}^{1} dp\ f(p) \approx \xi|\mathbf{q}|\ f(1) \ ,
$$

leading to

$$
\begin{aligned}
Q_{\mathbf{q}}(u) &\approx 2\pi \int_0^1 d\xi\ \xi|\mathbf{q}| \int_{-\infty}^{+\infty} dt\ e^{iu|\mathbf{q}|t - |\mathbf{q}||t|} \\
&= 2\pi \int_0^1 d\xi\ \xi \left[\int_0^{+\infty} ds\ e^{-s(\xi - iu)} + \int_{-\infty}^{0} ds\ e^{-s(\xi - iu)} \right] \\
&= 2\pi \int_0^1 d\xi\ \xi \left[\frac{1}{\xi - iu} + \frac{1}{\xi + iu} \right] = 4\pi \int_0^1 d\xi\ \frac{\xi^2}{\xi^2 + u^2} \\
&= 4\pi - 4\pi u^2 \int_0^1 d\xi\ \frac{1}{\xi^2 + u^2} = 4\pi \left(1 - u \arctan\frac{1}{u} \right) \equiv 4\pi R(u) \ .
\end{aligned}
$$

which after the change $s = |\mathbf{q}|t$ has become independent of $\mathbf{q}$. We have therefore

$$
\Delta E_{\text{div}} = -\left(\frac{3}{8\pi^5} \frac{e^2}{2a_0} N \right)
$$

$$\times \int_{-\infty}^{+\infty} du \ \int_0^\infty \frac{dq}{q} \frac{4\pi}{2\pi} \left[4\pi R(u)\right]^2 \sum_{n=2}^{\infty} \frac{(-1)^{n-2}}{n} \left(R(u)\frac{4\beta r_s}{\pi q^2}\right)^{n-2}$$
$$= -\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right) 32\pi^2 \int_{-\infty}^{+\infty} du \ R^2(u) \int_0^\infty \frac{dq}{q} \sum_{n=2}^{\infty} \frac{(-1)^{n-2}}{n} a^{n-2} \ .$$

It is easy to check, that for $|a| < 1$ the sum over n equals

$$\sum_{n=2}^{\infty} \frac{(-1)^{n-2}}{n} a^{n-2} = \frac{1}{a} - \frac{1}{a^2} \ln(1+a) \ .$$

In our case, of course, $|a| \gg 1$ as $|\mathbf{q}| equiv q \to 0$, but we will assume, that the right hand side can be continued to $a \gg 1$. This gives

$$\Delta E_{\mathrm{div}} = -\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right) 32\pi^2 \int_{-\infty}^{+\infty} du \ R^2(u)$$
$$\times \int_0^\infty \frac{dq}{q} \left[\frac{\pi q^2}{4\beta r_s R(u)} - \frac{\pi^2 q^4}{16\beta^2 r_s^2 R^2(u)} \ln\left(1 + \frac{4R(u)\beta r_s}{\pi q^2}\right)\right] \ .$$

Setting $b^2 \equiv 4\beta r_s R(u)/\pi$ we get an elementary integral

$$\int_0^\infty \frac{dq}{q} \left[\frac{q^2}{b^2} - \frac{q^4}{b^4} \ln\left(1 + \frac{b^2}{q^2}\right)\right] = \int_0^{1/b} dx \left(x + x^3 \ln x^2 - x^3 \ln(1+x^2)\right)$$
$$= \left[\frac{1}{2}x^2 + \frac{1}{4}x^4 \ln x^2 - \frac{x^4}{8} - \frac{1}{4}(x^4 - 1)\ln(1+x^2) + \frac{x^4}{8} - \frac{x^2}{4}\right]_0^{1/b}$$
$$= \left[\frac{1}{4b^2} - \frac{1}{4b^4} \ln(1+b^2) + \frac{1}{4} \ln\left(1 + \frac{1}{b^2}\right)\right] \to \frac{1}{4}\left(\frac{1}{2} - \ln b^2\right) \ ,$$

where we have taken the limit $r_s \to 0$ ($b \to 0$). Thus we get

$$\Delta E_{\mathrm{div}} = -\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right) 8\pi^2 \int_{-\infty}^{+\infty} du \ R^2(u) \left(\frac{1}{2} - \ln\frac{4\beta r_s R(u)}{\pi}\right)$$
$$\left(\frac{3}{8\pi^5}\frac{e^2}{2a_0}N\right) 8\pi^2 \int_{-\infty}^{+\infty} du \ R^2(u) \ \ln(r_s) + \ldots$$

In the second line we have retained only the term with $\ln(r_s)$. The remaining, perfectly finite, integral

$$\int_{-\infty}^{+\infty} du \ \left(1 - u \arctan\frac{1}{u}\right)^2 = \int_{-\infty}^{+\infty} dw \ \frac{1}{w^2} \left(1 - \frac{1}{w} \arctan w\right)^2$$

can be found in tables (Ryzhik & Gradsztajn) and equals $\frac{2}{3}\pi(1-\ln 2)$. Combining all the results, we get finally for the ground state energy the expression

$$
\begin{aligned}
E &= \frac{e^2}{2a_0}\, N \left[\frac{3}{5}\left(\frac{9}{4}\pi\right)^{\frac{2}{3}} \frac{1}{r_s^2} - \frac{3}{2\pi}\left(\frac{9}{4}\pi\right)^{\frac{1}{3}} \frac{1}{r_s} + \frac{2}{\pi^2}\pi(1-\ln 2)\ln r_s + \ldots \right] \\
&= \frac{e^2}{2a_0}\, N \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622 \ln r_s - 0.096 + \mathcal{O}(r_s) \right] \; .
\end{aligned}
$$

The r_s independent term in the last line is the contribution of the finite part of the $n = 2$ term which we have not attempted to compute here.