The mathematics of dilute quantum gases

3. Ground state energy of the dilute Fermi gas

We follow: E.H. Lieb, R. Seiringer, J.P. Solovej, "Ground state energy of the low density Fermi gas", Phys. Rev. A 71, 053605 (2005) [DFG]

1. The spin of a particle

Apart from their spatial degree of freedom, particles in quantum mechanics can carry an additional degree of freedom called spin. The spin is characterized by a number S that can take the values

$$0, 1/2, 1, 3/2, 2, 5/2 \dots \qquad (1)$$

From a mathematical point of view a particle with spin S has an additional degree of freedom living in a 2S+1 dimensional complex Hilbert space, that is, the wavefunction of a particle moving in $\mathbb{R}^3$ with spin S is of the form

$$\Psi \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2S+1} \, ; \quad \Psi(x,\sigma) \text{ with } x \in \mathbb{R}^d, \ \sigma \in \{1 \dots 2S+1\}.$$

The normalization condition now reads

$$\sum_{\sigma=1}^{2S+1} \int_{\mathbb{R}^3} |\Psi(x,\sigma)|^2 dx = 1 . \qquad (2)$$

From a physics point of view the spin has the interpretation of angular momentum attached to the particle. If the particle has electric charge the spin creates a magnetic moment that can couple to other degrees of freedom of a quantum system, as for example to the magnetic moment of another charged particle with spin. Spin-Spin interactions of this kind are crucial for the understanding of the light absorption spectra of atoms. The spins of the particles we are interested in do not interact with each other and so we do not go into more details here.

The particles we encounter in nature have the property that bosons have integer spin and fermions have half integer spin. This phenomenon cannot be explained with non-relativistic quantum mechanics, but only with its relativistic version, that is, with quantum field theory. An electron for example has spin $1/2$.

In cold quantum gases spin-spin interactions usually play no role, which is why we considered spinless bosons $(S=0)$ in the previous Chapter to keep the notation simple. The method of proof applies, however, also to particles with spin and gives the same result for the ground state energy.

This is because the position space part of the wavefunction and the spin part of the wavefunction can be symmetrized separately. (Think about this if you have never heard it before!)

Although there is no direct spin-spin interaction, the spin will play a role in the energy of a Fermi gas as we will see in the next section.

2. The ideal Fermi gas and the concept of the Fermi sea

Let us first consider N spinless (spin 0) fermions in the box $[0,L]^3$ and ask the question how their ground state energy looks like. The Hamiltonian of the system is given by

$$H_N^0 = \sum_{i=1}^{N} -\Delta_i \qquad (3)$$

with periodic boundary conditions. We know that the eigenvalues and eigenfunctions of $-\Delta$ defined on $L^2([0,L]^3)$

are given by $\varphi_p(x) = L^{-3/2} e^{ipx}$ and $e_p = p^2$ with $p \in \frac{2\pi}{L}\mathbb{Z}^3$, respectively. The operator H_N^0 now acts on $L^2_a([0,L]^{3N})$, the space of antisymmetric wave functions and we have

$$E_0^F(N,L) = \inf_{\substack{\|\Psi\|=1 \\ \Psi \in L^2_a([0,L]^{3N})}} \langle \Psi, H_N^0 \Psi \rangle. \qquad (4)$$

In case of bosons we could minimize each term in the energy separately. Here this is not possible because of the requirement of antisymmetry. The simplest antisymmetric wave function reads

$$\begin{aligned} \varphi_{p_1} \wedge \dots \wedge \varphi_{p_N}(x_1 \dots x_N) &= \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma)\, \varphi_{\sigma(p_1)} \otimes \dots \otimes \varphi_{\sigma(p_N)} (x_1 \dots x_N) \\ &= \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma)\, \varphi_{\sigma(p_1)}(x_1) \dots \varphi_{\sigma(p_N)}(x_N) \end{aligned} \qquad (5)$$

and is often called a Slater determinant. It is the closest one can get to a product wavefunction if one is restricted to wave functions in L^2_a. One can easily see that the lowest energy configuration is obtained by a Slater determinant with $p_1 \dots p_N$ chosen such that $p_1^2+\dots+p_N^2$ is minimized (in case of non-uniqueness any choice does the job). We check this statement for $N=2$ and leave the general case as an exercise.

A general two-particle wave function $\Psi \in L^2_a([0,L]^6)$ can be written as

$$\Psi = \sum_{\alpha\beta} c_{\alpha\beta} \, \varphi_{p_\alpha} \otimes \varphi_{p_\beta} , \text{ where } c_{\alpha\beta} = -c_{\beta\alpha} \text{ and } \sum_{\alpha\beta} |c_{\alpha\beta}|^2 = 1. \qquad (6)$$

We thus have

$$\langle \Psi, H_2^0 \Psi \rangle = \sum_{\alpha\beta\gamma\delta} \overline{c_{\alpha\beta}} c_{\gamma\delta} \left\langle \varphi_{p_\alpha} \otimes \varphi_{p_\beta} , \left(-\Delta_1 - \Delta_2\right) \varphi_{p_\gamma} \otimes \varphi_{p_\delta} \right\rangle$$
$$= \sum_{\alpha\beta} |c_{\alpha\beta}|^2 \left(e_{p_\alpha} + e_{p_\beta} \right). \qquad (7)$$

Since $c_{\alpha\alpha} = 0$ for all α, this expression is minimized for $c_{\alpha\beta} = \delta_{\alpha p_1} \delta_{\beta p_2}$, where $p_1 = (0,0,0)$ and e.g. $p_2 = (0,0,\frac{2\pi}{L})$, which proves the claim.

Let us assume that the momenta are enumerated s.t. $e_{p_\alpha} \le e_{p_\beta}$ if $\alpha \le \beta$ $(\alpha, \beta \in \mathbb{N})$. Then

$$E_0^F(N,L) = \sum_{\alpha=1}^{N} p_\alpha^2 . \qquad (8)$$

There is no closed form expression for (8) for finite N and L but we can evaluate the sum in the thermodynamic limit. This can be done as follows:

We choose $\mu > 0$ and consider

The sum counts the total number of momentum modes p with $p^2 \le \mu$

$$\rho = \frac{N}{L^3} \overset{!}{=} \lim_{\substack{N\to\infty \\ L\to\infty \\ N/L^3=\rho}} \underbrace{\frac{1}{L^3} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \mathbb{1}\left(p^2 \le \mu\right)}_{\text{This is a Riemann sum.}} \qquad (9)$$

Characteristic function of the set $\{p \in \frac{2\pi}{L}\mathbb{Z}^3 \mid p^2 \le \mu\}$

$$= \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} \mathbb{1}\left(p^2 \le \mu\right) dp = \underbrace{\left(\frac{1}{2\pi}\right)^3 \frac{4\pi}{3}}_{\frac{1}{6\pi^2}} \mu^{3/2}.$$

$$\Leftrightarrow \boxed{\mu = \left(6\pi^2 \varrho\right)^{2/3}} . \qquad (10)$$

The ball with radius $\sqrt{\mu}$ in momentum space is called the Fermi sea.

The result tells us that asymptotically in the thermodynamic limit we have to occupy all momenta with $|p| \leq \sqrt{\mu}$ to obtain the correct density. Using this, we can compute the ground state energy in the limit as follows

$$e_0^F(\varrho) = \lim_{\substack{N\to\infty \\ L\to\infty \\ N/L^3 = \varrho}} \frac{E_0^F(N,L)}{L^3} = \lim_{\substack{N\to\infty \\ L\to\infty \\ N/L^3=\varrho}} \frac{1}{L^3} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} p^2 \mathbb{1}\left(p^2 \leq \mu\right)$$

$$= \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} p^2 \mathbb{1}\left(p^2 \leq \mu\right) = \left(\frac{1}{2\pi}\right)^3 4\pi \int_0^{\sqrt{\mu}} p^4 dp \qquad (11)$$

$$= \frac{1}{10\pi^2} \mu^{5/2} = \frac{1}{10\pi^2}\left(6\pi^2 \varrho\right)^{5/3} = \underline{\underline{\frac{3}{5}\left(6\pi^2\right)^{2/3} \varrho^{5/3}.}}$$

The quantity μ is called the chemical potential of the system. It can be interpreted as the energy cost to add one additional particle to the system.

Our main theorem will be about spin 1/2 fermions, which we consider next. In this case we have more one-particle levels at our disposal because each particle may be in one of two spin states, which we denote by ↑ and ↓. The relevant one-particle eigenfunctions are thus

$$\{\varphi_{p,\uparrow}\}_{p\in\frac{2\pi}{L}\mathbb{Z}^3} \quad \text{and} \quad \{\varphi_{p,\downarrow}\}_{p\in\frac{2\pi}{L}\mathbb{Z}^3} . \qquad (12)$$

In this case the minimal energy for the two-particle problem equals 0 because because $\varphi_{0,\uparrow}$ and $\varphi_{0,\downarrow}$ are two basis functions with $\langle \varphi_{0,\uparrow}, \varphi_{0,\downarrow}\rangle = 0$.

Let us for the moment assume that we have a density $\rho_\uparrow$ of spin up particles and $\rho_\downarrow$ of spin down particles. The minimal energy of such a configuration is given by

$$e_0(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5}\left(6\pi^2\right)^{2/3}\left(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}\right). \qquad (13)$$

If we assume that $\rho = \rho_\uparrow + \rho_\downarrow$ is fixed we can minimize over $\rho_\uparrow$ and $\rho_\downarrow$ to obtain the energetically optimal spin configuration. A straight forward computation shows that the energy is minimized for $\rho_\uparrow = \rho_\downarrow$.

3. The main theorem for the dilute Fermi gas and heuristics

The main statement we are going to prove in the second Chapter is the following theorem for the interacting system in the dilute limit. The function v is chosen as in the theorem for the dilute Bose gas.

Theorem (Lieb, Seiringer, Solovej (2005): Fix $\rho_\uparrow = \frac{N_\uparrow}{L^3}$, $\rho_\downarrow = \frac{N_\downarrow}{L^3}$ and $\rho = \rho_\uparrow + \rho_\downarrow$, and let $E_0^F(N, N_\uparrow, N_\downarrow, L, v)$ denote the ground state energy of

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le i < j \le N} v(x_i - x_j) \qquad (14)$$

(with boundary conditions that make it self-adjoint) when restricted to $L^2_a([0,L]^{3N})$. In the dilute limit, that is, when $\rho^{1/3} a \to 0$, we then have

$$e_0^F(\rho,\rho_\uparrow,\rho_\downarrow,v) = \lim_{\substack{N\to\infty \\ L\to\infty \\ N/L^3=\rho,\ \frac{N_\uparrow}{L^3}=\rho_\uparrow \\ N_\downarrow/L^3=\rho_\downarrow}} \frac{E_0^F(N,N_\uparrow,N_\downarrow,L,v)}{L^3} \qquad (15)$$

$$= \frac{3}{5}\left(6\pi^2\right)^{2/3}\left(\rho_\uparrow^{5/3}+\rho_\downarrow^{5/3}\right) + 8\pi a\,\rho_\uparrow\rho_\downarrow + a\rho^2\,\mathcal{E}(\rho),$$

with $-\text{const.}\left(a\rho^{1/3}\right)^{1/13} \leq \mathcal{E}(\rho) \leq \text{const.}\left(a\rho^{1/3}\right)^{2/3}$.

Remark: The constants in the bounds on $\mathcal{E}(\rho)$ depend on the interaction potential only through the dimensionless ratio R_0/a. The explicit dependence could be displayed explicitly.

Before we start with the proof of the above Theorem let us argue why this is what one would expect.

Heuristics

(a) The interaction term in (15) is much smaller than the energy of the Fermi sea. Accordingly, one would expect that an approach based on first order perturbation theory should give a good result. Of course, as for the bosons, we need to take correlations due to the interactions between the particles into account.

(b) The interaction term in (15) is of the same order of magnitude as for the bosons, but now only particles in different spin states seem to interact. To explain this effect let us consider the interaction between two fermions with equal spin. Assume that the two particles have momenta p_1 and p_2, respectively, with $p_1^2 \leq \mu$ and $p_2^2 \leq \mu$. Their position space wavefunction is given by

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \Big(\varphi_{p_1}(x_1)\, \varphi_{p_2}(x_2) - \varphi_{p_2}(x_1)\, \varphi_{p_1}(x_2) \Big) \quad (16)$$

because the spin wavefunction is necessarily symmetric. The function Ψ describes two non-interaction particles and to obtain the wavefunction of an interacting system we have to multiply Ψ, as in the case of bosons, by the solution of the zero energy scattering equation. We obtain

$$\tilde{\Psi}(x_1,x_2) = f(x_1-x_2)\,\Psi(x_1,x_2).$$

(Note that $\|\tilde{\Psi}\| \neq 1$. This, however, plays no role in our discussion.) (17)

Let us compute the interaction energy of this function. We have

This function varies on the length scales $1/|p_1|$ and $1/|p_2|$ and we have $\Psi(x,x)=0$.

$$\int v(x-y)\,|\tilde{\Psi}(x,y)|^2\,d(x,y) = \int \underbrace{v(x-y)\,|f(x-y)|^2}_{\text{Those two functions vary on the length scale } a.}\,|\Psi(x,y)|^2\,d(x,y) \qquad (18)$$

We know that $1/|p_1| \geq \sqrt{\mu}^{-1}$; $\frac{1}{|p_2|} \geq \sqrt{\mu}^{-1}$ and that by (10) $\mu^{-1} \geq \text{const.}\,\rho^{-2/3}$. We thus know that Ψ varies on a length scale that is larger than a constant times $\rho^{-1/3}$, which is much larger than a in the dilute limit. But this implies

$$\int \underbrace{v(x-y)\,|f(x-y)|^2}_{\substack{\text{compactly}\\ \text{supported fct on}\\ \text{length scale } a.}}\,\underbrace{|\Psi(x,y)|^2}_{\simeq\, \rho^{2/3}\,\text{const.}\,|x-y|^2 \text{ for } x \text{ close to } y \text{ because } \Psi(x,x)=0.}\,d(x,y) \leq \text{const.}\,\overset{\text{small factor}}{\boxed{\rho^{2/3}a^2}}\int v(x)\,|f(x)|^2\,dx. \qquad (19)$$

While the interaction in (15) is of the order $\rho^2 a$, we expect that the interaction between particles of equal spin is because of (18) of the order $\rho^2 a\,(\rho^{2/3} a)$, which is much smaller in the dilute limit. Note that the source of this effect are the antisymmetrie of the wavefunction and the fact that the momenta in the Fermi sea lead to a spatial variation of the wavefunction that is large compared to the length scale of the interaction potential.

(c) In the case of the Bose gas the interaction energy is given by $4\pi a \rho^2$. In case of the Fermi gas it is $8\pi a \rho_\uparrow \rho_\downarrow$, that is, there seems to be an additional factor of 2. To explain where this factor comes from let us consider the interaction between two fermions of unequal spin. In this case the spin wave function can be chosen anti-symmetric, that is

$$|\Psi^s\rangle = \frac{1}{\sqrt{2}}\Big(\underbrace{|\uparrow\downarrow\rangle}_{=|\uparrow\rangle\otimes|\downarrow\rangle} - |\downarrow\uparrow\rangle\Big). \qquad (20)$$

$|\downarrow\rangle \leftarrow$ basis vector for spin ↓.

$|\uparrow\rangle \uparrow$ basis vector for spin ↑.

Accordingly, the position space wavefunction can be chosen symmetric:

$$\Psi^P(x_1,x_2) = f(x_1-x_2)\,\frac{1}{\sqrt{2}}\Big(\varphi_{p_1}(x_1)\varphi_{p_2}(x_2)+\varphi_{p_2}(x_1)\varphi_{p_1}(x_2)\Big). \quad (21)$$

Let us again compute the interaction energy. We have

$$\int V(x-y)\,|\Psi^P(x,y)|^2 f(x-y)^2\, d(x,y) \quad (22)$$

$$= \frac{1}{2}\int V(x-y)\,f(x-y)^2\,\big|\,\varphi_{p_1}(x)\varphi_{p_2}(y)+\varphi_{p_2}(x)\varphi_{p_1}(y)\,\big|^2\, d(x,y)$$

$$\simeq 2\,\underbrace{\int V(r)\,f(r)^2\,dr}\int\underbrace{|\varphi_{p_1}(x)|^2\,|\varphi_{p_2}(x)|^2}\,dx$$

Same considerations as before

This will contribute to the factor $4\pi a$. The other part comes from the kinetic energy.

This will give the density squared if we sum up all such contributions.

This is the factor 2 in the interaction energy relative to the bosons.

It is a consequence of the fact that the two fermions are sitting in two different one-particle functions (there is no condensate as in the case of bosons) and that the wavefunction is symmetrized. Note that this can only happen if the two fermions are in different spin states so the spin part of the wavefunction can be chosen antisymmetric.

The remainder of this Chapter is devoted to the proof of the Theorem. As in the case of bosons we start with the proof of an upper bound for the energy.

4. Upper bound to the ground state energy

Our starting point is the variational characterization for the energy in a finite box, that is,

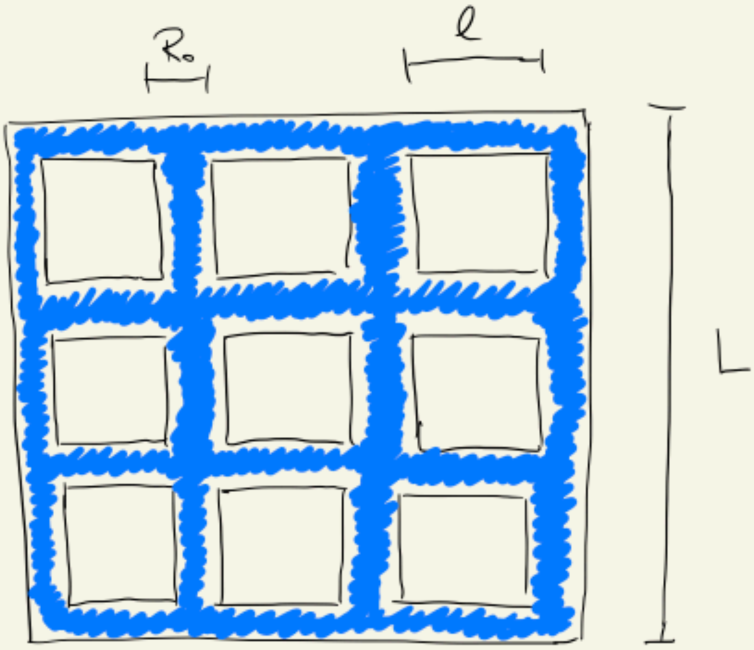
$$E_0^F(N_\uparrow, N_\downarrow, L, V) = \inf_{\substack{\|\phi\|=1 \\ \phi \in \underbrace{P_{N_\uparrow N_\downarrow}}_{\text{Projection onto the space with } N_\uparrow \text{ spin up and } N_\downarrow \text{ spin down particles}} \underbrace{L^2_{a,1/2}\left([0,L]^{3N}\right)}_{\text{Space of fermionic spin } 1/2 \text{ wave functions}}}} \langle \phi, H_N \phi \rangle \qquad (23)$$

For the upper bound it will be convenient to split the box $[0,L]^3$ into smaller boxes with side length l and to localize the particles into these smaller boxes. If we place these boxes a distance R_0 from each other, there will be no interaction between particles in different boxes. We want to put $n = \rho_\uparrow (\ell+R_0)^3$ spin up particles in each box and $m = \rho_\downarrow (\ell+R_0)^3$ spin down particles. Since n and m need not be integers, we will choose

$$n = \rho_\uparrow(\ell+R_0)^3+\varepsilon_1 \quad \text{and} \quad m = \rho_\downarrow(\ell+R_0)^3+\varepsilon_2 \qquad (24)$$

with $0 \le \varepsilon_1, \varepsilon_2 \le 1$ chosen s.t. n, m are integer. We then have too many particles in the system, but this is legitimate for an upper bound because all terms in the Hamiltonian are positive operators, and hence the energy is certainly an increasing function of the particle number.

Large and Small boxes:



When we restrict the minimization in (23) to a subclass of functions, we obtain an upper bound. This subclass is chosen to satisfy the following requirements:

- There are exactly n spin up and m spin down particles in each box.
- The wave function is smooth and compactly supported inside the open small boxes. That is, whenever one coordinate is at the boundary of a small box, or outside, it vanishes.

Minimization over such functions yields the upper bound

$$E_0^F(N_\uparrow, N_\downarrow, L, v) \le \underbrace{\frac{L^3}{(\ell+R_0)^3}}_{\text{\# of small boxes}} \underbrace{E_0^F(n, m, \ell, v)}_{\substack{\text{energy of the particles} \\ \text{in a small box with Laplacian} \\ \text{chosen with Dirichlet boundary} \\ \text{conditions (comes from choice} \\ \text{of functions.)}}}, \tag{25}$$

and hence

$$\lim_{\substack{N\to\infty \\ L\to\infty \\ N/L^3=\rho \\ \rho_\uparrow,\rho_\downarrow \text{ fixed}}} \frac{E_0^A(N, N_\uparrow, N_\downarrow, L, v)}{L^3} \le \frac{1}{(\ell+R_0)^3} E_0^A(n, m, \ell, v). \tag{26}$$

Next, we will construct the trial state. Why it is necessary to use the small boxes will become apparent later.

The trial state

Let $X = (x_1 \dots x_n)$ and $Y = (y_1 \dots y_m)$ be the collection of the coordinates of the spin up and the spin down particles, respectively. The trial state wavefunction on the small box $[0,\ell]^3$ will be chosen as

$$\Psi(X,Y) = D_n(X) D_m(Y) G_n(X) G_m(Y) F(X,Y). \quad (27)$$

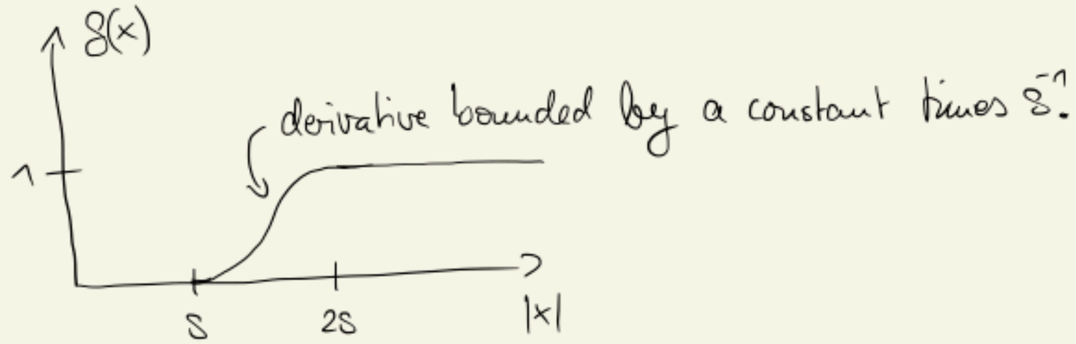
Here $D_n(X) = \varphi_{p_1} \wedge \dots \wedge \varphi_{p_n}(x_1, \dots, x_n)$ denotes the Slater determinant of the first n eigenfunctions of the Laplacian in the box $[0,\ell]^3$ with Dirichlet boundary conditions (in case of degeneracy any choice does the job). Moreover (28)

$$G_n(X) = \prod_{1 \le i < j \le n} g(x_i - x_j),$$

G_n assures that it is easy to show that the interaction between particles of equal spin plays no role.

for a radial function g with the following properties:

- $0 \leq g(x) \leq 1$ for all $x \in \mathbb{R}^3$
- $g(x) = 0$ for $|x| \leq s$ and $g(x) = 1$ for $|x| \geq 2s$ with $s > 2R_0$ to be chosen later.
- We can also assume that $|\nabla g(x)| \leq \text{const.}\, s^{-1}$ for a constant independent of s.



(Choose e.g. a fixed function $\tilde{g}$ with s replaced by 1 in the the above list and let $g(x) = \tilde{g}(x/s)$.)

Finally, let

$$f_R(x) = \begin{cases} f_0(|x|)/f_0(R) & \text{if } |x| \leq R \\ 1 & \text{if } |x| > R \end{cases} \qquad (29)$$

for some $R > R_0$ as in the case of the Bose gas and define (30)

$$F(X,Y) = \prod_{i=1}^{n} \prod_{j=1}^{m} f_R(x_i - x_j).$$

F is the correlation structure that allows us to obtain the correct interaction energy.

We also assume that $2R \leq S$.

Remark: To keep the notation simple we have suppressed spin indices in the trial state wavefunction. If we want to be more precise, we have to write

$$D_n = \varphi_{p_1,\uparrow} \wedge \cdots \wedge \varphi_{p_n,\uparrow} = \underbrace{\varphi_{p_1} \wedge \cdots \wedge \varphi_{p_n}}_{\text{position space part of WF}} \otimes \underbrace{\overset{|\uparrow\rangle \otimes |\uparrow\rangle \otimes \ldots \otimes |\uparrow\rangle}{\overset{\parallel}{|\uparrow, \ldots, \uparrow\rangle}}}_{\text{spin part of WF}} \quad (31)$$

and

$$D_m = \varphi_{p_1,\downarrow} \wedge \cdots \wedge \varphi_{p_m,\downarrow} = \varphi_{p_1} \wedge \cdots \wedge \varphi_{p_n} \otimes |\downarrow, \ldots, \downarrow\rangle . \quad (32)$$

The antisymmetric product of D_n and D_m would then be

$$D_n \wedge D_m (x_1, \nu_1, \ldots, x_n, \nu_n, x_{n+1}, \nu_{n+1}, \ldots x_{n+m}, \nu_{n+m}) \quad \text{spin index: } \uparrow \text{ or } \downarrow \quad (33)$$

$$= \frac{1}{\sqrt{(n+m)!\, n!\, m!}} \sum_{\sigma \in S_{n+m}} \operatorname{sgn}(\sigma)\, D_n(x_{\sigma(1)}, \nu_{\sigma(1)}, \ldots, x_{\sigma(n)}, \nu_{\sigma(n)})\, D_m(x_{\sigma(n+1)}, \nu_{\sigma(n+1)}, \ldots, x_{\sigma(n+m)}, \nu_{\sigma(n+m)}).$$

Note that $D_n \wedge D_m$ is again normalized in L^2 if we define the wedge product $\wedge$ with this normalization. It is not hard to check that the energy of this state is the same as the one of $D_n(X)D_m(Y)$ because the Hamiltonian H_N does not act on the spin indices. This is why we prefer to suppress spin indices. Note also that the functions G_n and F do not affect the antisymmetry of the wave-function because they are symmetric under an exchange of the coordinates.

By the variational principle we have

$$E_0^F(n,m,v) \le \frac{\langle \Psi, H_{n+m}\Psi\rangle}{\langle \Psi,\Psi\rangle} . \qquad (34)$$

In the case of the Bose gas the trial state wavefunction was considerably simpler and already in this case it was difficult to take the necessary cancellation in an expression of the form $\frac{\langle \Psi, H_{n+m}\Psi\rangle}{\langle \Psi,\Psi\rangle}$ between the numerator and the denominator into account. In the following we will see how this problem can be solved.

Since Ψ vanishes whenever two particles in the same spin state are closer together than the range of the interaction, we have

$$\langle \Psi, H_{n+m} \Psi \rangle = \sum_{i=1}^{n} \langle \Psi, -\Delta_{x_i} \Psi \rangle + \sum_{j=1}^{m} \langle \Psi, -\Delta_{y_j} \Psi \rangle \qquad (35)$$

$$+ \sum_{i=1}^{n} \sum_{j=1}^{m} \langle \Psi, v(x_i - y_j) \Psi \rangle .$$

We start by computing the kinetic energy.

The kinetic energy

We introduce the notation $\Delta_X = \sum_{i=1}^{n} \Delta_{x_i}$ as well as $\nabla_X = (\partial_{x_1}, \dots, \partial_{x_n})$. When we integrate by parts twice, we see that

$$\langle \Psi, -\Delta_X \Psi \rangle = \int D_m^2(Y)\, G_n^2(X)\, G_m^2(Y)\, F^2(X,Y) \qquad (36)$$

$$D_n(X) \left(-\Delta_X D_n(X) \right) d(X,Y) \; + \; \longrightarrow$$

$$+ \int D_n(X)^2 \, |\nabla_X G_n(X) F(X,Y)|^2 \, D_m(Y)^2 G_m(Y)^2 \, d(X,Y).$$

Note that the eigenfunctions of the Laplacian on $[0,\ell]^3$ can be chosen real because $\overline{-\Delta \varphi_p} = \overline{e_p \varphi_p} \iff -\Delta \overline{\varphi_p} = e_p \overline{\varphi_p}$. Accordingly, all functions in our trial state are real-valued.

Since $D_n(X)$ is an eigenfunction of $-\Delta_X$ whose eigenvalue is given by the sum of the n lowest one-particle energies, the first term on the right-hand side of (36) equals

$$\underbrace{E^D(n,\ell)}_{} \langle \Psi, \Psi \rangle. \tag{37}$$

Sum of lowest n eigenvalues of $-\Delta$ with Dirichlet boundary conditions in $[0,\ell]^3$.

To estimate the second term we pick $\varepsilon > 0$ to be chosen later and consider (38)

$$|\nabla_X G_n(X) F(X,Y)|^2 = F(X,Y)^2 |\nabla G_n(x)|^2 + G_n(x)^2 |\nabla_X F(X,Y)|^2$$

$xy \le \frac{\varepsilon}{2} x^2 + \frac{1}{2\varepsilon} y^2$ for $xy \ge 0$.

$$+ 2\, G_n(X) F(X,Y) \, \nabla_X G_n(X) \nabla_X F(X,Y)$$

$$\searrow \le (1+\varepsilon)\, G_n(X)^2 |\nabla_X F(X,Y)|^2 + (1+\varepsilon^{-1}) F(X,Y)^2 |\nabla_X G_n(X)|^2.$$

We use the same bounds for the kinetic energy of the Y particles (spin ↓ particles) and obtain the upper bound

$$\langle \Psi, H_{n+m} \Psi \rangle \leq (\mathrm{I}) + (1+\varepsilon)(\mathrm{II}) + (1+\varepsilon^{-1})(\mathrm{III}), \qquad (39)$$

where

$$(\mathrm{I}) = \left[E^D(n,\ell) + E^D(m,\ell) \right] \langle \Psi, \Psi \rangle, \qquad (40)$$

$$(\mathrm{II}) = \int \left[|\nabla_X F(X,Y)|^2 + |\nabla_Y F(X,Y)|^2 + V_{XY} F(X,Y)^2 \right] \times D_n(X)^2 D_m(Y)^2 G_n(X)^2 G_m(Y)^2 \, d(X,Y),$$

and

$$(\mathrm{III}) = \int \left[|\nabla_X G_n(X)|^2 G_m(Y)^2 + |\nabla_Y G_m(Y)|^2 G_n(X)^2 \right] \times F(X,Y)^2 D_n(X)^2 D_m(Y)^2 \, d(X,Y). \qquad (41)$$

To obtain the factor $(1+\varepsilon)$ in front of the interaction terms in (II) we used $v \geq 0$ and we denote $V_{XY} = \sum_{i=1}^{n} \sum_{j=1}^{m} v(x_i - y_j)$.

In the following we will derive appropriate upper bounds for these terms when divided by $\langle \Psi, \Psi \rangle$.

We start with (I):

$$\frac{(\mathrm{I})}{\langle \Psi, \Psi \rangle} = E^D(n,l) + E^D(m,l). \qquad (42)$$

A similar computation than on p.7 shows that $E^D(n,l)/l^3$ (note that we used periodic boundary conditions on p.7, while we have Dirichlet boundary conditions here) converges in the thermodynamic limit to $\frac{3}{5}(6\pi)^{2/3}\tilde{\rho}^{5/3}$, where $\tilde{\rho} = \frac{n}{l^3}$. We are however in a finite box and will choose l depending on the local parameters ρ and a. Accordingly, we need a quantitative estimate. Before we derive this estimate let us recall that the eigenvalues and eigenfunctions of the Dirichlet Laplacian are given by

$$e_p = p^2 \quad \text{and} \quad \Psi_p(x) = \left(\frac{2}{l}\right)^{3/2} \sin(p_1x_1)\sin(p_2x_2)\sin(p_3x_3),$$

where $p \in \left(\pi/l\,\mathbb{N}\right)^3$. (43)

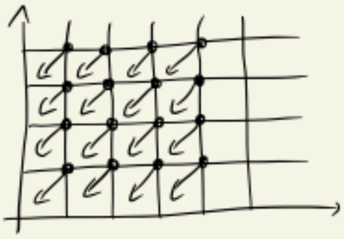
To continue with our analysis, we need the following Lemma.

Lemma 1: Let $f : \mathbb{R}_+ \to \mathbb{R}_+$ be a monotone decreasing measurable function with $\int_{\mathbb{R}^3} f(p^2)\,dp < +\infty$. We then have

$$\left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} f(p^2)\left[1 - \frac{3\pi}{2\ell|p|}\right] dp \leq \frac{1}{\ell^3} \sum_{p \in \frac{\pi}{\ell}\mathbb{N}^3} f(p^2) \tag{44}$$

$$\leq \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} f(p^2)\,dp.$$

Proof: By considering the sum as a lower Riemann sum we check the upper bound.



To obtain the second bound we consider the sum as an upper Riemann sum to the integral over the region

$$A = \{p \in \mathbb{R}^3 \mid p_i \geq \pi/\ell,\ i = 1,2,3\}. \tag{45}$$

Hence, the sum is bounded from below by $\left(\frac{1}{2\pi}\right)^3$ times

$$\int_{\mathbb{R}^3} f(p^2)\,dp - \sum_{i=1}^{3} \int_{0 \leq p_i \leq \pi/\ell} f(p^2)\,dp. \tag{46}$$

Since f is monotone decreasing, we can estimate

$$\int_{0\le p_i\le \pi/\ell} f(p^2)\,dp \le \frac{\pi}{\ell}\int_{\mathbb{R}^2} f(p^2)\,dp = \frac{1}{2}\,\frac{\pi}{\ell}\int_{\mathbb{R}^3} f(p^2)\,\frac{1}{|p|}\,dp. \qquad (47)$$

In combination, these considerations prove the claim. ∎

Our goal is to find an upper bound for the sum of the first n Dirichlet eigenvalues in the box $[0,\ell]^3$. We have

$$\sum_{j=1}^{n} p_j^2 \le \sum_{p\in\frac{\pi}{\ell}\mathbb{N}^3} p^2\,\mathbb{1}\left(|p|\le|p_n|\right). \qquad (48)$$

From the considerations on p. 6/7 we know that $p_n^2 \to \mu = \left(6\pi^2\frac{n}{\ell^3}\right)^{2/3}$ in the limit $n\to\infty$, $\ell\to\infty$ with n/ℓ^3 fixed. To obtain a bound for fixed n and ℓ, we consider

$$\frac{n}{\ell^3} \ge \frac{1}{\ell^3}\sum_{p\in\frac{\pi}{\ell}\mathbb{N}^3} \mathbb{1}\left(p^2\le \underset{\uparrow}{\tilde\mu}\right) \overset{\text{Lemma 1}}{\overset{\downarrow}{\ge}} \left(\frac{1}{2\pi}\right)^3\int_{\mathbb{R}^3}\mathbb{1}\left(p^2\le\tilde\mu\right)\left[1-\frac{3\pi}{2\ell|p|}\right]dp \qquad (49)$$

$$\sqrt{\tilde\mu} = \left|\,|p_n| - \text{const.}\,\frac{1}{\ell}\,\right|$$

$$= \frac{\tilde{\mu}^{3/2}}{6\pi^2} - \text{const.}\,\tilde{\mu}/\ell = \frac{\tilde{\mu}^{3/2}}{6\pi^2}\left(1 - \text{const.}\,\frac{1}{\tilde{\mu}^{1/2}\ell}\right) \qquad (50)$$

Hence, $\frac{n}{\ell^3} \geq \frac{\tilde{\mu}^{3/2}}{6\pi^2}\left(1 - \text{const.}\,\frac{1}{\ell\tilde{\mu}^{1/2}}\right)$. We know that $p_n^2 \to \mu = \left(6\pi^2 \frac{n}{\ell^3}\right)^{2/3}$ in the thermodynamic limit. In combination with the definition of $\tilde{\mu}$ we conclude that $\tilde{\mu} \leq \text{const.}\,(n/\ell^3)^{2/3}$.

Hence

$$\frac{n}{\ell^3} \geq \frac{|p_n|^3}{6\pi^2}\left(1 - \frac{\text{const.}}{|p_n|\ell}\right)\left(1 - \text{const.}\,\frac{1}{n^{1/3}}\right)$$

↳ bounded above and below by a constant times $(n/\ell^3)^{1/3}$

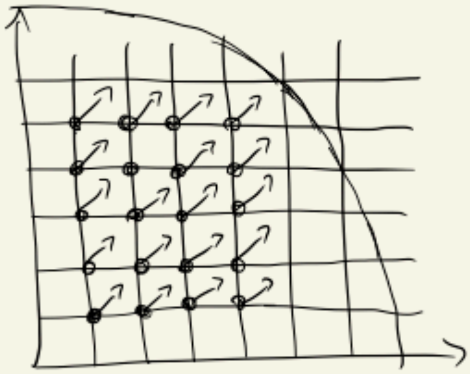
$$\geq \frac{|p_N|^3}{6\pi^2}\left(1 - \frac{\text{const.}}{n^{1/3}}\right)$$

$$\Rightarrow \boxed{|p_n| \leq \left(6\pi^2\,\frac{n}{\ell^3}\right)^{1/3}\left(\frac{1}{1 - \frac{\text{const.}}{n^{1/3}}}\right)^{1/3}}. \qquad (51)$$

Let us combine this result with Eq. (48). We claim that

$$\sum_{j=1}^{n} p_j^2 \leq \left(\frac{\ell}{2\pi}\right)^3 \int_{\mathbb{R}^3} \mathbb{1}\left(|p| \leq |p_n| + \sqrt{3}\,\frac{\pi}{\ell}\right) p^2\,dp. \qquad (52)$$

To see this we again interpret the relevant sum as a lower Riemann sum.



The right-hand side of (52) equals $\frac{\ell^3}{10\pi^2}\left(|p_n|+\sqrt{3}\,\frac{\pi}{\ell}\right)^5$

$$\le \frac{\ell^3}{10\pi^2}|p_n|^5\left(1+\text{const.}\,\frac{1}{n^{1/3}}\right) \quad \text{(see the argument in (51))}$$

$$\overset{(51)}{\le} \underbrace{\frac{\ell^3}{10\pi^2}\left(6\pi^2\,\frac{n}{\ell^3}\right)^{5/3}}_{\frac{3}{5}\left(6\pi^2\right)^{2/3}\left(\frac{n}{\ell^3}\right)^{5/3}\ell^3 \;=\; \frac{3}{5}\left(6\pi^2\right)^{2/3}\frac{n^{5/3}}{\ell^2}}\left(1+\text{const.}\,\frac{1}{n^{1/3}}\right) \qquad (53)$$

We conclude that there exist a constant such that

$$\boxed{E^D(n,\ell) \le \frac{3}{5}\left(6\pi^2\right)^{2/3}\frac{n^{5/3}}{\ell^2}\left(1+\text{const.}\,n^{-1/3}\right)} \qquad (54)$$

holds.

<u>Remark</u>: It can be shown that the exponent $-1/3$ in the remainder is optimal. We also note that this bound shows that we must not choose ℓ too small in order

to have an error term that is negligible compared with $\rho^2 a$.

We need

$$\frac{n^{5/3}}{\ell^5}\, n^{-1/3} \ll \rho^2 a \qquad (55)$$

↗ energy per volume, we will have $\frac{n}{\ell^3} \sim \rho$, and hence

$$\rho^{5/3} n^{-1/3} \ll \rho^2 a \iff n^{1/3} \gg \frac{1}{\rho^{1/3} a}$$

$$\iff \boxed{n \gg \frac{1}{\rho a^3}} . \qquad (56)$$

Our choice of ℓ below will guarantee that the number of particles n in the small boxes fulfills this requirement. In summary, we have shown:

$$(57)$$

$$\boxed{\begin{aligned}\frac{(\mathrm{I})}{(\Psi,\Psi)} = \left[E^D(n,\ell) + E^D(m,\ell)\right] &\le \frac{3}{5}\left(6\pi^2\right)^{2/3} \frac{n^{5/3}}{\ell^2}\left(1 + \text{Const.}\, n^{-1/3}\right) \\ &+ \frac{3}{5}\left(6\pi^2\right)^{2/3} \frac{m^{5/3}}{\ell^2}\left(1 + \text{Const.}\, m^{-1/3}\right)\end{aligned}} .$$

Upper bound on (II)

In the next step we derive an upper bound on (II). To that end, we need the following Lemma.

Lemma 2: Let $D_n(X)$ with $X = (x_1 \dots x_n)$ denote a Slater determinant of n linearly independent one-particle wave functions $\{\phi_\alpha\}_{\alpha=1}^{n}$. For a given function h of one variable, let

$$\Phi(X) = D_n(X) \prod_{i=1}^{n} h(x_i), \tag{58}$$

and let $\mathcal{M}$ denote the $n \times n$ matrix with components

$$\mathcal{M}_{\alpha\beta} = \int_{[0,\ell]^3} \overline{\phi_\alpha(x)}\, \phi_\beta(x)\, |h(x)|^2\, dx. \tag{59}$$

Then we have

(i) $\langle \Phi, \Phi \rangle = \det \mathcal{M}$ $\quad$ (norm of Φ) $\quad$ (60)

(ii) For $1 \leq k \leq n$, the k-particle densities $\rho_\Phi^{(k)}(x_1 \dots x_k)$ are given by

$$\rho_\Phi^{(k)}(x_1 \dots x_k) = \binom{n}{k} \frac{1}{\langle \Phi, \Phi \rangle} \int_{[0,\ell]^{3(N-k)}} |\Phi(X)|^2\, d(x_{k+1} \dots x_n) \tag{61}$$

$$= \frac{1}{k!} \prod_{i=1}^{k} |h(x_i)|^2 \left(\vec{\phi}(x_1) \wedge \dots \wedge \vec{\phi}(x_k),\ \overline{\mathcal{M}}^{-1} \otimes \dots \otimes \overline{\mathcal{M}}^{-1}\, \vec{\phi}(x_1) \wedge \dots \wedge \vec{\phi}(x_k) \right),$$

where $\vec{\phi}(x)$ denotes the n-dimensional vector $(\phi_1(x), \dots, \phi_n(x))$ and

and $$\vec{\phi}(x_1)\wedge\dots\wedge\vec{\phi}(x_k) = \sqrt{\frac{1}{k!}}\sum_{\sigma\in S_k} \mathrm{sgn}(\sigma)\,\vec{\phi}(x_{\sigma(1)})\otimes\dots\otimes\vec{\phi}(x_{\sigma(k)}) \,. \qquad (62)$$

(iii) If $\phi_i'(X) = \dfrac{\phi(X)\,k(x_i)}{h(x_i)}$ for some function $k(x)$, then

$$\sum_{i=1}^{n} \langle \phi_i', \phi_i' \rangle = \det(M)\,\mathrm{tr}\left[M^{-1}K\right] \qquad (63)$$

where K is the $n\times n$ matrix with components

$$K_{\alpha\beta} = \int_{[0,\ell]^3} \overline{\phi_\alpha(x)}\,\phi_\beta(x)\,|k(x)|^2 dx. \qquad (64)$$

<u>Proof:</u> Since the functions $\{\phi_\alpha\}_{\alpha=1}^{n}$ are only assumed to be linearly independent we can w.l.o.g. prove the Lemma for the choice $h\equiv 1$.

(i) $$\langle\Phi,\Phi\rangle = \frac{1}{n!}\sum_{\sigma,\sigma'\in S_n}\mathrm{sgn}(\sigma)\,\mathrm{sgn}(\sigma')\int \overline{\phi_{\sigma(1)}(x_1)\dots\phi_{\sigma(n)}(x_n)}\,\phi_{\sigma'(1)}(x_1)\dots\phi_{\sigma'(n)}\,d(x_1\dots x_n)$$

$$= \sum_{\sigma\in S_n}\mathrm{sgn}(\sigma)\int \overline{\phi_1(x_1)\dots\phi_n(x_n)}\,\phi_{\sigma(1)}(x_1)\dots\phi_{\sigma(n)}(x_n)\,d(x_1\dots x_n) \qquad (65)$$

$$= \sum_{\sigma\in S_n}\mathrm{sgn}(\sigma)\prod_{i=1}^{n} M_{i\sigma(i)} = \det(M).$$ This proves (i).

(ii) Let $A \in \mathbb{C}^{n\times n}$ be defined by $A_{i,\alpha} = \phi_\alpha(x_i)$. First we realize that

$$\frac{\int |\phi(x)|^2 \, d(x_{k+1},\dots,x_n)}{\int |\phi(x)|^2 \, d(x_1\dots x_n)} = \frac{1}{n!} \, \frac{\int \overset{\det(\bar{A}) = \det(A^*)}{\overline{\det(A)}} \det(A) \, d(x_{k+1},\dots,x_n)}{\det(M)} \qquad (66)$$

$$= \frac{1}{n!} \int \det(A M^{-1} A^*) \, d(x_{k+1},\dots,x_n).$$

The integrand can be written as

$$\det(A M^{-1} A^*) = \sum_{\sigma \in S_n} \mathrm{sgn}(\sigma) \prod_{i=1}^{n} (A M^{-1} A^*)_{i,\sigma(i)} . \quad \text{Hence,} \qquad (67)$$

$$\int \det(A M^{-1} A) \, dx_n = \sum_{\sigma \in S_n} \mathrm{sgn}(\sigma) \int \prod_{i=1}^{n} \sum_{\alpha\beta=1}^{n} \phi_\alpha(x_i) (M^{-1})_{\alpha\beta} \overline{\phi_\beta(x_{\sigma(i)})} \, dx_n \qquad (68)$$

Denote for any σ, $n_\sigma = \sigma^{-1}(n)$ such that $\sigma(n_\sigma) = n$. Then the above equals (We assume $n_\sigma \neq n$. If $n_\sigma = n$ the argument is almost the same.)

$$\sum_{\sigma\in S_n} \operatorname{sgn}(\sigma) \prod_{\substack{i=1\\ i\neq n_\sigma}}^{n-1} \sum_{\alpha\beta=1}^{n} \phi_\alpha(x_i)\left(M^{-1}\right)_{\alpha\beta} \overline{\phi_\beta(x_{\sigma(i)})} \tag{69}$$

$$\underbrace{\times \sum_{\alpha\beta\alpha'\beta'=1}^{n} \int \phi_\alpha(x_n)\left(M^{-1}\right)_{\alpha\beta} \overline{\phi_\beta(x_{\sigma(n)})}\, \phi_{\alpha'}(x_{n_\sigma})\left(M^{-1}\right)_{\alpha'\beta'} \overline{\phi_{\beta'}(x_{\underbrace{\sigma(n_\sigma)}_{n}})}\, dx_n}_{}$$

$$= \sum_{\alpha\beta\alpha'\beta'=1}^{n} \phi_{\alpha'}(x_{n_\sigma}) \overline{\phi_\beta(x_{\sigma(n)})}\, M_{\beta'\alpha} \left(M^{-1}\right)_{\alpha\beta} \left(M^{-1}\right)_{\alpha'\beta'}$$

$$= \sum_{\alpha\beta=1}^{n} \phi_\alpha(x_{n_\sigma}) \overline{\phi_\beta(x_{\sigma(n)})} \left(M^{-1}\right)_{\alpha\beta} = \left(AM^{-1}A^*\right)_{n_\sigma,\sigma(n)}$$

We thus have

$$\int \det\left(AM^{-1}A^*\right) dx_n = \sum_{\sigma\in S_{n-1}} \operatorname{sgn}(\sigma) \prod_{\substack{i=1\\ i\neq n_\sigma}}^{n-1} \left(AM^{-1}A^*\right)_{i,\sigma(i)} \left(AM^{-1}A^*\right)_{n_\sigma,\sigma(n)}$$

$$= \det\left(\tilde{A} M^{-1} \tilde{A}^*\right), \tag{70}$$

where $\tilde{A}\in\mathbb{C}^{(n-1)\times n}$, $\tilde{A}_{i\alpha} = \phi_\alpha(x_i)$ with $\alpha = 1\ldots n$, $i = 1\ldots(n-1)$. Using the same argument, we also check that

$$\int \det\left(A M^{-1} A^*\right) d(x_{k+1},\dots,x_n) = (n-k)!\, \det\left(A^{(k)} M^{-1} A^{(k)*}\right), \qquad (71)$$

with $A^{(k)} \in \mathbb{C}^{k\times n}$, $A^{(k)}_{i\alpha} = \phi_\alpha(x_i)$. This implies

$$\binom{n}{k} \frac{\int |\Phi(x)|^2 d(x_{k+1},\dots,x_n)}{\int |\Phi(x)|^2 d(x_1 \dots x_n)} = \frac{1}{k!\,(n-k)!} \int \det\left(A M^{-1} A^*\right) d(x_{k+1},\dots,x_n)$$

$$= \frac{1}{k!} \det\left(A^{(k)} M^{-1} A^{(k)*}\right). \qquad (72)$$

Next, we compute

$$\left(\vec{\phi}(x_1) \wedge \dots \wedge \vec{\phi}(x_k),\ \overline{M^{-1}} \otimes \dots \otimes \overline{M^{-1}}\, \vec{\phi}(x_1) \wedge \dots \wedge \vec{\phi}(x_k) \right)$$

$$= \frac{1}{k!} \sum_{\sigma,\sigma' \in S_k} \operatorname{sgn}(\sigma) \operatorname{sgn}(\sigma') \left(\vec{\phi}(x_{\sigma(1)}) \otimes \dots \otimes \vec{\phi}(x_{\sigma(k)}),\ \left(\overline{M^{-1}}\vec{\phi}\right)(x_{\sigma'(1)}) \otimes \dots \otimes \left(\overline{M^{-1}}\vec{\phi}\right)(x_{\sigma(k)}) \right)$$

$$= \frac{1}{k!} \sum_{\sigma,\sigma' \in S_k} \operatorname{sgn}(\sigma) \operatorname{sgn}(\sigma') \prod_{i=1}^{k} \left(\vec{\phi}(x_{\sigma(i)}),\ \overline{M^{-1}}\vec{\phi}(x_{\sigma'(i)}) \right) \qquad (73)$$

$$= \sum_{\sigma \in S_k} \operatorname{sgn}(\sigma) \prod_{i=1}^{k} \Bigg(\underbrace{\sum_{\alpha\beta=1}^{n} \overline{\phi_\alpha(x_{\sigma(i)})}\, \overline{\left(M^{-1}\right)}_{\alpha\beta}\, \phi_\beta(x_i)}_{\sum_{\alpha\beta=1}^{n} A_{i,\beta} \left(M^{-1}\right)_{\beta\alpha} \left(A^*\right)_{\alpha,\sigma(i)} = \left(A M^{-1} A^*\right)_{i,\sigma(i)}} \Bigg)$$

$= \det\left(A^{(k)} M^{-1} (A^{(k)})^* \right)$. This proves (ii).

(iii) Let $\phi_i'(X) = \phi(X)\, k(x_i)$ and consider (74)

$$\sum_{i=1}^{n} \langle \phi_i, \phi_i \rangle = \sum_{i=1}^{n} \int |\phi(X)|^2 \, d(x_2 \ldots x_n)\, |k(x_1)|^2 \, dx_1$$

$$= \det(M) \underbrace{\binom{n}{1}^{-1}}_{\frac{n!}{(n-1)!}} \sum_{i=1}^{n} \int \underbrace{\rho_\phi^{(1)}(x)}_{\left(\vec{\Phi}(x),\, \overline{M^{-1}}\, \vec{\phi}(x)\right)} |k(x)|^2 \, dx$$

$$= \det(M) \sum_{\alpha\beta=1}^{n} \underbrace{\int \overline{\phi_\alpha(x)}\, \overline{(M^{-1})}_{\alpha\beta}\, \phi_\beta(x)\, |k(x)|^2}_{\overline{(M^{-1})}_{\alpha\beta} K_{\alpha\beta} = (M^{-1})_{\beta\alpha} K_{\alpha\beta}}$$

$= \det(M)\, \mathrm{tr}\left(M^{-1} K \right)$. This proves (iii), and therewith the Lemma.

∎

Let us use Lemma 2 to derive an appropriate upper bound for (II) in (40). With $G_n(X) \le 1$, we see that for fixed Y,

$$\int \left[|\nabla_X F(X,Y)|^2 + \tfrac{1}{2} V_{XY} F(X,Y)^2 \right] D_n(X)^2 G_n(X)^2 \, dX$$

$$\le \int \left[|\nabla_X F(X,Y)|^2 + \tfrac{1}{2} V_{XY} F(X,Y)^2 \right] D_n(X)^2 \, dX = (*) . \qquad (75)$$

We also have $$\nabla_{x_i} F(X,Y) = \nabla_{x_i} \prod_{l=1}^{n} \prod_{j=1}^{m} f_R(x_l - y_j) \qquad (76)$$

$$= \left(\nabla_{x_i} \prod_{j=1}^{m} f_R(x_i - y_j) \right) \prod_{\substack{l=1 \\ l \neq i}}^{n} \prod_{j=1}^{m} f_R(x_l - y_j)$$

$$= \left[\sum_{k=1}^{m} \nabla f_R(x_i - y_k) \prod_{\substack{j=1 \\ j \neq k}}^{m} f_R(x_i - x_j) \right] \frac{F(X,Y)}{\prod_{j=1}^{m} f_R(x_i - y_j)}$$

$$= \left[\sum_{k=1}^{m} \frac{\nabla f_R(x_i - y_k)}{f(x_i - y_k)} \right] \prod_{j=1}^{m} f_R(x_i - y_j) \; \frac{F(X,Y)}{\prod_{j=1}^{m} f_R(x_i - y_j)}$$

$$= F(X,Y) \sum_{k=1}^{m} \frac{\nabla f_R(x_i - y_k)}{f_R(x_i - y_k)} .$$

$$\Rightarrow (*) = \sum_{i=1}^{n} \int \Big\{ \Big[\big|\nabla_{x_i} F(X,Y)\big|^2 + \frac{1}{2} \sum_{j=1}^{m} V(x_i - y_j) \, \big|F(X,Y)\big|^2 \Big\} D_n(x) \, dX$$

$$= \sum_{i=1}^{n} \int D_n^2(x) \big|F(X,Y)\big|^2 \Big\{ \sum_{k,l=1}^{m} \frac{\nabla f_R(x_i - y_k) \cdot \nabla f_R(x_i - y_l)}{f_R(x_i - y_k) \, f_R(x_i - y_l)} + \frac{1}{2} \sum_{j=1}^{m} V(x_i - y_j) \Big\} \, dX \qquad (77)$$

$$= \sum_{i=1}^{n} \int D_n^2(x) \prod_{j=1}^{n} |h(x_j)|^2 \, \frac{|k(x_i)|^2}{|h(x_i)|^2} \, dX \, ,$$

where h and k are defined by

$$h(x) = \prod_{j=1}^{m} f(x - y_j) \quad \text{and} \qquad (78)$$

$$k(x) = \sqrt{ \Big| \nabla_x \prod_{j=1}^{n} f(x - y_j) \Big|^2 + \frac{1}{2} \sum_{j=1}^{m} v(x - y_j) \prod_{k=1}^{m} f(x - y_k)^2 } \, .$$

When we apply Lemma 2,(iii) to the right-hand side (r.h.s.) of (77), we find

$$(*) = \mathrm{tr}\big[K_Y M_Y^{-1}\big] \int D_n(x)^2 \, |F(X,Y)|^2 \, dX. \qquad (79)$$

The matrices M_Y and K_Y are defined by

$$\left(\mathbb{U}_Y\right)_{\alpha\beta} = \int_{[0,\ell]^3} \overline{\phi_\alpha(x)}\,\phi_\beta(x)\,|h(x)|^2\,dx \quad \text{and} \tag{80}$$

$$\left(K_Y\right)_{\alpha\beta} = \int_{[0,\ell]^3} \overline{\phi_\alpha(x)}\,\phi_\beta(x)\,|k(x)|^2\,dx,$$

where by $\{\phi_\alpha\}_{\alpha=1}^n$ we have denoted the first n eigenfunctions of the Dirichlet Laplacian in $[0,\ell]^3$ (as before in case of degeneracy any choice does the job).

We note that the matrices $\mathbb{U}_Y$ and K_Y are both positive definite (check!). This allows us to bound (81)

$$\operatorname{tr}\left[K_Y\,\mathbb{U}_Y^{-1}\right] \leq \|\mathbb{U}_Y^{-1}\|\,\operatorname{tr}\left[K_Y\right], \longleftarrow \boxed{\text{Exercise: Prove this if you have not seen it before.}}$$

where $\|\circ\|$ denotes the operatornorm defined by

$$\|A\| = \sup_{\|v\|=1} \|Av\|. \tag{82}$$

To continue we need a bound for the two terms on the r.h.s. of (81). Note that we can assume that all the y_i's are separated by at least a distance δ, because the integrand of (II) in (40) vanishes otherwise.

Let us define $\xi(x) = |\nabla f(x)|^2 + \frac{1}{2} v(x) |f(x)|^2.$ (83)

Since $s \geq 2R$ by assumption, we have

$$|Q_y(x)|^2 = \left| \nabla_x \prod_{j=1}^{m} f(x-y_j) \right|^2 + \frac{1}{2} \sum_{k=1}^{m} v(x-y_k) \prod_{j=1}^{m} f(x-y_j)^2 \qquad (84)$$

$$= \sum_{j=1}^{m} \xi(x-y_j).$$

Let $\rho_n^D(x)$ be the one-particle density of $D_n(X)$, that is,

$$\rho_n^D(x) = n \int |D_n(x, x_2 \ldots x_n)|^2 \, d(x_2 \ldots x_n) \qquad (85)$$

Lemma 2,(ii)
$h \equiv 1 \Rightarrow M_{\alpha\beta} = \delta_{\alpha\beta}$

$$= (\vec{\phi}(x), \vec{\phi}(x)) = \sum_{\alpha=1}^{n} |\phi_\alpha(x)|^2.$$

In combination, (84) and (85) imply

$$\operatorname{tr} K_y = \sum_{\alpha=1}^{n} \int |\phi_\alpha(x)|^2 |Q_y(x)|^2 \, dx \qquad (86)$$

$$= \sum_{\alpha=1}^{n} \sum_{j=1}^{m} \int |\phi_\alpha(x)|^2 \xi(x-y_j) \, dx$$

$$= \sum_{j=1}^{m} \int \rho_n^D(x) \xi(x-y_j) \, dx = \sum_{j=1}^{m} \rho_n^D \overset{\substack{\text{Convolution} \\ \downarrow}}{*} \xi(y_j).$$

To bound $\|\mathcal{U}_y^{-1}\|$ we need the following Lemma.

Lemma 3: Assume that $|y_i - y_j| \geq S \geq 2R$ for all $i \neq j$. Then

$$\|1 - \mathcal{U}_y\| \leq \text{const.} \left(\frac{aR^2}{S^3} + n^{2/3} \frac{S^2}{\ell^2} \right). \tag{87}$$

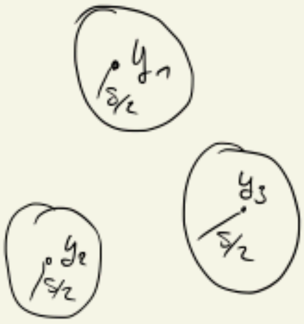
Proof: Let $b \in \mathbb{C}^n$ with components $\{b_\alpha\}_{\alpha=1}^n$, define
$q(x) = 1 - \prod_{j=1}^m f(x-y_j)^2 \geq 0$ and consider

$$(b, (1-\mathcal{U}_y)b) = \sum_\alpha |b_\alpha|^2 - \sum_{\alpha\beta} \overline{b_\alpha} b_\beta \int \overline{\phi_\alpha(x)} \phi_\beta(x) \prod_{j=1}^m f(x-y_j)^2 dx$$

$$= \int q(x) \left| \sum_\alpha b_\alpha \phi_\alpha(x) \right|^2 dx . \tag{88}$$

Let us interpret $q(x)$ as an external potential and $\sum_\alpha b_\alpha \phi_\alpha(x)$ as a wavefunction with a bound on the kinetic energy that follows from the fact that $\{\phi_\alpha\}_{\alpha=1}^n$ are the first n eigenfunctions of the Dirichlet Laplacian in $[0,\ell]^3$. Then we have transformed the question to finding a bound on the maximal potential energy of such a wave function in the potential q. In view of (51) the kinetic energy of $\sum_\alpha b_\alpha \phi_\alpha$ is certainly bounded from above by a constant times $n^{2/3} \ell^{-2}$, that is, the Fermi energy for n particles. Recall that the chemical potential μ is of that order.

Let B_j denote the ball of radius $\delta/2$ around y_j. By assumption these balls are not overlapping. Since $\delta \geq 2R$ we have $q(x) = 0$ if x is an element of the complement of $\bigcup_{j=1}^{m} B_j$.



For a given function $\phi(x)$ denote by

$$\phi_j = \frac{1}{|B_j|} \int_{B_j} \phi(x)\, dx \qquad (89)$$

the average of ϕ in B_j and let $\eta(x) = \phi(x) - \phi_j$.

We have

$$\int_{B_j} q(x) |\underset{\substack{\downarrow \\ \eta(x)+\phi_j}}{\phi(x)}|^2 dx \overset{\substack{(a+b)^2 \leq 2(a^2+b^2) \\ \downarrow}}{\leq} 2 \int_{B_j} q(x) |\eta(x)|^2 dx + 2\, |\phi_j|^2 \int_{B_j} q(x)\, dx \qquad (90)$$

as well as

$$\frac{\delta^3}{8} \frac{4\pi}{3} = \frac{\delta^3 \pi}{6}$$

$$|\phi_j|^2 = \frac{1}{|B_j|^2} \int_{B_j \times B_j} \phi(x) \phi(y)\, d(x,y) \overset{\substack{\text{Cauchy-Schwarz} \\ \downarrow}}{\leq} \frac{1}{\underbrace{|B_j|}_{\frac{4\pi}{3}(\delta/2)^3}} \int_{B_j} |\phi(x)|^2 dx \qquad (91)$$

$$= \frac{6}{\pi \delta^3} \int_{B_j} |\phi(x)|^2 dx.$$

Since $s \geq R$,

$$\int_{B_j} q(x)\,dx = \int_{\mathbb{R}^3} \left(1-f(x)^2\right)dx \overset{\substack{(45)\text{ Dilute Bose gas}\\ \downarrow}}{\leq} 4\pi a R^2. \tag{92}$$

Note that $\eta(x)$ is a function whose average over the ball B_j is zero. In the next step we need the following version of the Poincaré inequality:

(Poincaré inequality): Let $\Omega \subset \mathbb{R}^n$ be a bounded connected open set that has the cone property for some Θ, r. Let $1 \leq p < \infty$ and let $1 \leq q \leq \frac{np}{n-p}$ when $p<n$, $q < \infty$ when $p=n$, and $1 \leq q \leq \infty$ when $p>n$. Let g be a function in $L^{p'}(\Omega)$ $\left(\frac{1}{p'}+\frac{1}{q}=1\right)$ with $\int_\Omega g(x)dx = 1$. Then there is a finite number $S>0$, which depends on Ω, q, p such that for any $f \in H^{1,p}(\Omega)$

$$\left\| f - \int_\Omega f(x)g(x)\,dx \right\|_{L^q(\Omega)} \leq S \, \|\nabla f\|_{L^p(\Omega)}. \tag{93}$$

Proof: See Lieb/Loss Theorem 8.11./8.12.

We use $q(x) \le 1$, the Poincaré inequality and the fact that η is orthogonal to the constant function to see that

$$\int_{B_j} q(x)|\eta(x)|^2dx \le \int_{B_j} |\eta(x)|^2dx \underset{\substack{\uparrow \\ \text{Holder}}}{\le} \left(\int_{B_j} dx\right)^{2/3}\left(\int_{B_j}|\eta(x)|^6dx\right)^{1/3}$$

$$\underset{\substack{\nearrow \\ \text{Poincaré} \\ q=6,\ p=2,\ n=3}}{\le} \text{const.}\, \delta^2 \int_{B_j} |\nabla\eta(x)|^2dx \tag{94}$$

$$= \text{const.}\, \delta^2 \int_{B_j} |\nabla\phi(x)|^2dx.$$

Let us sum over the balls:

$$\int q(x)|\phi(x)|^2dx = \sum_{j=1}^{m} \int_{B_j} q(x)|\phi(x)|^2dx \overset{\substack{(90),(91),(92),(94) \\ \downarrow}}{\le} \text{const.}\, \delta^2 \int |\nabla\phi(x)|^2dx$$

$$+\, 2\cdot 4\pi a R^2\left(\frac{6}{\pi\delta^3}\right)^2 \int |\phi(x)|^2dx$$

$$\le \text{const.}\left[\delta^2 \underbrace{\int|\nabla\phi(x)|^2dx}_{\text{By assumption } \le \text{ const. } n^{2/3}\ell^{-2}.} + \frac{aR^2}{\delta^3}\underbrace{\int|\phi(x)|^2dx}_{=1 \text{ by assumption}}\right] \tag{95}$$

(To bound the relevant operator norm we only need to consider functions with norm 1.)

This proves the claim. ∎

Since $0 \le \mathcal{M}_Y \le 1$ in the sense of operators $\left(\Leftrightarrow 0 \le (\psi, \mathcal{M}_Y \psi) \le 1 \;\; \forall \psi \right)$, we have

$$\| \mathcal{M}_Y^{-1} \| = \frac{1}{1 - \| 1 - \mathcal{M}_Y \|} \overset{\substack{\text{Lemma 3} \\ \downarrow}}{\le} A_n = \frac{1}{1 - \text{const.} \left[\frac{a R^2}{S^3} + n^{2/3} (S/\ell)^2 \right]} , \qquad (86)$$

provided the denominator is positive. We insert (86) and (86) into (79) and obtain

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \tfrac{1}{2} V_{XY} |F(X,Y)|^2 \right] dX \qquad (87)$$

$$\le A_n \sum_{j=1}^{m} \rho_n^D * \xi(y_j) \int D_n(X)^2 F(X,Y)^2 \, dX .$$

To be able to compare the r.h.s. of (87) with $\langle \psi, \psi \rangle$ we have to put $G_n(X)^2$ back into the integrand. For this purpose we need the following Lemma, which compares the integrals with and without the factor $G_n(X)^2$.

Lemma 4: For any fixed Y we have

$$\int D_n(X)^2 F(X,Y)^2 G_n(X)^2 \, dX \ge \int D_n(X)^2 F(X,Y)^2 \, dX \qquad (88)$$

$$\times \left[1 - \text{const.}\, n^{8/3} \| \mathcal{M}_Y^{-1} \|^2 (S/\ell)^5 \right].$$

Proof: Since $g(x) = 1$ for $|x| \geq 2s$, we have

$$G_n(X)^2 = \prod_{1\le i<j\le n} g(x_i-x_j)^2 \underset{\substack{\uparrow \\ \text{Lemma, Chapter 2} \\ \text{p.17}}}{\geq} 1 - \sum_{1\le i<j\le n} \mathbb{1}\left(|x_i-x_j| \le 2s\right). \qquad (99)$$

To evaluate the second term on the r.h.s. of (99) in the relevant integral, we need the two-particle density of the state $D_n(X)\,F(X,Y)$, that is,

$$\rho^{(2)}_{D_nF}(x,x') = \binom{n}{2} \frac{\int D_n(x,x',x_3\ldots x_n)^2\, F(x,x',x_3\ldots x_n;Y)^2\, d(x_3\ldots x_n)}{\int D_n(X)^2\, F(X,Y)^2\, dX} \qquad (100)$$

$h(x) = \prod_{j=1}^{m} f(x-y_j)$, Lemma 2

$$\overset{\downarrow}{=} \frac{1}{2} \underbrace{|h(x)|^2 |h(x')|^2}_{\le 1 \text{ because } f \le 1} \Big(\vec{\phi}(x) \wedge \vec{\phi}(x'),\ \underset{\downarrow}{M_Y^{-1}} \otimes M_Y^{-1}\, \vec{\phi}(x) \wedge \vec{\phi}(x') \Big)$$

$$(M_Y)_{\alpha\beta} = \int \overline{\phi_\alpha(x)}\, \phi_\beta(x)\, |h(x)|^2 dx$$

$$\le \|M_Y^{-1}\|^2 \underbrace{\tfrac{1}{2}\Big(\vec{\phi}(x) \wedge \vec{\phi}(x'),\ \vec{\phi}(x) \wedge \vec{\phi}(x') \Big)}$$

$\rho_n^{D,(2)}(x,x')$ = two-particle density of $D_n(X)$.

We claim that $\rho_n^{D,(2)}(x,x') \le \text{const.}\, |x-x'|^2 \left(n/\ell^3\right)^{8/3}$ holds for some constant independent of ℓ and n (Check!).

Hence,

$$\int D_n(X)^2 F(X,Y)^2 G_n(X)^2 dX \tag{101}$$

$$\geq \int D_n(X)^2 F(X,Y)^2 dX - \underset{n(n-1)}{\nearrow} \underbrace{\int D_n(X)^2 F(X,Y)\, 1\!\!1(|x_1-x_2| \leq 2s)\, dX}$$

$$\geq -\tfrac{1}{2} \| \mathcal{U}_Y^{-1} \|^2 \int \rho_n^{D,(2)}(x,x')\, 1\!\!1(|x-x'| \leq 2s)\, d(x,x')$$

$$\geq -\text{const.}\ \| \mathcal{U}_Y^{-1} \|^2 \underbrace{\int |x-x'|^2 \left(n/\ell^3\right)^{8/3} 1\!\!1(|x-x'| \leq 2s)\, d(x,x')}_{\text{const.}\ \frac{n^{8/3}}{\ell^8} s^5 \ell^3}$$

$$\geq \int D_n(X)^2 F(X,Y)^2 dX - \text{const.}\ \| \mathcal{U}_Y^{-1} \|^2 n^{8/3} (s/\ell)^5$$

$$\geq \int D_n(X)^2 F(X,Y)^2 dX \left(1 - \text{const.}\ \| \mathcal{U}_Y^{-1} \|^2 n^{8/3} (s/\ell)^5 \right)$$

$\blacksquare$

This proves the claim.

Remark: It is the n-dependence in the error term in (98) that forces us to introduce the small boxes with a controllable particle number.

Note also the exponent 5 in Eq. (58), which comes from the fact that the two-particle density vanishes as $|x-x'|^2$ for x close to x'. Had we not taken this into account, we would get an error term of the order $n^2(\delta/\ell)^3$. Since necessarily $\delta > a$ this error would be huge if $n \gg (a^3\rho)^{-1}$, which is demanded by Eq. (55).

Let us combine (57) with Lemma 4. We find

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \tfrac{1}{2} V_{XY} F(X,Y)^2 \right] D_m(Y)^2 G_m(Y)^2 \, d(X,Y) \tag{102}$$

$$\leq A_n \sum_{j=1}^{m} \int \rho_n^D * \xi(y_j)\, D_n^2(X) F(X,Y)^2 D_m(Y)^2 G_m(Y)^2 \, d(X,Y)$$

$$\leq A_n \frac{\sum_{j=1}^{m} \int \rho_n^D * \xi(y_j)\, D_n^2(X) G_n^2(X) F(X,Y)^2 \cdots \qquad d(X,Y)}{\left[1 - \text{const.}\, n^{8/3} \|\mathcal{U}_Y^{-1}\|^2 (\delta/\ell)^5 \right] \longleftarrow =: B_n^{-1}}$$

$$= A_n B_n \sum_{j=1}^{n} \int \rho_n^D * \xi(y_i)\, D_n^2(X) G_n^2(X) F(X,Y)^2 D_m^2(Y) G_m^2(Y) \, d(X,Y)$$

Next, we do similar estimates for the Y integration, use $|G_m(Y)| \leq 1$, Lemma 3 and Lemma 4 and find

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \tfrac{1}{2} v_{XY} F(X,Y)^2 \right] D_m(Y)^2 G_m(Y)^2 \, d(X,Y) \tag{103}$$

$$\leq A_n B_n B_m \int D_n^2(X) G_n^2(X) F(X,Y)^2 D_m^2(Y) G_m^2(Y) \, \mathrm{tr}\left[\hat{K}_X \mathbb{M}_X^{-1}\right] d(X,Y).$$

The matrix $\mathbb{M}_X$ is the same as before, with Y replaced by X and n replaced by m, and $\hat{K}_X$ is the $m \times m$ matrix with components

$$\left(\hat{K}_X\right)_{\alpha\beta} = \int \overline{\phi_\alpha(y)} \phi_\beta(y) \prod_{i=1}^{n} f(y-x_i)^2 \rho_n^D * \xi(y) \, dy . \tag{104}$$

We use $|f(x)| \leq 1$ and $\|\mathbb{M}_Y^{-1}\| \overset{\text{Lemma 3}}{\leq} A_m$ and the fact that the x_i's are separated at least by a distance S to see that

$$\mathrm{tr}\, \hat{K}_X \mathbb{M}_Y^{-1} \leq A_m \underbrace{\mathrm{tr}\, \hat{K}_X}_{\sum_{\alpha=1}^{m} \underbrace{\int |\phi_\alpha(y)|^2}_{= \rho_m^D(y)} \underbrace{\prod_{i=1}^{n} f(y-x_i)^2}_{\leq 1} \rho_n^D * \xi(y) \, dy} \overset{|f| \leq 1}{\leq} A_m \int \rho_n^D(x) \xi(x-y) \rho_m^D(y) \, d(x,y). \tag{105}$$

We recall that $\int \xi(y) \, dy = \int \left\{ |\nabla f(y)|^2 + \frac{1}{2} v(x) |f(y)|^2 \right\} dy = \dfrac{4\pi a}{1 - a/R}$.

Using this and Young's inequality we show that

Young's inequality: Let $p,q,r \geq 1$ and $\frac{1}{p}+\frac{1}{q}+\frac{1}{r}=2$. Let $f \in L^p(\mathbb{R}^n)$, $g \in L^q(\mathbb{R}^n)$ and $h \in L^r(\mathbb{R}^n)$. Then

$$\left| \int_{\mathbb{R}^n} f(x)\, g(x-y)\, h(y)\, d(x,y) \right| \leq C_{p,q,r,n} \, \|f\|_p \, \|g\|_q \, \|h\|_r$$

See Lieb/Loss Analysis, Theorem 4.2.

$$\operatorname{tr} \hat{K}_x M_y^{-1} \leq A_m \left(\int \rho_n^D(x)^2 dx \right)^{1/2} \left(\int \rho_m^D(y)^2 dy \right)^{1/2} \frac{4\pi a}{1-a/R} . \quad (106)$$

When we write $\rho^D(x)^2$ in terms of plane waves we see that

$$\int \rho_n^D(x)^2 dx = \frac{1}{\ell^3} \sum_{p,q} \prod_{a=1}^{3} \left(1 + \frac{1}{2} \delta_{p_a,q_a} \right), \quad (107)$$

where p_a denotes the components of the wave vector p and the sums are over the n lowest eigenstates of the Dirichlet Laplacian. Using (107) we check that

$$\int \rho_n^D(x)^2\,dx \le \frac{n^2}{\ell^3}\left(1+\text{const.}\, n^{-1/3}\right). \quad \left(\text{Exercise}\right) \qquad (108)$$

Eq. (103) therefore implies the bound

$$\int G_n(X)^2 D_n(X)^2\left[|\nabla_X F(X,Y)|^2+\tfrac{1}{2}v_{XY}\,F(X,Y)^2\right]D_m(Y)^2 G_m(Y)^2\,d(X,Y)$$

$$\le \langle\Psi,\Psi\rangle\,\frac{4\pi a n m}{\ell^3(1-c/R)}A_nA_mB_nB_m\left(1+\text{const.}\,n^{-1/3}\right)\left(1+\text{const.}\,m^{-1/3}\right). \qquad (109)$$

The same bound holds with X and Y replaced, and we thus obtain

$$(\text{II}) \le \langle\Psi,\Psi\rangle\,\frac{8\pi a n m}{\ell^3(1-c/R)}A_nA_mB_nB_m\left(1+\text{const.}\,n^{-1/3}\right)\left(1+\text{const.}\,m^{-1/3}\right). \qquad (110)$$

It remains to bound the term (III). This term can be estimated with similar techniques than (II). Since it does not contribute to the leading order the analysis is a little simpler.

We have

$$(\text{III}) \le \langle\Psi,\Psi\rangle\,\text{const.}\times\left(n^{8/3}+m^{8/3}\right)\frac{s^3}{\ell^5}. \qquad (111)$$

For a proof of this see Eqs. (42) – (44) in the reference on the first page (the red one) of this Chapter.

Putting our results together, we have shown that there exists a constant $C>0$ (independent of the parameters) such that

$$\begin{aligned} E_0^F(n,m,\ell) \leq \frac{3}{5}\left(6\pi^2\right)^{2/3} \frac{n^{5/3}+m^{5/3}}{\ell^2}\left(1+Cn^{-1/3}+Cm^{-1/3}\right) \qquad (112) \\ +8\pi a \frac{nm}{\ell^3}\Big(1+\varepsilon+C\Big[\frac{aR^2}{s^3}+(n+m)^{2/3}(s/\ell)^2+\frac{a}{R} \\ +n^{-1/3}+m^{-1/3}+(n+m)^{8/3}(s/\ell)^5\Big]\Big) \\ +\frac{Cs}{\varepsilon}\frac{(n+m)^2}{\ell^3}\left[(n+m)^{2/3}(s/\ell)^2\right]. \end{aligned}$$

To obtain (112) we have assumed that the error terms are small, which will be fulfilled for small $\rho^{1/3}a$ by our choice of R, s, n, m and ℓ.

The optimal choice for ε in the above equation is

$$\varepsilon^2 = \text{const.}\,(n+m)^{8/3}\, s^3 \big/ (\ell^2 a n m) \tag{113}$$

and yields the bound

$$\begin{aligned} E_0(n,m,\ell) \le{}& \frac{3}{5}(6\pi^2)^{2/3}\,\frac{n^{5/3}+m^{5/3}}{\ell^2}\left(1 + Cn^{-1/3} + Cm^{-1/3}\right) \\ &+ 8\pi a \frac{nm}{\ell^3}\left(1 + C\left[\frac{aR^2}{s^3} + (n+m)^{2/3}(s/\ell)^2 + \frac{a}{R} + n^{-1/3} + n^{-1/3} \right.\right. \\ &\qquad\qquad \left.\left. + (n+m)^{8/5}(s/\ell)^5\right]\right) \\ &+ C\,(n+m)^{7/3}\,\frac{s^{3/2}a^{1/2}}{\ell^4}\,. \end{aligned} \tag{114}$$

The optimal choice of R, s and ℓ turns out to be

$$R = a\left(a\rho^{1/3}\right)^{-2/9}, \quad s = 2R, \quad \ell = \rho^{-1/3}\left(a\rho^{1/3}\right)^{-11/9} \tag{115}$$

and implies the final upper bound

$$\boxed{\begin{aligned} \underset{\substack{\uparrow \\ \text{(needs to be replaced} \\ \text{by } (\ell+R_0)^3)}}{\frac{1}{\ell^3}}\, E_0^{\mp}(n,m,\ell) \le{}& \frac{3}{5}(6\pi^2)^{2/3}\left[\rho_1^{5/3} + \rho_2^{5/3}\right] + 8\pi a \rho_1\rho_2 \\ &+ \text{const.}\; a\rho^2\left(a\rho^{1/3}\right)^{2/9} \end{aligned}}\,. \tag{116}$$

This concludes the proof of the upper bound.

5. Lower bound for the ground state energy

The proof of the lower bound for E_0^F will be split into three parts. In the first part we state an improved version of the Dyson Lemma. This is necessary because we need a sufficient amount of kinetic energy to built up the Fermi sea, which would not be possible to obtain with the version of the Dyson Lemma we used for the Bose gas. In the second part we establish properties that any approximate minimizer of the energy necessarily has. In the third and final part we use the Dyson Lemma and these estimates to prove the desired lower bound for E_0^F.

For the lower bound we choose Dirichlet boundary conditions for the Laplacian in the definition of H_N.

5.1 Dyson Lemma

We recall that $\hat{f}(k) = \left(\frac{1}{2\pi}\right)^{3/2} \int f(x)\, e^{-ikx}\, dx$. The following Lemma is a generalization of the Dyson Lemma we used in the case of the Bose gas. This time we keep certain low momentum modes in the kinetic energy to built up the Fermi sea and only use the high momentum modes to obtain the softer and longer ranged potential U with the scattering length in front. Here high momentum means of the order $1/a$ while low momentum means smaller than or equal to $\rho^{1/3}$.

Lemma 5 (Dyson Lemma): For $R > R_0$ let $\mathbb{1}(|x| \leq R)$ be the characteristic function of the ball of radius R centered at the origin. Let $\chi(p)$ be a radial function, $0 \leq \chi(p) \leq 1$, such that $h(x) = \overset{\leftarrow \text{ inverse Fourier transform}}{\widecheck{(1-\chi)}}(x)$ is bounded and integrable. Let

$$f_R(x) = \sup_{|y| \leq R} |h(x-y) - h(x)| \tag{117}$$

and

$$w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{\mathbb{R}^3} f_R(y)\,dy. \qquad (118)$$

Then for any positive radial function $\mathcal{U}(x)$, supported in the annulus $\{x\in\mathbb{R}^3 \mid R_0 \le |x| \le R\}$ with $\int_{\mathbb{R}^3} \mathcal{U}(x)dx \le 4\pi$, and for any $\varepsilon>0$,

$$-\nabla \chi(p)\, \mathbb{1}(|x|\le R)\, \chi(p) \nabla + \tfrac{1}{2}V(x) \geq (1-\varepsilon)\, a\, \mathcal{U}(x) - \frac{a}{\varepsilon} w_R(x). \qquad (119)$$

Here, $\mathbb{1}(|x|\le R)$ is a multiplication operator in x-space, whereas $\chi(p)$ is a multiplication operator in momentum space. Thus, $\nabla\chi(p)\,\mathbb{1}(|x|\le R)\,\chi(p)\nabla$ is an operator version of ∇^2, which is cut-off in both configuration and momentum space.

Remark. The original version of the Dyson Lemma has $\chi(p)\equiv 1$ and $w_R(x)\equiv 0$. The cutoff $\chi(p)$ in (119) essentially says that only the high-momentum part of ∇ is needed to give a good account of the scattering of two particles. The (relatively) low-momentum part of ∇ is not used in (119) and is thereby saved for later use to give a good estimate of the part of the kinetic energy needed to fill the Fermi sea. The price we pay is the error term $a\omega_R(x)/\varepsilon$, which does not appear in the original version of the Dyson Lemma. If $\chi(p)\equiv 1$ then $\omega_R(x)\equiv 0$ and we recover the original version of the Dyson Lemma.

As in case of the Bose gas we need a many-particle version of the Dyson Lemma, which we state in the form of a Corollary.

<u>Corollary 1</u>: If $y_1 \cdots y_N$ are N points in $\mathbb{R}^3$, with $|y_i-y_j|\geq 2R$ for all $i\neq j$, then, as an operator on functions of x,

$$-\nabla\chi(p)\nabla + \frac{1}{2}\sum_{i=1}^{N} v(x-y_i) \geq \sum_{i=1}^{N}\Big((1-\varepsilon)a\,U(x-y_i) - \frac{a}{\varepsilon}\omega_R(x-y_i)\Big). \tag{120}$$

<u>Proof</u>: The Corollary follows from the Dyson Lemma using translation invariance of the relevant operators and the fact that

$$\sum_{i=1}^{N} \mathbb{1}\big(|x-y_i|\leq R\big) \leq 1, \tag{121}$$

which follows since by the assumption the balls are not overlapping.

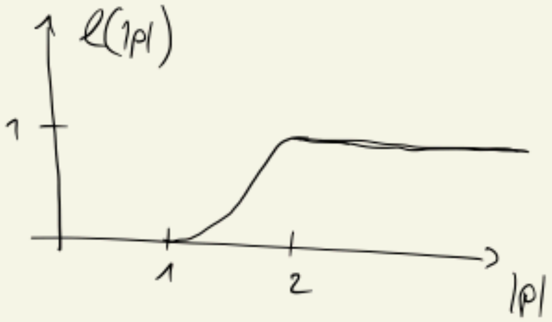
▨

We will not prove the generalized Dyson Lemma here. If you are interested you can find its proof in [DFG] in the Appendix (See cover page of this Chapter for the reference. A link to the paper can be found on the course webpage.)

We apply the corollary with the cut-off function

$$\chi_s(p) = \ell(sp) , \tag{122}$$

where ℓ denotes a smooth, radial, positive function with $\ell(p) = 0$ for $|p| \leq 1$, $\ell(p) = 1$ for $|p| \geq 2$, and $0 \leq \ell(p) \leq 1$ in between.



For this choice of $\chi_s(p)$ the corresponding function

$u(x) = (\widehat{1-\chi_S})(S)$ is a smooth function that decays faster than any inverse power. Accordingly, by scaling $\omega_R(x)$ satisfies for $R \leq \text{const.} S$ the bounds

$$|\omega_R(x)| \leq \text{const.} \frac{R^2}{S^5}, \qquad \int |\omega_R(x)|\, dx \leq \text{const.} \frac{R^2}{S^2} \tag{123}$$

for some constants only depending on the function ℓ. Moreover, if $|y_i - y_j| \geq 2R$ for all $i \neq j$, then

$$\sum_{i=1}^{N} \omega_R(x-y_j) \leq \text{const.} \frac{1}{RS^2} \tag{124}$$

independent of x and N. Later we are going to choose $R \ll S \ll \varrho^{-1/3}$.

5.2. A priori bounds

Let $N_1, N_2, N \in \mathbb{N}$ with $N_1+N_2=N$ and let $\Psi_N(X,Y)$ be a sequence of normalized wave functions that is separately antisymmetric in the X and the Y coordinates. As $N\to\infty$ we assume that $N_1/L^3 \to \rho_1$, $N_2/L^3 \to \rho_2$ and denote $\rho = \rho_1+\rho_2$. Let the one-particle density matrices γ_1 and γ_2 be defined by

$$\gamma_1(x,x') = N_1 \int \Psi(x, x_2 \dots x_{N_1}; Y)\overline{\Psi(x', x_2 \dots x_N; Y)}\, d(x_2 \dots x_{N_1}, Y),$$

$$\gamma_2(y,y') = N_2 \int \Psi(X, y, y_2 \dots y_{N_2})\Psi(X, y', y_2 \dots y_{N_2})\, d(X, y_2 \dots y_{N_2}).$$

Moreover let P_μ denote the following spectral projection of the Laplacian with periodic boundary conditions on $[0,L]^3$, given by the integral kernel:

$$P_\mu(x,x') = \frac{1}{L^3} \sum_{\substack{p \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |p| \le (6\pi^2 M/L^3)^{1/3}}} e^{ip(x-x')}. \qquad (125)$$

Intermezzo (Definition of the trace for positive Operators on a separable Hilbert space):

Let $\mathcal{H}$ be a separable Hilbert space, $\{\varphi_n\}_{n=1}^{\infty}$ an orthonormal basis, and define for any positive bounded operator A on $\mathcal{H}$ its trace by $\operatorname{tr} A = \sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle$. The trace of A has has the following properties:

(a) $\operatorname{tr} A$ is independent of the choice of basis

(b) $\operatorname{tr} A \in \mathbb{R}_+ \cup \{0\} \cup \{+\infty\}$

(c) $\operatorname{tr}(A+B) = \operatorname{tr} A + \operatorname{tr} B$

(d) $\operatorname{tr} \lambda A = \lambda \operatorname{tr} A$ for all $\lambda \geq 0$

(e) $\operatorname{tr} \mathcal{U}A\mathcal{U}^{-1} = \operatorname{tr} A$ for any unitary $\mathcal{U}$. $\mathcal{U}$ is called unitary if $\langle \mathcal{U}\psi, \mathcal{U}\varphi \rangle = \langle \psi, \varphi \rangle$ for all $\psi, \varphi \in \mathcal{H}$.

(f) If $0 \leq A \leq B$, then $\operatorname{tr} A \leq \operatorname{tr} B$.

(g) $\operatorname{tr} AB = \operatorname{tr} BA$ if $\operatorname{tr} A < +\infty$ and B bounded.

To prove the above statement, we need the square root lemma (see Reed, Simon 1 (Functional analysis, Theorem IV.5)).

<u>Square root lemma</u>: Let $A \geq 0$ be a bounded operator. Then there is a unique bounded operator $B \geq 0$ with $B^2 = A$.

Remark: B can be defined via the power series of the square root.

To prove (a) let $\{\psi_m\}_{m=1}^{\infty}$ be another orthonormal basis and consider

$$\mathrm{tr}_\varphi A = \sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle = \sum_{n=1}^{\infty} \langle A^{1/2}\varphi_n, A^{1/2}\varphi_n \rangle$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \langle A^{1/2}\varphi_n, \psi_m \rangle \langle \psi_m, A^{1/2}\varphi_n \rangle$$

$A \geq 0$ implies A s.a.

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \langle A^{1/2}\psi_m, \varphi_n \rangle \langle \varphi_n, A^{1/2}\psi_m \rangle$$

Sum over positive terms $\Rightarrow$ interchanging sums is OK

$$= \sum_{m=1}^{\infty} \langle \psi_m, A\psi_m \rangle.$$

This proves (a). (b)-(g) are straight forward.

☒

The trace has the same properties for operators A with

$$\operatorname{tr}(A^*A)^{1/2} < +\infty,$$

see Reed, Simon 1 (Functional analysis, Section VI.6). For such operators we write $A \in \mathcal{J}_1$.

If $A \in \mathcal{J}_1$ has an integral kernel (all such operators do although we will not discuss this), then

$$\operatorname{tr} A = \int A(x,x)\, dx.$$

If you are not familiar with these things I recommend some reading. You can also discuss this issue with me.

By scaling $\mathrm{tr}[P_\mu]$ does not depend on L and we have

$$\lim_{\mu\to\infty} \frac{1}{\mu} \mathrm{tr}\left[P_\mu\right] = 1. \qquad (126)$$

In the following two lemmas we prove a-priori bounds for wave functions satisfying certain energy bounds (from the upper bound we know that such functions exist). These lemmas, in particular, apply to the true ground state.

<u>Lemma 6</u>: Assume that, in the thermodynamic limit $N\to\infty$, $L\to\infty$ with $\rho_i = N_i/L^3$ fixed, there is a sequence of states $\Psi_N(X,Y)$ such that

$$\limsup_{L\to\infty} \frac{1}{L^3} \langle \Psi_N, H_N \Psi_N \rangle \leq \frac{3}{5}\left(6\pi^2\right)^{2/3}\left[\rho_1^{5/3} + \rho_2^{5/3}\right] + Ca\rho^2 \qquad (127)$$

for some $C>0$ independent of ρ. Then for $i=1,2$

$$\limsup_{L\to\infty} \frac{1}{L^3} \mathrm{tr}\left[\gamma_i\left(1-P_{N_i}\right)\right] \leq \text{const.} \times \rho\sqrt{a\rho^{1/3}}. \qquad (128)$$

<u>Proof</u>: We immediately have the trivial lower bound for

for noninteracting fermions $(V \geq 0)$

$$\liminf_{L\to\infty} \frac{1}{L^3} \langle \Psi_N, H_N \Psi_N \rangle \geq \frac{3}{5}(6\pi^2)^{2/3}\left[\varrho_1^{5/3} + \varrho_2^{5/3}\right]. \qquad (129)$$

To prove (128), however, we need the following refinement:

$$\liminf_{L\to\infty} \frac{1}{L^3} \langle \Psi_N, (-\Delta_x - \Delta_y)\Psi_N \rangle \qquad (130)$$

$$\geq \frac{3}{5}(6\pi^2)^{2/3} \limsup_{L\to\infty}\Big[\varrho_1^{5/3}\left(1 + \text{const.}\ \zeta_1^2\right) + \varrho_2^{5/3}\left(1 + \text{const.}\ \zeta_2^2\right)\Big],$$

where $\zeta_i = N_i^{-1}\,\mathrm{tr}\left[\gamma_i(1-P_{N_i})\right]$ for $i = 1,2$. Using (130), $V \geq 0$ and (127) we easily check that (128) holds. It remains to prove (130).

We consider the case of the Laplacian acting on the X variables and denote $\gamma = \gamma_1$ and $P = P_{N_1}$ for simplicity. Denote

$$\delta(\gamma, P) = \mathrm{tr}\left[\gamma(1-P)\right] \qquad (131)$$

and consider for $\alpha \geq 0$

$$\underbrace{\langle \Psi_N, \sum_{i=1}^{N_1} -\Delta_i \Psi_N \rangle} - \alpha\, \mathcal{S}(\gamma, P) = (*) \tag{132}$$

$$= N_1 \int \left[-\Delta_x \Psi(x, x_2 \dots x_{N_1}, Y) \right) \Psi(x, x_2 \dots x_{N_1}, Y)\, d(x_2 \dots x_{N_1}, Y)\, dx$$

$$= \int \left[-\Delta_x \gamma_1(x, x') \right]_{x = x'} dx$$

$$\frac{1}{L^{3/2}} e^{ipx}$$

$$= \mathrm{tr}\left[-\Delta \gamma_1 \right] = \sum_{p \in \frac{2\pi}{L} \mathbb{Z}^3} \langle \varphi_p, -\Delta \gamma_1 \varphi_p \rangle = \sum_{p \in \frac{2\pi}{L} \mathbb{Z}^3} p^2\, u(p)$$

with $u(p) = \langle \varphi_p, \gamma_1 \varphi_p \rangle$. Note that $0 \leq u(p) \leq 1$ and $\mathrm{tr}\, \gamma_1 = N_1$. We also have

$$\mathcal{S}(\gamma, P) = \sum_{|p| > p_F} u(p) \quad \text{with} \quad p_F = \left(6\pi^2 \rho_1 \right)^{1/3}. \tag{133}$$

Accordingly,

$$(*) = \sum_{p \in \frac{2\pi}{L} \mathbb{Z}^3} \left(p^2 - \alpha \mathbb{1}\left(|p| > p_F \right) \right) u(p) \tag{134}$$

$$\geq \inf_{\substack{0 \leq u(p) \leq 1 \\ \sum_p u(p) = N_1}} \left\{ \sum_{p \in \frac{2\pi}{L} \mathbb{Z}^3} \left(p^2 - \alpha \mathbb{1}\left(|p| > p_F \right) \right) u(p) \right\}.$$

Next we write

$$\sum_p \left(p^2 - \alpha \mathbb{1}\left(|p| > p_F\right)\right) u(p) = \sum_p \left(p^2 - \alpha \left(\mathbb{1} - \mathbb{1}\left(|p| \le p_F \right)\right)\right) u(p)$$

$$= \sum_p \left(p^2 - p_F^2 + \alpha \mathbb{1}(|p| \le p_F)\right) u(p) \qquad (135)$$

$$+ \left(p_F^2 - \alpha\right) N_1 .$$

We insert (135) into (134) and obtain

$$(*) = \underbrace{\inf_{\substack{0 \le u(p) \le 1 \\ \sum_p u(p) = N_1}} \left\{ \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \left(p^2 - p_F^2 + \alpha \mathbb{1}\left(|p| \le p_F \right)\right) u(p) \right\}} + \left(p_F^2 - \alpha\right) N_1 \qquad (136)$$

When we drop the restriction $\sum_p u(p) = N_1$ we obtain a lower bound. With the remaining constraint $0 \le u(p) \le 1$, the minimizer of the above minimization problem is given by

$$u(p) = \mathbb{1}\left(p^2 - p_F^2 + \alpha \mathbb{1}\left(|p| \le p_F\right) \le 0 \right)$$

$$= \mathbb{1}\left(p^2 - p_F^2 + \alpha \le 0 \right)$$

$$\ge \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \left[p^2 - p_F^2 + \alpha \right]_- + \left(p_F^2 - \alpha\right) N_1, \quad \text{where } [x]_- = \min\{x, 0\}.$$

Since we are interested in the thermodynamic limit, we can compute the sum (up to terms that do not grow proportionally to L^3) by an integral. We have

$$\sum_{|p|\le\sqrt{p_\mp^2-\alpha}} \left(p^2-p_\mp^2+\alpha\right) = \frac{L^3}{(2\pi)^3}\int_{|p|\le\sqrt{p_\mp^2-\alpha}} \left(p^2-p_\mp^2+\alpha\right) dp + o(L^3) \qquad (137)$$

$$= \frac{L^3}{10\pi^2}\left[p_\mp^2-\alpha\right]_+^{5/2} + \frac{L^3}{6\pi^2}\left(-p_\mp^2+\alpha\right)\left[p_\mp^2-\alpha\right]_+^{3/2} + o(L^3)$$

Assume that $p_\mp^2-\alpha\ge 0$

$$= \frac{L^3}{\pi^2}\left(\frac{1}{10}-\frac{1}{6}\right)\left[p_\mp^2-\alpha\right]^{5/2} + o(L^3) = -\frac{L^3}{15\pi^2}\left(p_\mp^2-\alpha\right)^{5/2} + o(L^3).$$

For (*) this implies

$$(*) \ge -\frac{L^3}{15\pi^2}\left(p_\mp^2-\alpha\right)^{5/2} + \left(p_\mp^2-\alpha\right)N_1. \qquad (138)$$

Next, we write our bound as

$$\left\langle \Psi_N, \sum_{i=1}^{N_1} -\Delta_i \Psi_N \right\rangle - \frac{3L^3}{5}(6\pi^2)^{2/3}\rho^{5/3} - \alpha\, S(\gamma,P) \qquad (139)$$

$$\ge -\frac{L^3}{15\pi^2}\left(p_\mp^2-\alpha\right)^{5/2} - \frac{3}{5}\frac{L^3}{6\pi^2}p_\mp^5 + \left(p_\mp^2-\alpha\right)N_1 + o(L^3),$$

where we have used that

$p_F^2 = (6\pi^2 \varrho)^{2/3} \iff p_F = (6\pi^2 \varrho)^{1/3} \iff \varrho = p_F^3 \, \frac{1}{6\pi^2}$, and therefore

$$\underline{\underline{\frac{3}{5}(6\pi^2)^{2/3} \varrho^{5/3}}} = \frac{3}{5}(6\pi^2)^{2/3}\left(p_F^3 \, \frac{1}{6\pi^2}\right)^{5/3} = \underline{\underline{\frac{3}{5}\, \frac{1}{6\pi^2}\, p_F^5}}. \tag{140}$$

We also write $N_1 = L^3 \frac{1}{6\pi^2} \mu_1^{3/2} = \frac{L^3}{6\pi^2} p_F^3$ in the term proportional to N_1 in (139). Hence,

$$\left\langle \Psi_N, \sum_{i=1}^{N_1} -\Delta_i \Psi_N \right\rangle - \frac{3L^3}{5}(6\pi^2)^{2/3} \varrho^{5/3} - \alpha\, \mathcal{S}(\varrho, P) \tag{141}$$

$$\geq -\frac{L^3}{6\pi^2}\left\{ \frac{2}{5}\left(p_F^2 - \alpha\right)^{5/2} + \frac{3}{5} p_F^5 - p_F^5 + \alpha\, p_F^3 \right\} + o(L^3)$$

$$= -\frac{L^3}{6\pi^2}\left\{ \frac{2}{5}\left(p_F^2 - \alpha\right)^{5/2} - \frac{2}{5} p_F^5 + \alpha\, p_F^3 \right\} + o(L^3)$$

$$\left[\frac{2}{5}\left(p_F^2 - \alpha\right)^{5/2} = \frac{2}{5} p_F^5 - p_F^3 \alpha + \frac{1}{2}\, \frac{3}{2}\left(p_F^2 - \alpha'\right)^{1/2} \alpha^2 \quad \text{for some } 0 \leq \alpha' \leq \alpha \right]$$

↑ Second order Taylor approx. with remainder

$$= -\frac{L^3}{6\pi^2}\, \frac{3}{4}\left(p_F^2 - \alpha'\right)^{1/2} \alpha^2 + o(L^3) \geq -\frac{L^3}{6\pi^2} \frac{3}{4} p_F\, \alpha^2 + o(L^3).$$

For $0 \leq \alpha \leq p_F^2$ we have shown:

$$\left\langle \Psi_N, \sum_{i=1}^{N} -\Delta_i \Psi_N \right\rangle \geq \frac{3L^3}{5} (6\pi^2)^{2/3} \rho^{5/3} + \alpha\, \delta(\gamma,P) - \frac{L^3}{6\pi^2} \frac{3}{4} p_F \alpha^2 + o(L^3). \tag{142}$$

We note that $\delta(\gamma,P) \geq 0$.

Optimize : $\frac{1}{2}\alpha\delta = \frac{1}{6\pi^2}\frac{3}{4} L^3 \overset{(6\pi^2\rho_1)^{1/3}}{\overset{\uparrow}{p_F}} \alpha^2$ (Keep $\frac{1}{2}\alpha\delta$)

$$\Leftrightarrow \alpha = \frac{2}{3} 6\pi^2 \underbrace{\frac{\delta}{L^3}}_{\leq \rho_1} \frac{1}{p_F}$$

→ (Fulfills $p_F^2 - \alpha \geq 0$ because $\delta \leq N$)

$$\leq \frac{2}{3} (6\pi^2)^{2/3} \rho_1^{2/3} = \frac{2}{3} p_F^2$$

This implies

$$\boxed{\frac{\left\langle \Psi_N, \sum_{i=1}^{N} -\Delta_i \Psi_N \right\rangle}{L^3} \geq \frac{3}{5} (6\pi^2)^{2/3} \rho^{5/3} + \text{const.}\, \rho^{-1/3} \left(\frac{\delta(\gamma,P)}{L^3} \right)^2}, \tag{143}$$

which is the bound we were looking for (see Eq. 130).

In particular, this finishes the proof of Lemma 6. ▨

The second a-priori bound concerns the nearest neighbor distance among particles. For given points $y_1 \cdots y_{N_2} \in \mathbb{R}^3$, let $J_R(y_1 \cdots y_{N_2})$ be the number of y_i's with the property that the distance to the nearest neighbor among the other y_i's is less than $2R$.

Lemma 7: Assume that there exists a constant $C>0$, independent of $\rho = N/L^3$, such that

$$\frac{1}{N} \langle \Psi_N, H_N \Psi_N \rangle \leq C \rho^{2/3}. \qquad (144)$$

Then

$$\langle \Psi_N, J_R(y_1, \dots, y_{N_2}) \Psi_N \rangle \leq \text{const.} \times N \left(R^3 \rho\right)^{2/3}. \qquad (145)$$

Proof: Let S_i denote the distance of the coordinate y_i to its nearest neighbor among the coordinates y_j with $j \neq i$. We have

$$J_R(y_1 \cdots y_{N_2}) \leq (2R^2) \sum_{i=1}^{N_2} \frac{1}{S_i^2}. \qquad (146)$$

To prove the claim we use the following bound from Lieb, Yau, "The stability and instability of relativistic matter", Communications in Mathematical Physics 118, 177–213 (1988) (see Theorem 5 therein)

$$\sum_{i=1}^{N_2} \frac{1}{\delta_i^2} \leq \text{const.} \sum_{i=1}^{N_2} -\Delta_i \,, \tag{147}$$

which holds in the sense of operators. We combine (144), (146), (147) and $V \geq 0$ to prove the claim. ☒

<u>Remark 1</u>: If you are interested in the proof of (147) and you have no access to the reference please let me know.

<u>Remark 2</u>: Let us consider (147) in the special case $N_2 = 2$ to get some intuition. The full case is a many-particle version of what we discuss here. In the $N_2 = 2$ we will also assume that the particles live in $\mathbb{R}^3$ to keep the discussion simple. We need to show that

$$\frac{1}{|x_1 - x_2|^2} \leq \text{const.} \left(-\Delta_1 - \Delta_2 \right) \tag{148}$$

holds. To that end, we introduce relative and center-of-mass coordinates

$$r = x_1 - x_2 \quad \text{and} \quad R = \frac{x_1 + x_2}{2} \qquad (149)$$

with related momenta

$$p_r = \frac{p_1 - p_2}{2} \quad \text{and} \quad P_R = p_1 + p_2 . \qquad (150)$$

Eq. (148) reads

$$\frac{1}{r^2} \leq \text{const.} \left(\overset{P_R^2/2}{\overset{\downarrow}{\frac{-\Delta_R}{2}}} - \overset{2p_r^2}{\overset{\downarrow}{2\Delta_r}} \right). \qquad (151)$$

The statement now follows from Hardy's inequality (see e.g. wikipedia) in the form

Note that this holds for all f, that is, we do not need the antisymmetry of the wave function for $N_2 = 2$. For $N_2 \geq 3$ it is needed, however.

$$\int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|^2} dx \leq \overset{\swarrow}{4} \int_{\mathbb{R}^3} |\nabla f(x)|^2 dx , \qquad (152)$$

where 4 is the best possible constant. Since $-\Delta_R \geq 0$ and $\frac{-\Delta_R}{2} - 2\Delta_r = -\Delta_{x_1} - \Delta_{x_2}$ this proves (148). Eq. (147) is a many-particle version of (148) for particles in a box described by antisymmetric wave functions.

5.3. Putting it together

We can neglect the interaction between the X-particles and between the Y-particles for a lower bound, that is, we have

$$H_N \geq \Big(-\overset{\overset{\text{Dirichlet boundary conditions}}{\swarrow}}{\Delta}_X + \frac{1}{2} V_{XY} \Big) + \Big(-\overset{\downarrow}{\Delta}_Y + \frac{1}{2} V_{XY} \Big). \qquad (153)$$

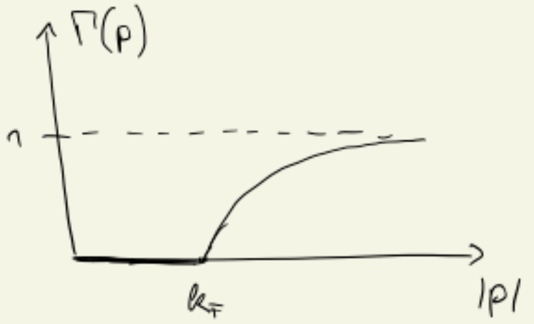
In the following we will use the Dyson Lemma and the a-priori bounds from the previous section to prove a lower bound for the first term on the r.h.s. of (153). The second term can be estimated in the same way.

We start by decomposing the kinetic energy into low and high momentum modes. Let

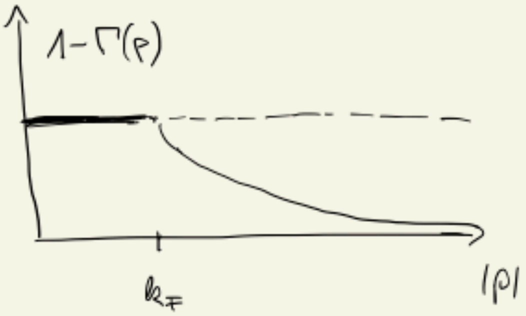
$$\Gamma(p) = \max\Big\{ 1 - \frac{k_F^2}{p^2}, 0 \Big\} \qquad (154)$$

with $k_F = (6\pi^2 \rho)^{1/3}$ and write the Laplacian as

$$\Delta = \nabla \Gamma(p) \nabla + \nabla (1 - \Gamma(p)) \nabla. \qquad (155)$$



high momentum part



low momentum part

For the low momentum part of the Laplacian we claim that

$$\sum_{i=1}^{N_1} -\nabla_i\left(1-\Gamma(p_i)\right)\nabla_i \geq \frac{3}{5}\left(6\pi^2\right)^{2/3}\frac{N_1^{5/3}}{L^2} \qquad (156)$$

holds. Note that the inequality has to be understood in the sense that the left and right-hand side are tested with functions in $L^2_a([0,L]^{3N_1})$ that satisfy Dirichlet boundary conditions. Let us prove this claim.

We know that the left-hand side of (156) is minimized by a Slater determinant. Let $\{\phi_i\}_{i=1}^{N_1}$ be a set of orthonormal functions and denote by Ψ the related Slater determinant. The l.h.s. of (156) tested with Ψ reads

$$\langle \Psi, \sum_{i=1}^{N_1} -\nabla_i \left(1-\Gamma(p)\right)\nabla_i \Psi \rangle = \sum_{i=1}^{N_1} - \langle \phi_i, \nabla \left(1-\Gamma(p)\right) \nabla \phi_i \rangle$$

$$= \sum_{i=1}^{N_1} \int_{\mathbb{R}^3} p^2 \left[1-\Gamma(p)\right] |\hat{\phi}_i(p)|^2 dp, \qquad (157)$$

where $\hat{\phi}_i(p) = \left(\frac{1}{2\pi}\right)^{-3/2} \int_{[0,L]^3} e^{-ipx} \phi_i(x) dx$. Note that this is nothing but the Fouriertransform on $\mathbb{R}^3$ if one extends ϕ_i outside the cube by 0 (this is reasonable because $\phi_i \big|_{\partial[0,L]^3} \equiv 0$).

Since the functions $\phi_i(x)$ are orthonormal, we have that

$$\sum_{i=1}^{N_1} |\hat{\phi}_i(p)|^2 = \left(\frac{1}{2\pi}\right)^3 \sum_{i=1}^{N_1} \langle e^{ipx}, \phi_i \rangle \langle \phi_i, e^{ipx} \rangle \qquad (158)$$

$$\leq \left(\frac{1}{2\pi}\right)^3 \langle e^{ipx}, e^{ipx} \rangle = \left(\frac{L}{2\pi}\right)^3.$$

Additionally,

$$\int \sum_{i=1}^{N_1} |\hat{\phi}_i(p)|^2 dp = N_1. \qquad (159)$$

Eq. (158), (159) and (157) motivate the bound

$$\left\langle \Psi, \sum_{i=1}^{N_1} -\nabla_i \left(1-\Gamma(p)\right)\nabla_i \Psi \right\rangle \tag{160}$$

$$\geqslant \inf_{\substack{\int \xi(p)dp = N_1 \\ 0 \leq \xi(p) \leq \left(\frac{L}{2\pi}\right)^3}} \int_{\mathbb{R}^3} p^2 \left[1-\Gamma(p)\right] \xi(p) \, dp.$$

Since $p^2[1-\Gamma(p)]$ is a monotonically increasing function of $|p|$, the above infimum is attained by

$$\xi(p) = \mathbb{1}\left(|p| \leq \left(\frac{6\pi^2 N_1}{L^3}\right)^{1/3}\right). \quad \text{(Check!)} \tag{161}$$

It remains to compute

$$\int_{\mathbb{R}^3} \underbrace{p^2\left[1-\Gamma(p)\right]} \, \mathbb{1}\left(|p| \leq \left(\frac{6\pi^2 N_1}{L^3}\right)^{1/3}\right) dp \tag{162}$$

$$= \begin{cases} p^2 & \text{if } |p| \leq k_F = (6\pi^2 \rho)^{1/3} \\ k_F^2 & \text{if } |p| > k_F \end{cases} \qquad \Bigg| \quad \frac{N_1}{L^3} \leq \frac{N_1+N_2}{L^3} = \rho$$

$$= \frac{3}{5}\left(6\pi^2\right)^{2/3} \frac{N_1^{5/3}}{L^2}.$$ This proves (156).

Remark 1: Please note the similarity of this argument and the one in the proof of Lemma 6.

Remark 2: Note that the above technique can be used to prove lower bounds for the sum of the first N eigenvalues of an operator (this is what we do here).

To treat the high momentum part we use that

$$\Gamma(p) \geq \left(1 - s^2 k_F^2\right) \chi_s^2(p) \qquad (163)$$

for any $s \leq \frac{1}{k_F}$, with χ_s defined in (122). Hence, we can use corollary 1 to get a lower bound on this term. In order to apply the corollary, however, we have to make sure that the y_j's are separated at least a distance $2R$. Let $\tilde{Y} \subset Y$ be the set of y_j's whose distance to the nearest neighbor is at least $2R$. Note that, by definition, $|\tilde{Y}| = N_2 - J_R(Y)$. We are going to neglect the interaction with y_j's that are not in the set $\tilde{Y}$, which can only lower the energy. Hence, we obtain, for a given configuration of Y,

$$\sum_{i=1}^{N_1} -\nabla_i \Gamma(p) \nabla_i + \frac{1}{2} \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} V(x_i - y_j) \geqslant \left(1 - \delta^2 k_F^2\right) \sum_{i=1}^{N_1} W_Y(x_i), \qquad (164)$$

with

$$W_Y(x) = \sum_{\{j \,|\, y_j \in \tilde{Y}\}} \left(\left(1-\varepsilon\right) a\, \mathcal{U}(x - y_j) - \frac{a}{\varepsilon} w_R(x - y_j) \right), \qquad (165)$$

depending on ε, a, R, and δ.

A convenient choice for $\mathcal{U}(x)$ is (as in case of the Bose gas)

$$\mathcal{U}(x) = \begin{cases} 3\left(R^3 - R_0^3\right)^{-1} & \text{for } R_0 \leq |x| \leq R, \\ 0 & \text{otherwise.} \end{cases} \qquad (166)$$

Now let $\Psi_N(X,Y)$ be a normalized fermionic wave function. We can express the expectation value of $\sum_i W_Y(x_i)$ as

$$\left\langle \Psi_N, \sum_{i=1}^{N_1} W_Y(x_i) \Psi_N \right\rangle = \int n_Y \operatorname{tr}\left[\gamma_Y W_Y\right] dY, \qquad (167)$$

where
$$n_Y = \int |\Psi_N(X,Y)|^2 dX \qquad (168)$$

and γ_Y denotes the one-particle density matrix of $\Psi_N(X,Y)$ for fixed Y, that is,

$$\gamma_Y(x,x') = \frac{N_1}{n_Y}\int \Psi_N(x,x_2\ldots x_{N_1},Y)\overline{\Psi_N(x',x_2\ldots x_{N_1},Y)}\,d(x_2\ldots x_{N_1}). \qquad (169)$$

We claim that $0 \leq \gamma_Y \leq 1$, $\mathrm{tr}\,\gamma_Y = N_1$, $\int n_Y\, dY = 1$ and $\int n_Y \gamma_Y\, dY = \gamma_1$. The first claim follows because for almost every Y, γ_Y denotes the 1-pdm (one-particle density matrix) of a fermionic wave function. The other properties follow immediately.

Let P be an orthogonal projection ($P^* = P$, $P^2 = P$) on the one-particle Hilbert space and let γ be any fermionic 1-pdm.

↙ Pauli principle

That is, $0 \leq \gamma \leq 1$ and $\mathrm{tr}[\gamma] = N_1$, see e.g. Lieb, Seiringer, "The stability of matter in quantum mechanics", Cambridge University press, Chapter 3.1.5. Reduced density matrices.

Also let W_+, W_- be two positive operators and denote $W = W_+ - W_-$. For any $\delta > 0$, we claim that

$$\mathrm{tr}\left[\gamma W\right] = \mathrm{tr}\left[PW\right] + \mathrm{tr}\left[(\gamma-1)PWP\right] + \mathrm{tr}\left[\gamma\,(1-P)WP)\right]$$

$$+ \mathrm{tr}\left[\gamma\Big(PW(1-P)\Big)\right] + \mathrm{tr}\left[\gamma\Big((1-P)W(1-P)\Big)\right] \qquad (170)$$

$$\geq \mathrm{tr}\left[PW_+\right](1-\delta) - \mathrm{tr}\left[PW_-\right](1+\delta)$$

$$- \left(1+\delta^{-1}\right) \times \Big(\|W_+\| + \|W_-\| \Big)\, \mathrm{tr}\left[\gamma(1-P)\right] - \|W\|\, \mathrm{tr}\left[P(1-\gamma)\right],$$

with $\|\cdot\|$ denoting operator norm. This follows from

- $\mathrm{tr}\, PW = \mathrm{tr}\, PW_+ - \mathrm{tr}\, PW_- \qquad (171)$
- $$\mathrm{tr}\,\gamma(1-P)W(1-P) = \mathrm{tr}\left[(1-P)\gamma(1-P)\right]^{1/2}(W_+ - W_-)\left[(1-P)\gamma(1-P)\right]^{1/2}$$
  $$\geq -\mathrm{tr}\left[(1-P)\gamma(1-P)\right]^{1/2} W_-\left[(1-P)\gamma(1-P)\right]^{1/2}$$
  $$\geq -\|W_-\|\, \mathrm{tr}\,\gamma(1-P) \qquad (172)$$
- $$\mathrm{tr}\underbrace{(\gamma-1)}_{\leq 0}PWP \underset{\uparrow}{\geq} -\|W_+\|\, \mathrm{tr}\, P(1-\gamma) \qquad (173)$$

  argue as for the previous point

Intermezzo: Hilbert-Schmidt and trace norm

For an operator A denote $|A| = (A^*A)^{1/2}$. The trace norm of A is defined by $\|A\|_1 = \mathrm{tr}|A|$ and we have

$$|\mathrm{tr}A| \leq \|A\|_1 .$$

Similarly we define the Hilbert-Schmidt norm by $\|A\|_2 = (\mathrm{tr}A^*A)^{1/2}$. For two operators A and B we have

$$|\mathrm{tr}AB| \leq \|A\|_2 \|B\|_2 .$$

We also note that the trace norm bounds the Hilbert-Schmidt norm, more precisely

$$\|A\|_2 \leq \|A\|_1 .$$

Finally, we note that

$$\|AB\|_1 \leq \|B\| \, \|A\|_1 ,$$
$$\|AB\|_2 \leq \underset{\substack{\nearrow \\ \text{operator norm}}}{\|B\|} \, \|A\|_2 .$$

$$
\begin{aligned}
\cdot]\quad \mathrm{tr}\,\gamma(1-P)WP &= \mathrm{tr}\,P\gamma(1-P)W_+ - \mathrm{tr}\,P\gamma(1-P)W_- \\
&= \mathrm{tr}\,W_+^{1/2}P\gamma^{1/2}\gamma^{1/2}(1-P)W_+^{1/2} \qquad (174)\\
&\quad - \mathrm{tr}\,W_-^{1/2}P\gamma^{1/2}\gamma^{1/2}(1-P)W_-^{1/2}
\end{aligned}
$$

$$
\begin{aligned}
&\geq -\|W_+^{1/2}P\gamma^{1/2}\|_2 \, \|\gamma^{1/2}(1-P)W_+^{1/2}\|_2 \\
&\quad - \|W_-^{1/2}P\gamma^{1/2}\|_2 \, \|\gamma^{1/2}(1-P)W_-^{1/2}\|_2
\end{aligned}
$$

$$
\begin{aligned}
&\geq -\frac{\delta}{2}\|W_+^{1/2}P\gamma^{1/2}\|_2^2 - \frac{1}{2\delta}\|\gamma^{1/2}(1-P)W_+^{1/2}\|_2^2 \\
&\quad -\frac{\delta}{2}\|W_-^{1/2}P\gamma^{1/2}\|_2^2 - \frac{1}{2\delta}\|\gamma^{1/2}(1-P)W_-^{1/2}\|_2^2
\end{aligned}
$$

$$
\begin{aligned}
&= -\delta/2\,\mathrm{tr}\,P\gamma P W_+ - \frac{1}{2\delta}\,\mathrm{tr}\,(1-P)\gamma(1-P)W_+ \\
&\quad -\delta/2\,\underbrace{\mathrm{tr}\,P\gamma P W_-} - \frac{1}{2\delta}\,\mathrm{tr}(1-P)\gamma(1-P)W_-
\end{aligned}
$$

$$
= \mathrm{tr}\,(PW_-P)^{1/2}\underbrace{\gamma}_{\leq 1}(PW_-P)^{1/2} \leq \mathrm{tr}\,PW_-
$$

$$
\begin{aligned}
&\geq -\frac{\delta}{2}\,\mathrm{tr}\,PW_+ - \frac{\delta}{2}\,\mathrm{tr}\,PW_- - \frac{1}{2\delta}\|W_+\|\,\mathrm{tr}(1-P)\gamma \\
&\quad - \frac{1}{2\delta}\|W_-\|\,\mathrm{tr}(1-P)\gamma
\end{aligned}
$$

$$\uparrow$$

$\cdot]$ $\mathrm{tr}\,\gamma PW(1-P) \geq$ the same as before. (175)

Now let $P = P_{N_1}$ defined in Eq. (125) and $W = W_Y$. We choose W_+ to be the terms in (165) containing $\mathcal{U}(x)$ and W_- the ones containing $w_R(x)$. Using $\int \mathcal{U}(x)dx = 4\pi$, we then find

$$\mathrm{tr}\, P W_+ = (1-\varepsilon)\, a \sum_{\{j\,:\, y_j \in \tilde{Y}\}} \mathrm{tr}\left[P_{N_1} \mathcal{U}(x-y_j)\right] \qquad (176)$$

$$= \int P_{N_1}(x,x)\, \mathcal{U}(x-y_j)\, dx$$

kernel

$$= \frac{1}{L^3} \sum_{\substack{p \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |p| \leq \left(6\pi^2 N_1/L^3\right)^{1/3}}} e^{ip(x-x')}$$

$$= \frac{(1-\varepsilon)a}{L^3} \underbrace{\left(\sum_{\substack{p \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |p| \leq \left(6\pi^2 N_1/L^3\right)^{1/3}}} 1 \right)}_{= \mathrm{tr}\left[P_{N_1}\right]} \sum_{\underbrace{\{j\,:\, y_j \in \tilde{Y}\}}_{N_2 - J_R(Y)}} \int_{[0,L]^3} \mathcal{U}(x-y_j)\, dx$$

$$\geq \frac{\mathrm{tr}\left[P_{N_1}\right]}{L^3} (1-\varepsilon)\, 4\pi a \left[N_2 - J_R(Y) - \text{const.} \times \frac{L^2}{R^2} \right].$$

The last term in the square brackets bounds the number of y_j's in $\tilde{Y}$ that are at least a distance R away from the boundary of the box. Since the distance between the y_j's is bigger than $2R$ by assumption, the number of such y_j's close to the boundary of the box is bounded by a constant times L^2/R^2.

When we interpret the relevant sum as a Riemann sum, we check that

$$\frac{\operatorname{tr} P_{N_1}}{N_1} = \frac{\int_{[0,L]^3} P_{N_1}(x,x)\,dx}{N_1} = \frac{1}{N_1} \sum_{\substack{p \in \frac{2\pi}{L}\mathbb{Z}^3 \\ |p| \leq \left(6\pi^2 \frac{N_1}{L^3}\right)^{1/3}}} 1 \qquad (177)$$

$$\xrightarrow[\substack{N_1 \to \infty \\ L \to \infty \\ N_1/L^3 = \rho_1}]{} 1$$

in the thermodynamic limit. That is, we can replace $\operatorname{tr} P_{N_1}$ by N_1 in (176) at the expense of a correction that vanishes in the thermodynamic limit.

To estimate the term proportional to $J_R(Y)$ in (176) when inserted into (167) we note that

$$\int u_Y J_R(Y)\,dY = \langle \Psi_N, J_R(Y) \Psi_N \rangle. \qquad (178)$$

We can without loss of generality assume that

$$\frac{1}{N}\langle \Psi_N, H_N \Psi_N\rangle \leq 2\,\frac{3}{5}\,(6\pi^2)^{2/3}\,\rho^{2/3} \qquad (179)$$

holds, which allows us to apply Lemma 7 to estimate the term in (178). This is because if $N^{-1}\langle \Psi_N, H_N\Psi_N\rangle > 2\,\frac{3}{5}(6\pi^2)^{2/3}\,\rho^{2/3}$ then there is nothing to prove because the r.h.s. is larger than the lower bound we intend to show. Lemma 7 applied to (178) shows

$$\int u_Y\, J_R(Y)\, dY \leq \text{const. } N\,(R^3\rho)^{2/3}. \qquad (180)$$

Analogously, we see that

$$\begin{aligned} \operatorname{tr}[PW_-] &= \sum_{\{j:\, j\in\tilde{Y}\}} \frac{a}{\varepsilon}\, \operatorname{tr}\left[P_{N_1} w_R(x-y_j)\right] \qquad (181) \\ &= \frac{\operatorname{tr}[P_{N_1}]}{L^3}\, \underbrace{\sum_{\{j:\, j\in\tilde{Y}\}}}_{\leq N_2} \frac{a}{\varepsilon}\, \underbrace{\int_{[0L]^3} w_R(x-y_j)\, dx}_{\substack{\leq \text{ const. } R^2/\delta^2 \\ \uparrow (123)}} \\ &\leq \text{const. } \frac{aR^2}{\varepsilon\delta^2}\, \frac{N_2 \operatorname{tr}[P_{N_1}]}{L^3}. \end{aligned}$$

Moreover, using (124) and the fact that the distance between y_j's contributing to w_Y is at least $2R$, we find that

$$\|w_Y\| \le \underbrace{\|w_+\|}_{\le \frac{3a}{R^3-R_0^3}} + \underbrace{\|w_-\|}_{\underset{\overset{\uparrow}{(124)}}{\le} \text{const.}\,\frac{a}{\varepsilon}\frac{1}{R\delta^2}} \le \left(\frac{3a}{R^3-R_0^3} + \text{const.}\,\frac{a}{\varepsilon\delta^2 R}\right). \qquad (182)$$

The a-priori bound in Lemma 6 implies that, for large enough N,

$$\int u_Y \operatorname{tr}\left[\gamma_Y(1-P)\right] dY = \operatorname{tr}\left[\gamma_1(1-P)\right] \le CN\left(a^3\rho\right)^{1/6}, \qquad (183)$$

where γ_1 is the 1-pdm for the X particles of any approximate ground state in the sense that

$$\limsup_{L\to\infty}\left\langle \Psi_N, H_N\Psi_N\right\rangle \le \frac{3}{5}\left(6\pi^2\right)^{2/3}\left(\rho_1^{5/3}+\rho_2^{5/3}\right) + Ca\rho^2 \qquad (184)$$

for an appropriately chosen $C>0$. As before, the argument is (for a reasonable choice of C) that if (184) does not hold then there is nothing to prove, so we can restrict attention to such Ψ_N.

To see that the same bound is true for $\operatorname{tr}[P(1-\gamma_1)]$ we note that

$$\operatorname{tr}\left[P(1-\gamma_1)\right] = \underbrace{\operatorname{tr}\left[\gamma_1(1-P)\right]}_{\substack{\le C N (a^3\rho)^{1/6} \\ \uparrow \\ (183)}} + \underbrace{\operatorname{tr}\left[P-\gamma_1\right]}_{} \tag{185}$$

$$= \operatorname{tr}P - \underbrace{\operatorname{tr}\gamma_1}_{=N_1}$$

$$= \underbrace{\frac{\operatorname{tr}P}{N_1}}_{\substack{\to 1 \text{ in thermodynamic limit} \\ \nearrow \\ (177)}} N_1 - N_1 \overset{\uparrow}{\to} 0$$

$$\le \text{const.}\ N \left(a^3\rho\right)^{1/6}.$$

When we collect our estimates and use the same bound with X and Y interchanged for the second term on the r.h.s. of (153), we arrive at the lower bound

$$\lim_{\substack{L\to\infty \\ N_1\to\infty \\ N_2\to\infty \\ N_1/L^3=\rho_1 \\ N_2/L^3=\rho_2}} \frac{E_0^F(N_1,N_2,L)}{L^3} \geq \frac{3}{5}\left(6\pi^2\right)^{2/3}\left(\rho_1^{5/3}+\rho_2^{5/3}\right) + 8\pi a\rho_1\rho_2 \tag{186}$$

$$\times\left(1-\varepsilon-\delta-s^2\left(6\pi^2\rho\right)^{2/3} - \text{const.}\ \frac{R^2}{\varepsilon s^2}\right)$$

$$-\text{const.}\ a\rho^2\left(R^3\rho\right)^{2/3} - \text{const.}\ \rho\left(a^3\rho\right)^{\frac{1}{6}}\left(1+\frac{1}{s}\right)$$

$$\times\left(\frac{a}{R^3-R_0^3}+\frac{a}{\varepsilon s^2 R}\right).$$

The optimal choice of the parameters is

$$R = \rho^{-1/3}\left(a\rho^{1/3}\right)^{\frac{3}{26}}, \quad \delta = \rho^{-1/3}\left(a\rho^{1/3}\right)^{\frac{1}{26}}, \quad \varepsilon = s = \left(a\rho^{1/3}\right)^{\frac{1}{13}}. \qquad (187)$$

We thus obtain the lower bound

$$\lim_{\substack{L\to\infty \\ N_1\to\infty \\ N_2\to\infty \\ N_1/L^3 = \rho_1 \\ N_2/L^3 = \rho_2}} \frac{E_0^F(N_1,N_2,L)}{L^3} \geq \frac{3}{5}\left(6\pi^2\right)^{2/3}\left(\rho_1^{5/3} + \rho_2^{5/3}\right) + 8\pi a \rho_1\rho_2 \qquad (188)$$

$$- \text{const.}\ a\rho^2\left(a\rho^{1/3}\right)^{\frac{1}{13}}.$$

This finishes the proof of the lower bound. In combination with the upper bound in (116), (188) proves the Theorem on page 8 and 10. It also ends our discussion of the dilute Fermi gas.