

Notes on 1D bosons

Johannes Agerskov

Dated: December 9, 2021

We consider the dilute Bose gas in one dimension, where we seek to prove the formula for the ground state energy

$$\frac{E}{L} = \frac{\pi^2}{3} \rho^3 (1 + 2\rho a + o(\rho)). \quad (0.1)$$

We assume that the interaction potential v has compact support, say in the ball of radius R_0 , B_{R_0} .

1 Upper bound

1.1 Periodic boundary conditions

We provide the upper bound for (0.1), by using the variational principle with a suitable trial state. We assume for simplicity periodic boundary conditions to begin with. Consider the trial state

$$\Psi(x) = \begin{cases} \omega(\mathcal{R}(x)) \frac{\tilde{\Psi}_F(x)}{\sin(\frac{\pi}{L}\mathcal{R}(x))} & \text{if } \mathcal{R}(x) < b, \\ \tilde{\Psi}_F(x) & \text{if } \mathcal{R}(x) \geq b, \end{cases} \quad (1.1)$$

where ω is the suitably normalized solution to the two-body scattering equation, *i.e.* $\omega(x) = f(x) \frac{\sin(\frac{\pi}{L}b)}{f(b)}$ where f is any solution of the two-body scattering equation and $b \geq R_0$. $\tilde{\Psi}_F(x) = \mathcal{N}^{1/2} \prod_{i < j}^N \sin(\frac{\pi}{L}|x_i - x_j|)$ is the absolute value of the free fermionic ground state, and $\mathcal{R}(x) = \min_{i < j}(|x_i - x_j|)$ is uniquely defined a.e.

The energy of this trial state is then

$$\mathcal{E}(\Psi) = \int \sum_{i=1}^N |\nabla_i \Psi|^2 + \sum_{i < j}^N v_{ij} |\Psi|^2, \quad (1.2)$$

where $v_{ij}(x) = v(x_i - x_j)$. Since v is supported in B_b and $\Psi = \tilde{\Psi}_F$ except in the region $B = \{x \in \mathbb{R}^N | \mathcal{R}(x) < b\}$, we may rewrite this as

$$\mathcal{E}(\Psi) = E_0 + \int_B \sum_{i=1}^N |\nabla_i \Psi|^2 + \sum_{i < j}^N v_{ij} |\Psi|^2 - \sum_{i=1}^N \left| \nabla_i \tilde{\Psi}_F \right|^2, \quad (1.3)$$

where $E_0 = N \frac{\pi^2}{3} \rho^2$ is the ground state energy of the free Fermi gas. Using that $v \geq 0$, symmetry of exchange of particles, and defining the set $B_{12} = \{x \in \mathbb{R}^N | \mathcal{R}(x) < b, \mathcal{R}(x) = |x_1 - x_2|\} \subset A_{12} = \{x \in \mathbb{R}^N | |x_1 - x_2| < b\}$ which up to a set of measure zero is the intersection of B and $\{1 \text{ and } 2 \text{ are closest}\}$, we find

$$\begin{aligned}
\mathcal{E}(\Psi) &= E_0 + \binom{N}{2} \int_{B_{12}} \sum_{i=1}^N |\nabla_i \Psi|^2 + \sum_{i < j}^N v_{ij} |\Psi|^2 - \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \\
&= E_0 + \binom{N}{2} \int_{B_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}|^2 + \sum_{i < j}^N v_{ij} |\tilde{\Psi}|^2 - \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \\
&= E_0 + \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}|^2 + \sum_{i < j}^N v_{ij} |\tilde{\Psi}|^2 - \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \\
&\quad - \binom{N}{2} \int_{A_{12} \setminus B_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}|^2 + \sum_{i < j}^N v_{ij} |\tilde{\Psi}|^2 - \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \\
&\leq E_0 + E_1 + \binom{N}{2} \int_{A_{12} \setminus B_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2
\end{aligned} \tag{1.4}$$

where we have defined

$$\tilde{\Psi} = \begin{cases} \omega(x_1 - x_2) \frac{\tilde{\Psi}_F(x)}{\sin(\frac{\pi}{L}|x_1 - x_2|)} & \text{if } |x_1 - x_2| < b, \\ \tilde{\Psi}_F(x) & \text{if } |x_1 - x_2| \geq b, \end{cases}$$

and $E_1 = \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}|^2 + \sum_{i < j}^N v_{ij} |\tilde{\Psi}|^2 - \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2$.

We may estimate

$$\begin{aligned}
\binom{N}{2} \int_{A_{12} \setminus B_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 &= \binom{N}{2} \left(2N \left[\int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 - \int_{B_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \right] \right. \\
&\quad \left. + \binom{N-2}{2} \left[\int_{A_{12} \cap A_{34}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 - \int_{B_{12} \cap A_{34}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \right] \right) \\
&\leq \binom{N}{2} \left[2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 + \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \right]
\end{aligned} \tag{1.5}$$

Thus we find

$$\mathcal{E}(\Psi) \leq E_0 + E_1 + E_2^{(1)} + E_2^{(2)} \tag{1.6}$$

with $E_2^{(1)} = \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2$ and $E_2^{(2)} = \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2$.

We notice that since $\tilde{\Psi}_F = |\Psi_F|$ so by the diamagnetic inequality we have $|\nabla_i \tilde{\Psi}_F| \leq |\nabla_i \Psi_F|$, which implies that $\tilde{\Psi}_F$ is in $H^1(\Lambda_L)$. Furthermore, Ψ_F is $C^1(\Lambda_L)$ with a zero set $\{\Psi_F = 0\}$ of measure zero, $|\nabla_i \tilde{\Psi}_F|^2$ and $|\nabla_i \Psi_F|^2$ are equal a.e. But then $|\nabla_i \tilde{\Psi}_F| = |\nabla_i \Psi_F|$ as $L^2(\Lambda_L)$ functions. Hence we may replace $\tilde{\Psi}_F$ with Ψ_F in all integrals above.

1.1.1 Reduced density matrices

We recall briefly the definition of the reduced density matrices, as we will use some fact about these frequently in the subsequent calculations. For an N -(identical)particle state Ψ , the n -particle reduced density matrix is defined by

$$\gamma^{(n)}(x_1, \dots, x_n; y_1, \dots, y_n) = \frac{N!}{(N-n)!} \int \overline{\Psi(x_1, \dots, x_N)} \Psi(y_1, \dots, y_N) dx_{n+1} \dots dx_N. \quad (1.7)$$

For a determinant state $\Psi = \det(u_i(x_j))$ with u_i orthonormal states, the one-particle reduced density matrix is given by

$$\gamma^{(1)}(x, y) = \sum_{i=1}^N \overline{u_i(x)} u_i(y). \quad (1.8)$$

The n -particle reduced density matrix may be expressed in terms of creation and annihilation operators as

$$\gamma^{(n)}(x_1, \dots, x_n; y_1, \dots, y_n) = \left\langle a_{x_1}^\dagger \dots a_{x_n}^\dagger a_{y_n} \dots a_{y_1} \right\rangle. \quad (1.9)$$

For the groundstate of a free Hamiltonian (or any quasi free state), Wick's theorem applies and n -particle reduced density matrix of the Fermi groundstate may be computed recursively by

$$\left\langle c_{x_1}^\dagger \dots c_{x_n}^\dagger c_{y_n} \dots c_{y_1} \right\rangle = \sum_{i=1}^n (-1)^{i-1} \left\langle c_{x_1}^\dagger c_{y_i} \right\rangle \left\langle c_{x_2}^\dagger \dots c_{x_n}^\dagger c_{y_n} \dots c_{y_{i+1}} c_{y_{i-1}} \dots c_{y_1} \right\rangle. \quad (1.10)$$

For the Fermi ground state with periodic boundary conditions, we also have

$$\begin{aligned} \gamma^{(1)}(x, y) &= \left\langle c_x^\dagger c_y \right\rangle = \frac{1}{L} \sum_{j=-(N-1)/2}^{(N-1)/2} e^{i2\pi(x-y)j/L} = \frac{1}{L} e^{-i\pi(x-y)(\rho-1/L)} \sum_{j=0}^{N-1} \left(e^{i2\pi(x-y)/L} \right)^j \\ &= \frac{1}{L} e^{-i\pi(x-y)(N-1)/L} \frac{1 - e^{2\pi(x-y)\rho}}{1 - e^{2\pi(x-y)/L}} = \frac{1}{L} \frac{e^{-i\pi\rho(x-y)} - e^{i\pi\rho(x-y)}}{e^{-i\pi(x-y)/L} - e^{i\pi(x-y)/L}} = \frac{1}{L} \frac{\sin(\pi\rho(x-y))}{\sin\left(\frac{\pi}{L}(x-y)\right)}. \end{aligned} \quad (1.11)$$

For $x - y \ll \rho^{-1}$ we may use the relation

$$\gamma^{(1)}(x, y) = \rho + \frac{\pi^2}{6} \left(\frac{\rho}{L^2} - \rho^3 \right) (x - y)^2 + \mathcal{O}((x - y)^3). \quad (1.12)$$

1.1.2 Calculating E_1

Recall the definition

$$E_1 = \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N \left| \nabla_i \tilde{\Psi} \right|^2 + \sum_{i < j}^N v_{ij} \left| \tilde{\Psi} \right|^2 - \sum_{i=1}^N \left| \nabla_i \tilde{\Psi}_F \right|^2 \quad (1.13)$$

We estimate E_1 by splitting it in three terms. First we have

$$\begin{aligned} E_1^{(1)} &= 2 \binom{N}{2} \int_{A_{12}} |\nabla_1 \tilde{\Psi}|^2 \\ &= 2 \binom{N}{2} \int_{A_{12}} \bar{\tilde{\Psi}} (-\Delta_1 \tilde{\Psi}) + 2 \binom{N}{2} \int \left[\bar{\tilde{\Psi}} \nabla_1 \tilde{\Psi} \right]_{x_1=x_2-b}^{x_1=x_2+b}. \end{aligned} \quad (1.14)$$

The boundary term can be explicitly calculated, and to lowest order in b we find

$$\begin{aligned} 2 \binom{N}{2} \int \left[\bar{\tilde{\Psi}} \nabla_1 \tilde{\Psi} \right]_{x_1=x_2-b}^{x_1=x_2+b} &= L \left[\frac{\omega(x)}{\sin(\pi x/L)} \partial_x \left(\frac{\omega(x)}{\sin(\pi x/L)} \right) \gamma^{(2)}(x, 0) \right]_{-b}^b \\ &\quad + L \left[\left(\frac{\omega(x)}{\sin(\pi x/L)} \right)^2 \partial_x \left(\gamma^{(2)}(x, 0; y, 0) \right) \right]_{y=x}^b. \end{aligned} \quad (1.15)$$

Since the continuous function $\frac{\omega(x)}{\sin(\pi x/L)} = \frac{x-a}{b-a} \frac{\sin(\pi b/L)}{\sin(\pi x/L)}$ for $|x| > b$, we see that

$$\partial_x \left(\frac{\omega(x)}{\sin(\pi x/L)} \right) \Big|_{x=\pm b} \approx \pm \pi b/L \frac{\frac{1}{b-a} - 1}{(\pi b/L)} = \pm \frac{a}{b^2} \quad (1.16)$$

and we know that $\gamma^{(2)}(x, 0) = \frac{\pi^2}{3} \rho^4 x^2$. Furthermore, by Wick's theorem it is straightforward to show that

$$\partial_x \left(\gamma^{(2)}(x, 0; y, 0) \right) \Big|_{y=x} = \frac{\pi^2}{3} N \rho^3 x + \rho^2 o(\rho x) \quad (1.17)$$

Thus we have

$$E_1^{(1)} = \frac{\pi^2}{3} N \rho^3 (2a + 2b) + 2 \binom{N}{2} \int_{A_{12}} \bar{\tilde{\Psi}} (-\Delta_1 \tilde{\Psi}) \quad (1.18)$$

Another contribution to E_1 is

$$\begin{aligned} E_1^{(2)} &= - \binom{N}{2} \int_{A_{12}} 2 |\nabla_1 \Psi_F|^2 + \sum_{i=3}^N |\nabla_i \Psi_F|^2 = \\ &\quad - \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N \bar{\Psi}_F (-\Delta_i \Psi_F) - 2 \binom{N}{2} \int \left[\bar{\Psi}_F \nabla_1 \Psi_F \right]_{x_1=x_2-b}^{x_1=x_2+b} \\ &= -E_0 \binom{N}{2} \int_{A_{12}} |\Psi_F|^2 - L \left[\partial_y \gamma^{(2)}(x, 0; y, 0) \Big|_{y=x} \right]_{-b}^b \end{aligned} \quad (1.19)$$

Again using (1.17) and $\gamma^{(2)}$ we find

$$E_1^{(2)} = -E_0 \frac{1}{2} \frac{\pi^2}{9} N \rho^3 b^3 - \frac{\pi^2}{3} N \rho^3 (2b). \quad (1.20)$$

The last contributions are $E_1^{(3)} = \binom{N}{2} \int_{A_{12}} \sum_{i < j}^N v_{ij} \left| \tilde{\Psi} \right|^2 = \binom{N}{2} \int_{A_{12}} v_{12} \left| \tilde{\Psi} \right|^2 + \binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} \left| \tilde{\Psi} \right|^2$ and $E_1^{(4)} = \int_{A_{12}} \sum_{i=3}^N \left| \nabla_i \tilde{\Psi} \right|^2$. First we notice that

$$\begin{aligned} & \binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} \left| \tilde{\Psi} \right|^2 \\ & \leq C'_1 \int_{A_{12} \cap \text{supp}(v_{34})} v(x_3 - x_4) \gamma^{(4)}(x_1, x_2, x_3, x_4) + C'_2 \int_{A_{12} \cap \text{supp}(v_{23})} v(x_2 - x_3) \gamma^{(3)}(x_1, x_2, x_3). \end{aligned} \quad (1.21)$$

To leading order in L , $|x_3 - x_4|$ and $|x_1 - x_2|$ we find that

$$\gamma^{(4)}(x_1, x_2, x_3, x_4) = \frac{\pi^4}{9} \rho^8 (x_1 - x_2)^2 (x_3 - x_4)^2 \quad (1.22)$$

and to leading order in L , $|x_1 - x_2|$ and $|x_2 - x_3|$ we find

$$\gamma^{(3)}(x_1, x_2, x_3) = \frac{\pi^6}{135} \rho^9 \underbrace{(x_1 - x_3)^2}_{=[(x_1 - x_2) + (x_2 - x_3)]^2} (x_1 - x_2)^2 (x_2 - x_3)^2. \quad (1.23)$$

Therefore we have

$$\begin{aligned} & \binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} \left| \tilde{\Psi} \right|^2 \\ & \leq C' \left(N^2 (\rho b)^3 \rho^3 \int x^2 v(x) dx + N(\rho b)^3 \rho^5 \int x^4 v(x) dx + N(\rho b)^4 \rho^4 \int x^3 v(x) dx \right. \\ & \quad \left. + N(\rho b)^5 \rho^3 \int x^2 v(x) dx \right) \\ & \leq C' N^2 (\rho b)^5 \rho \int v = \text{const. } E_0 N(\rho b)^3 \left(b \int v \right) \end{aligned} \quad (1.24)$$

and then we find that

$$\begin{aligned} E_1 &= E_1^{(1)} + E_1^{(2)} + E_1^{(3)} + E_1^{(4)} \\ &\leq \frac{2\pi^2}{3} N \rho^3 a + 2 \binom{N}{2} \int_{A_{12}} \left(\tilde{\Psi}(-\Delta_1) \tilde{\Psi} + \frac{1}{2} \sum_{i=3}^N \left| \nabla_i \tilde{\Psi} \right|^2 + \frac{1}{2} v_{12} \left| \tilde{\Psi} \right|^2 \right) + E_0 N(\rho b)^3 \left(-\frac{1}{2} \frac{\pi^2}{9} + \frac{1}{2} \rho \int v \right) \end{aligned} \quad (1.25)$$

Using the two body scattering equation this implies

$$\begin{aligned}
E_1 &\leq \frac{2\pi^2}{3} N \rho^3 a + 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \omega(-\Delta_1) \frac{\Psi_F}{\sin(\pi(x_1 - x_2)/L)} \\
&\quad + 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} (\nabla_1 \omega) \nabla_1 \frac{\Psi_F}{\sin(\pi(x_1 - x_2)/L)} \\
&\quad + \binom{N}{2} \int_{A_{12}} \sum_{i=3}^N \bar{\Psi} \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} (-\Delta_i) \Psi_F \\
&\quad - E_0 \frac{1}{2} \frac{\pi^2}{9} N \rho^3 b^3 + \text{const. } E_0 N (\rho b)^3 \left(b \int v \right)
\end{aligned} \tag{1.26}$$

Now using that

$$\begin{aligned}
&\binom{N}{2} \int_{A_{12}} \sum_{i=3}^N \bar{\Psi} \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} (-\Delta_i) \Psi_F \\
&= E_0 \binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} \tilde{\Psi} \right|^2 - 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} (-\Delta_1) \Psi_F,
\end{aligned} \tag{1.27}$$

$$\binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} \Psi_F \right|^2 \leq C_1 \left(\frac{b}{L} \right)^2 \pi^2 \rho^4 \left(\frac{L}{\pi} \right)^2 L b = C_1 N \rho^3 b^3 \tag{1.28}$$

and that

$$2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} (-\Delta_1) \Psi_F \leq C_2 E_0 N \rho^3 b^3 \tag{1.29}$$

we find that

$$\binom{N}{2} \int_{A_{12}} \sum_{i=3}^N \bar{\Psi} \frac{\omega}{\sin(\pi(x_1 - x_2)/L)} (-\Delta_i) \Psi_F \leq C E_0 N (\rho b)^3. \tag{1.30}$$

Furhtermore we find to leading order in N and ρb that

$$2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \omega(-\Delta_1) \frac{\Psi_F}{\sin(\pi(x_1 - x_2)/L)} = \frac{\pi^2}{15} N \rho^2 (\rho b)^3, \tag{1.31}$$

and that

$$2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} (\nabla_1 \omega) \nabla_1 \frac{\Psi_F}{\sin(\pi(x_1 - x_2)/L)} = \frac{\pi^2}{45} N \rho^2 (\rho b)^3. \tag{1.32}$$

Combining everything we find

$$E_1 \leq E_0 \left(2\rho a + \text{const. } N (\rho b)^3 \left[1 + b \int v \right] \right). \tag{1.33}$$

1.1.3 A remark about the hard core potential

Notice that it appears that we cannot deal with the hard core case. However, in the above calculation we threw away the term $\int_{A_{12} \setminus B_{12}} \sum_{2 \leq i < j}^N v_{ij} |\Psi|^2$. Adding this back in, we get the error $\binom{N}{2} \int_{B_{12}} \sum_{2 \leq i < j}^N v_{ij} |\tilde{\Psi}|^2$ instead of $\binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} |\tilde{\Psi}|^2$. In doing so, we immediately see that in the presence of a hard core potential wall, $\tilde{\Psi}$ is zero, whenever two coordinates are

within the hard core. Thus we may replace v_{ij} by \tilde{v}_{ij} which is zero whenever $|x_i - x_j|$ is within the range of the hard core. Thus our result, generalizes to the case of a hard core, plus an integrable potential.

1.1.4 Calculating E_2

Recall that $E_2 = E_2^{(1)} + E_2^{(2)}$ with

$$\begin{aligned} E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \Psi_F|^2 \\ E_2^{(2)} &= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^N |\nabla_i \Psi_F|^2 \end{aligned} \quad (1.34)$$

To estimate these, we first split them in two terms each and use partial integration. Consider first $E_2^{(1)}$:

$$\begin{aligned} E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \Psi_F|^2 \\ &= \binom{N}{2} 2N \left(\int_{A_{12} \cap A_{13}} |\nabla_1 \Psi_F|^2 + 2 \int_{A_{12} \cap A_{13}} |\nabla_2 \Psi_F|^2 \right) + \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=4}^N |\nabla_i \Psi_F|^2 \end{aligned} \quad (1.35)$$

For the second term, we can perform partial integration directly, in order to obtain

$$\begin{aligned} \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=3}^N |\nabla_i \Psi_F|^2 &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=3}^N \overline{\Psi_F} (-\Delta_i \Psi_F) \\ &\leq E_0 N^3 \int_{A_{12} \cap A_{23}} |\Psi_F|^2 - N^3 \int_{A_{12} \cap A_{23}} \sum_{i=1}^3 \overline{\Psi_F} (-\Delta_i \Psi_F) \\ &\leq 2E_0 \int_{[0,L]} \int_{[x_2-b, x_2+b]} \int_{x_2-b, x_2+b} \gamma^{(3)}(x_1, x_2, x_3) dx_3 dx_1 dx_2 - N^3 \int_{A_{12} \cap A_{23}} \sum_{i=1}^3 \overline{\Psi_F} (-\Delta_i \Psi_F) \end{aligned} \quad (1.36)$$

Changing variable $y_1 = x_1 - x_2$, $y_3 = x_3 - x_2$ and using translational invariance, we find

$$\begin{aligned} 2E_0 L \int_{[-b,b]} \int_{[-b,b]} \gamma^{(3)}(y_1, 0, y_3) dy_1 dy_3 &\approx 8E_0 L \frac{\pi^6}{135} \rho^9 \int_{[-b,b]} \int_{[-b,b]} y_1^4 y_3^2 dy_1 dy_3 \\ &= E_0 N \frac{8\pi^6}{15 \cdot 135} (b\rho)^8. \end{aligned} \quad (1.37)$$

Using Wick's theorem, we find that to leading order in $L\rho$, $|x_1 - x_2|$, $\rho|x_2 - x_3|$, and $\rho|x_1 - x_3|$ we have

$$\left(\partial_{x_1} \partial_{y_1} \gamma^{(3)}(x_1, x_2, x_3; y_1, y_2, y_3) \right) \Big|_{y=x} = \frac{\pi^6}{135} \rho^9 (x_2 - x_3)^2 ((x_1 - x_3) + (x_1 - x_2))^2 \quad (1.38)$$

and

$$\left(\partial_{y_1}^2 \gamma^{(3)}(x_1, x_2, x_3; y_1, y_2, y_3) \right) \Big|_{y=x} = \frac{2\pi^6}{135} \rho^9 (x_1 - x_2)(x_1 - x_3)(x_2 - x_3)^2 \quad (1.39)$$

Thus we find

$$\binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^3 \left(|\nabla_i \Psi_F|^2 - \overline{\Psi_F}(-\Delta_i \Psi_F) \right) \leq \tilde{C}_1 \frac{\pi^2}{3} \rho^9 L b^6 = \tilde{C}_1 E_0 (b\rho)^6. \quad (1.40)$$

Collecting everything we find

$$E_2^{(1)} \leq \text{const. } E_0(\rho b)^6 (1 + N(\rho b)^2). \quad (1.41)$$

To estimate $E_2^{(2)}$ use integration by parts

$$\begin{aligned} E_2^{(2)} &= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \left(4 |\nabla_1 \Psi_F|^2 + \sum_{i=5}^N |\nabla_i \Psi_F|^2 \right) \\ &= \binom{N}{2} \binom{N-2}{2} \left(4 \int_{|x_3-x_4|<b} [\overline{\Psi_F} \nabla_1 \Psi_F]_{x_1=x_2-b}^{x_1=x_2+b} + \int_{A_{12} \cap A_{34}} \sum_{i=1}^N \overline{\Psi_F}(-\Delta_i \Psi_F) \right) \\ &= 4 \int_{x_2 \in [0, L]} \int_{|x_3-x_4|<b} \left[\partial_{y_1} \gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, y_2, y_3, y_4) \Big|_{y_1=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} + E_0 \int_{A_{12} \cap A_{34}} \gamma^{(4)}(x_1, \dots, x_4). \end{aligned} \quad (1.42)$$

Using translational invariance, we have

$$\begin{aligned} \left[\partial_{y_1} \gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, y_2, y_3, y_4) \Big|_{y_1=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} &= \left[\partial_y \gamma^{(4)}(x, 0, x_3, x_4; y, 0, x_3, x_4) \Big|_{y=x} \right]_{x=-b}^{x=b} \\ &= 2b \partial_x \left[\partial_y \gamma^{(4)}(x, 0, x_3, x_4; y, 0, x_3, x_4) \Big|_{y=x} \right]_{x=0} + o(b) \end{aligned} \quad (1.43)$$

We find by straightforward computation that to leading order in ρL and $|x_3 - x_4|$ we have

$$\partial_x \left[\partial_y \gamma^{(4)}(x, 0, x_3, x_4; y, 0, x_3, x_4) \Big|_{y=x} \right]_{x=0} = \frac{1}{9} \pi^4 \rho^8 (x_3 - x_4)^2 \quad (1.44)$$

and we therefore get

$$4 \int_{x_2 \in [0, L]} \int_{|x_3-x_4|<b} \left[\partial_{y_1} \gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, y_2, y_3, y_4) \Big|_{y_1=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} = \frac{2}{9} \pi^2 E_0 N(\rho b)^4 \quad (1.45)$$

Furthermore we find that to leading order in L , $|x_1 - x_2|$, and $|x_3 - x_4|$ we have

$$\gamma^{(4)}(x_1, x_2, x_3, x_4) \leq 9 \hat{C}_2 \rho^8 (x_1 - x_2)^2 (x_3 - x_4)^2 \quad (1.46)$$

from which it follows that

$$E_0 \int_{A_{12} \cap A_{34}} \gamma^{(4)}(x_1, \dots, x_4) \leq \hat{C}_2 E_0 N^2 (\rho b)^6. \quad (1.47)$$

Collecting all terms we find the upper bound

$$E \leq E_0 \left(1 + 2\rho a + \text{const. } N(\rho b)^3 \left(1 + b \int v \right) \right) \quad (1.48)$$

1.1.5 Proof of bounds

We will now provide more general proofs for the above performed expansions. We start by considering the $\gamma^{(2)}(x_1, x_2; y_1, x_2)$, for which we show the following result

Proposition 1. *Let $|x_1 - x_2| < b \ll \rho^{-1}$ then*

$$\left| \gamma^{(2)}(x_1, x_2; y_1, x_2) \right| \leq C \rho^4 |(x_1 - x_2)(y_1 - x_2)| + o(\rho^4 |(x_1 - x_2)(y_1 - x_2)|), \quad (1.49)$$

where C is dimensionless and independent of ρ , L and N .

Proof. By antisymmetry of the wave function, it is clear that $\gamma^{(2)}(x_2, x_2; x_2, x_2) = 0$. Thus by Taylor's theorem for multivariate functions we have

$$\gamma^{(2)}(x_1, x_2; y_1, x_2) = c_1(x_2) \rho^3 (x_1 - x_2) + c_2 \rho^3 (x_2)(y_1 - x_2) + C(x_2, N) \rho^4 (x_1 - x_2)(y_1 - x_2) + \epsilon_T(x_1, x_2, y_1) \quad (1.50)$$

where $\epsilon_T(x_1, x_2, y_1)$ denotes the Taylor error term. Clearly, by antisymmetry we have $c_1 = c_2 = 0$, since $\gamma(x_2, x_2; y_1, x_2) = 0$ and vice versa. Now by dimensions and translational invariance $C(x_2)$ can be chosen to only depend on N . However, assume for contradiction that $C(N)$ is unbounded as a function of N . Then $\partial_{x_1} \partial_{y_1} \gamma^{(2)}(x_1, 0; y_1, 0)|_{y_1, x_1=0}$ is unbounded as a function of N . However, this contradicts the fact that $\gamma^{(2)}$ by Wick's theorem is a finite sum of products of $\gamma^{(1)}$ which all are finite and have finite derivatives. Thus we may conclude that there exist $C > 0$ such that $C > |C(x_2, N)|$ and the result now follows from the triangle inequality. \square

Alternatively, we find the bounds by row and column expansions of the determinant in Wick's theorem. Consider *e.g.* the following example

Proposition 2. *Let $|x_1 - x_2| \leq b \ll \rho^{-1}$ and $|x_3 - x_3| \leq b \ll \rho^{-1}$ then*

$$\rho^{(4)}(x_1, \dots, x_4) \leq C(x_1 - x_2)^2 (x_3 - x_4)^2. \quad (1.51)$$

Proof. Recall that Wick's theorem states that

$$\rho^{(4)}(x_1, \dots, x_4) = \begin{vmatrix} \gamma^{(1)}(x_1, x_1) & \gamma^{(1)}(x_1, x_2) & \gamma^{(1)}(x_1, x_3) & \gamma^{(1)}(x_1, x_4) \\ \gamma^{(1)}(x_2, x_1) & \gamma^{(1)}(x_2, x_2) & \gamma^{(1)}(x_2, x_3) & \gamma^{(1)}(x_2, x_4) \\ \gamma^{(1)}(x_3, x_1) & \gamma^{(1)}(x_3, x_2) & \gamma^{(1)}(x_3, x_3) & \gamma^{(1)}(x_3, x_4) \\ \gamma^{(1)}(x_4, x_1) & \gamma^{(1)}(x_4, x_2) & \gamma^{(1)}(x_4, x_3) & \gamma^{(1)}(x_4, x_4) \end{vmatrix} \quad (1.52)$$

where $\gamma^{(1)}(x, x) = \lim_{y \rightarrow x} \gamma^{(1)}(x, y) = \rho$. Now subtraction row 2 from 1 followed by subtracting column 2 from column 1 and then subtracting row 3 from row 4 followed by subtracting column 3 from column 4, we obtain denoting $\gamma^{(1)}(x_i, x_j)$ by $\gamma_{ij}^{(1)}$

$$\rho^{(4)}(x_1, \dots, x_4) = \begin{vmatrix} \gamma_{11}^{(1)} - \gamma_{21}^{(1)} - \gamma_{12}^{(1)} + \gamma_{22}^{(1)} & \gamma_{12}^{(1)} - \gamma_{22}^{(1)} & \gamma_{13}^{(1)} - \gamma_{23}^{(1)} & \gamma_{14}^{(1)} - \gamma_{24}^{(1)} - \gamma_{13}^{(1)} + \gamma_{23}^{(1)} \\ \gamma_{21}^{(1)} - \gamma_{22}^{(1)} & \gamma_{22}^{(1)} & \gamma_{23}^{(1)} & \gamma_{24}^{(1)} - \gamma_{23}^{(1)} \\ \gamma_{31}^{(1)} - \gamma_{32}^{(1)} & \gamma_{32}^{(1)} & \gamma_{33}^{(1)} & \gamma_{34}^{(1)} - \gamma_{33}^{(1)} \\ \gamma_{41}^{(1)} - \gamma_{42}^{(1)} - \gamma_{31}^{(1)} + \gamma_{32}^{(1)} & \gamma_{42}^{(1)} - \gamma_{32}^{(1)} & \gamma_{43}^{(1)} - \gamma_{33}^{(1)} & \gamma_{44}^{(1)} - \gamma_{34}^{(1)} - \gamma_{43}^{(1)} + \gamma_{33}^{(1)} \end{vmatrix} \quad (1.53)$$

We then bound this by the corresponding permanent

$$\rho^{(4)}(x_1, \dots, x_4) \leq \begin{vmatrix} \left| \gamma_{11}^{(1)} - \gamma_{21}^{(1)} - \gamma_{12}^{(1)} + \gamma_{22}^{(1)} \right| & \left| \gamma_{12}^{(1)} - \gamma_{22}^{(1)} \right| & \left| \gamma_{13}^{(1)} - \gamma_{23}^{(1)} \right| & \left| \gamma_{14}^{(1)} - \gamma_{24}^{(1)} - \gamma_{13}^{(1)} + \gamma_{23}^{(1)} \right| \\ \left| \gamma_{21}^{(1)} - \gamma_{22}^{(1)} \right| & \left| \gamma_{22}^{(1)} \right| & \left| \gamma_{23}^{(1)} \right| & \left| \gamma_{24}^{(1)} - \gamma_{23}^{(1)} \right| \\ \left| \gamma_{31}^{(1)} - \gamma_{32}^{(1)} \right| & \left| \gamma_{32}^{(1)} \right| & \left| \gamma_{33}^{(1)} \right| & \left| \gamma_{34}^{(1)} - \gamma_{33}^{(1)} \right| \\ \left| \gamma_{41}^{(1)} - \gamma_{42}^{(1)} - \gamma_{31}^{(1)} + \gamma_{32}^{(1)} \right| & \left| \gamma_{42}^{(1)} - \gamma_{32}^{(1)} \right| & \left| \gamma_{43}^{(1)} - \gamma_{33}^{(1)} \right| & \left| \gamma_{44}^{(1)} - \gamma_{34}^{(1)} - \gamma_{43}^{(1)} + \gamma_{33}^{(1)} \right| \end{vmatrix}_+ \quad (1.54)$$

Furhtermore, we use that $\sup |\partial^k \gamma^{(1)}| \leq \text{const. } \rho^{k+1}$, the mean value theorem, and translational invariance to obtain $\gamma_{1j} - \gamma_{2j} \leq \text{const. } \rho^2(x_1 - x_2)$ for $j > 2$ and $\gamma_{12} - \gamma_{22} \leq \text{const. } \rho^3(x_1 - x_2)^2$ (requires MVT twice). Notice also that for example if $|x_1 - x_2| < |x_3 - x_4|$ we have by the MVT

$$\gamma_{14}^{(1)} - \gamma_{24}^{(1)} - \gamma_{13}^{(1)} + \gamma_{23}^{(1)} = \gamma^{(1)'}(\xi_1 - x_4)(x_1 - x_2) - \gamma^{(1)'}(\xi_2 - x_3)(x_1 - x_2) = \gamma^{(1)''}(\xi)(x_1 - x_2)((x_3 - x_4) + (\xi_2 - \xi_1)) \quad (1.55)$$

such that $\left| \gamma_{14}^{(1)} - \gamma_{24}^{(1)} - \gamma_{13}^{(1)} + \gamma_{23}^{(1)} \right| \leq \text{const. } \rho^3 |(x_1 - x_2)(x_3 - x_4)|$. Similarly for $|x_3 - x_4| \leq |x_1 - x_2|$ we could have argued that $\left| \gamma_{14}^{(1)} - \gamma_{24}^{(1)} - \gamma_{13}^{(1)} + \gamma_{23}^{(1)} \right| \leq \text{const. } \rho^3 |(x_1 - x_2)(x_3 - x_4)|$. Thus we get

$$\rho^{(4)} \leq \text{const. } \rho^4 \begin{vmatrix} \rho^2(x_1 - x_2)^2 & \rho^2(x_1 - x_2)^2 & \rho(x_1 - x_2) & \rho^2(x_1 - x_2)(x_3 - x_4) \\ \rho^2(x_1 - x_2)^2 & 1 & 1 & \rho(x_3 - x_4) \\ \rho(x_1 - x_2) & 1 & 1 & \rho^2(x_3 - x_4)^2 \\ \rho^2(x_1 - x_2)(x_3 - x_4) & \rho(x_3 - x_4) & \rho^2(x_3 - x_4)^2 & \rho^2(x_3 - x_4)^2 \end{vmatrix}_+ \quad (1.56)$$

It is then straightforward to see that

$$\rho^{(4)} \leq \text{const. } \rho^8(x_1 - x_2)^2(x_3 - x_4)^2 \quad (1.57)$$

□

Remark: Notice that for Dirichlet boundary conditions we do not have $\gamma_{12} - \gamma_{22} \leq$

const. $\rho^3(x_1 - x_2)^2$, nevertheless we do have

$$\begin{aligned} \gamma_{11}^{(1)} - \gamma_{21}^{(1)} - \gamma_{12}^{(1)} + \gamma_{22}^{(1)} &= \partial_{x_1} \gamma^{(1)}(\xi_1, x_1)(x_1 - x_2) - \partial_{x_1} \gamma^{(1)}(\xi_2, x_2)(x_1 - x_2) \\ &= \partial_{x_1} \gamma^{(1)}(\xi_2, x_1)(x_1 - x_2) + \partial_{x_1}^2 \gamma(\xi_3, x_1)(x_1 - x_2)(\xi_1 - \xi_2) - \partial_{x_1} \gamma^{(1)}(\xi_2, x_2)(x_1 - x_2) \\ &= \partial_{x_2} \partial_{x_1} \gamma^{(1)}(\xi_2, \xi_4)(x_1 - x_2)^2 + \partial_{x_1}^2 \gamma(\xi_3, x_1)(x_1 - x_2)(\xi_1 - \xi_2) \end{aligned} \quad (1.58)$$

and by triangle inequality we have

$$\left| \gamma_{11}^{(1)} - \gamma_{21}^{(1)} - \gamma_{12}^{(1)} + \gamma_{22}^{(1)} \right| \leq \text{const. } \rho^3(x_1 - x_2)^2 \quad (1.59)$$

together with $\gamma_{11}^{(1)} - \gamma_{21}^{(1)} \leq \text{const. } \rho^2(x_1 - x_2)$ it is clear that it holds even in the Dirichlet case that $\rho^{(4)} \leq \text{const. } \rho^8(x_1 - x_2)^2(x_3 - x_4)^2$

Proposition 3. *Let $|x_1 - x_2| < b \ll \rho^{-1}$ then*

$$\left| \partial_{x_1} \partial_{y_1} \gamma^4(x_1, x_2, x_3, x_4, y_1, x_2, x_3, x_4) \right| \leq \text{const. } \rho^8(x_3 - x_4)^2 \quad (1.60)$$

Proof. By Wick's theorem we have

$$\begin{aligned} &\partial_{x_1} \partial_{y_1} \gamma^4(x_1, x_2, x_3, x_4, y_1, x_2, x_3, x_4) \\ &= \begin{vmatrix} \partial_{x_1} \partial_{y_1} \gamma^{(1)}(x_1, y_1) & \partial_{x_1} \gamma^{(1)}(x_1, x_2) & \partial_{x_1} \gamma^{(1)}(x_1, x_3) & \partial_{x_1} \gamma^{(1)}(x_1, x_4) \\ \partial_{y_1} \gamma^{(1)}(x_2, y_1) & \gamma^{(1)}(x_2, x_2) & \gamma^{(1)}(x_2, x_3) & \gamma^{(1)}(x_2, x_4) \\ \partial_{y_1} \gamma^{(1)}(x_3, y_1) & \gamma^{(1)}(x_3, x_2) & \gamma^{(1)}(x_3, x_3) & \gamma^{(1)}(x_3, x_4) \\ \partial_{y_1} \gamma^{(1)}(x_4, y_1) & \gamma^{(1)}(x_4, x_2) & \gamma^{(1)}(x_4, x_3) & \gamma^{(1)}(x_4, x_4) \end{vmatrix}. \end{aligned} \quad (1.61)$$

Subtracting row 3 from row 4 followed by column 3 from column 4 we obtain

$$\begin{aligned} &\partial_{x_1} \partial_{y_1} \gamma^4(x_1, x_2, x_3, x_4, y_1, x_2, x_3, x_4) \\ &= \begin{vmatrix} \partial_{x_1} \partial_{y_1} \gamma_{11}^{(1)} & \partial_{x_1} \gamma_{12}^{(1)} & \partial_{x_1} \gamma_{13}^{(1)} & \partial_{x_1} \gamma_{14}^{(1)} - \partial_{x_1} \gamma_{13}^{(1)} \\ \partial_{y_1} \gamma_{21}^{(1)} & \gamma_{22}^{(1)} & \gamma_{23}^{(1)} & \gamma_{24}^{(1)} - \gamma_{23}^{(1)} \\ \partial_{y_1} \gamma_{31}^{(1)} & \gamma_{32}^{(1)} & \gamma_{33}^{(1)} & \gamma_{34}^{(1)} - \gamma_{33}^{(1)} \\ \partial_{y_1} \gamma_{41}^{(1)} - \partial_{y_1} \gamma_{31}^{(1)} & \gamma_{42}^{(1)} - \gamma_{32}^{(1)} & \gamma_{43}^{(1)} - \gamma_{33}^{(1)} & \gamma_{44}^{(1)} - \gamma_{34}^{(1)} - \gamma_{43}^{(1)} + \gamma_{33}^{(1)} \end{vmatrix}. \end{aligned} \quad (1.62)$$

where $\gamma_{j1}^{(1)}$ denotes $\gamma^{(1)}(x_j, y_1)$ and $\gamma_{ji}^{(1)} = \gamma^{(1)}(x_j, x_i)$ for $i > 1$. By same arguments as above $\left| \gamma_{3j}^{(1)} - \gamma_{4j}^{(1)} \right| \leq \text{const. } \rho^2 |x_3 - x_4|$ and $\left| \gamma_{44}^{(1)} - \gamma_{34}^{(1)} - \gamma_{43}^{(1)} + \gamma_{33}^{(1)} \right| \leq \text{const. } \rho^3(x_3 - x_4)^2$. Further-

more, by the MVT we have $\left| \partial_{x_1} \gamma_{14}^{(1)} - \partial_{x_1} \gamma_{13}^{(1)} \right| \leq \text{const. } \rho^3 |x_3 - x_4|$. Thus we obtain

$$\begin{aligned} & \left| \partial_{x_1} \partial_{y_1} \gamma^4(x_1, x_2, x_3, x_4, y_1, x_2, x_3, x_4) \right| \\ & \leq \text{const. } \rho^4 \begin{vmatrix} \rho^2 & \rho & \rho & \rho^2(x_3 - x_4) \\ \rho & 1 & 1 & \rho(x_3 - x_4) \\ \rho & 1 & 1 & \rho^2(x_3 - x_4)^2 \\ \rho^2(x_3 - x_4) & \rho(x_3 - x_4) & \rho^2(x_3 - x_4)^2 & \rho^2(x_3 - x_4)^2 \end{vmatrix}_+ \end{aligned} \quad (1.63)$$

from which it follows that $\left| \partial_{x_1} \partial_{y_1} \gamma^4(x_1, x_2, x_3, x_4, y_1, x_2, x_3, x_4) \right| \leq \text{const. } \rho^8(x_3 - x_4)^2$ \square

We present a more abstract argument for the following bounds. Notice that all derivatives of $\gamma^{(1)}$ are uniformly bounded by some power of ρ . Thus this is also true, by Wick's theorem, for any $\gamma^{(k)}$. Using this and the fact that Ψ_F is antisymmetric we prove

Proposition 4. $\gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, x_2, x_3, x_4) \leq \text{const. } \rho^8(x_1 - x_2)(y_1 - x_2)(x_3 - x_4)^2$

Proof. Recall that

$$\gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, x_2, x_3, x_4) = \frac{N!}{(N-4)!} \int \overline{\Psi_F(x_1, x_2, x_3, x_4, \dots, x_N)} \Psi_F(y_1, x_2, x_3, x_4, \dots, x_N) dx_5 \dots dx_N \quad (1.64)$$

it is clear by antisymmetry of Ψ_F and symmetry when exchanging x_3 and x_4 that by the mean value theorem used multiple times we have

$$\gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, x_2, x_3, x_4) \leq \text{const. } \rho^8(x_1 - x_2)(y_1 - x_2)(x_3 - x_4)^2 \quad (1.65)$$

\square

1.2 Dirichlet boundary conditions

We will now do the computation again, this time using Dirichlet boundary conditions instead of periodic. To begin with, we construct the free Fermi groundstate. The Dirichlet eigenstates of the Laplacian are $\phi_j(x) = \sqrt{2/L} \sin(\pi j x / L)$. Thus the free Fermi groundstate is

$$\Psi_F(x) = \det(\phi_j(x_i))_{i,j=1}^N = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i} \right)^N \begin{vmatrix} e^{iy_1} - e^{-iy_1} & e^{i2y_1} - e^{-i2y_1} & \dots & e^{iNy_1} - e^{-iNy_1} \\ e^{iy_2} - e^{-iy_2} & e^{i2y_2} - e^{-i2y_2} & \dots & e^{iNy_2} - e^{-iNy_2} \\ \vdots & \vdots & \ddots & \vdots \\ e^{iy_N} - e^{-iy_N} & e^{i2y_N} - e^{-i2y_N} & \dots & e^{iNy_N} - e^{-iNy_N} \end{vmatrix}, \quad (1.66)$$

where we defined $y_i = \frac{\pi}{L}x_i$. Defining $z = e^{iy}$ and using the relation $(x^n - y^n)/(x - y) = \sum_{k=0}^{n-1} x^k y^{n-1-k}$ we find

$$\Psi_f(x) = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{i=1}^N (z_i - z_i^{-1}) \begin{vmatrix} 1 & z_1 + z_1^{-1} & \dots & \sum_{k=0}^{N-1} z_1^{2k-N+1} \\ 1 & z_2 + z_2^{-1} & \dots & \sum_{k=0}^{N-1} z_2^{2k-N+1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & z_N + z_N^{-1} & \dots & \sum_{k=0}^{N-1} z_N^{2k-N+1} \end{vmatrix}. \quad (1.67)$$

Notice now that $(z + z^{-1})^n = \sum_{k=0}^n \binom{n}{k} z^{2k-n}$. Now for i from 1 to $N-1$ we add $\left(\binom{N-1}{i} - \binom{N-1}{i-1}\right)$ times column $N-i$ to column N . This of course does not change the determinant, and we find

$$\Psi_f(x) = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{i=1}^N (z_i - z_i^{-1}) \begin{vmatrix} 1 & z_1 + z_1^{-1} & \dots & \sum_{k=0}^{N-2} z_1^{2k-N+1} & (z_1 + z_1^{-1})^{N-1} \\ 1 & z_2 + z_2^{-1} & \dots & \sum_{k=0}^{N-2} z_2^{2k-N+1} & (z_2 + z_2^{-1})^{N-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & z_N + z_N^{-1} & \dots & \sum_{k=0}^{N-2} z_N^{2k-N+1} & (z_N + z_N^{-1})^{N-1} \end{vmatrix}. \quad (1.68)$$

Now for $i = 1$ to $N-2$ we add $\left(\binom{N-2}{i} - \binom{N-2}{i-1}\right)$ times column $N-1-i$ to column $N-1$, continue this process, *i.e.* for $j = 3$ to N : for $i = 1$ to $N-j$ add $\left(\binom{N-j}{i} - \binom{N-j}{i-1}\right)$ times column $N-1-i$ to column $N-j+1$. Then we obtain

$$\Psi_f(x) = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{i=1}^N (z_i - z_i^{-1}) \begin{vmatrix} 1 & z_1 + z_1^{-1} & (z_1 + z_1^{-1})^2 & \dots & (z_1 + z_1^{-1})^{N-1} \\ 1 & z_2 + z_2^{-1} & (z_2 + z_2^{-1})^2 & \dots & (z_2 + z_2^{-1})^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & z_N + z_N^{-1} & (z_N + z_N^{-1})^2 & \dots & (z_N + z_N^{-1})^{N-1} \end{vmatrix}. \quad (1.69)$$

The determinant is recognized as a Vandermonde determinant and thus we have

$$\begin{aligned} \Psi_f(x) &= \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{k=1}^N (z_k - z_k^{-1}) \prod_{i < j}^N \left((z_i + z_i^{-1}) - (z_j + z_j^{-1})\right) \\ &= 2^{\binom{N}{2}} \sqrt{\frac{2}{L}}^N \prod_{k=1}^N \sin\left(\frac{\pi}{L}x_k\right) \prod_{i < j}^N \left[\cos\left(\frac{\pi}{L}x_i\right) - \cos\left(\frac{\pi}{L}x_j\right)\right] \\ &= -2^{\binom{N}{2}+1} \sqrt{\frac{2}{L}}^N \prod_{k=1}^N \sin\left(\frac{\pi}{L}x_k\right) \prod_{i < j}^N \sin\left(\frac{\pi(x_i - x_j)}{2L}\right) \sin\left(\frac{\pi(x_i + x_j)}{2L}\right). \end{aligned} \quad (1.70)$$

We construct our trial state, similarly to the construction for periodic b.c. by

$$\Psi(x) = \begin{cases} \omega(\mathcal{R}(x)) \frac{\tilde{\Psi}_F(x)}{\mathcal{R}(x)} & \text{if } \mathcal{R}(x) < b, \\ \tilde{\Psi}_F(x) & \text{if } \mathcal{R}(x) \geq b, \end{cases} \quad (1.71)$$

where ω is the suitably normalized solution to the two-body scattering equation, *i.e.* $\omega(x) = f(x) \frac{b}{f(b)}$ where f is any solution of the two-body scattering equation. $\tilde{\Psi}_F(x) = |\Psi_F|$ is the

absolute value of the free fermionic ground state. Obviously (1.6) still holds with Dirichlet b.c. and thus we need only recalculate the corrections and errors E_1 , $E_2^{(1)}$ and $E_2^{(2)}$.

1.2.1 Reduced density matrices

We compute the one-particle reduced density matrix of the free Fermi groundstate with Dirichlet b.c. in the usual way

$$\begin{aligned}\gamma^{(1)}(x, y) &= \frac{2}{L} \sum_{j=1}^N \sin\left(\frac{\pi}{L} jx\right) \sin\left(\frac{\pi}{L} jy\right) \\ &= \frac{\cos\left(\pi\left[\left(\rho + \frac{1}{L}\right)x + \rho y\right]\right) - \cos\left(\pi\left[\left(\rho + \frac{1}{L}\right)x - \rho y\right]\right) - \cos\left(\pi\left[\left(\rho + \frac{1}{L}\right)y + \rho x\right]\right) + \cos\left(\pi\left[\left(\rho + \frac{1}{L}\right)y - \rho x\right]\right)}{4L \sin\left(\frac{\pi}{2L}(x-y)\right) \sin\left(\frac{\pi}{2L}(x+y)\right)} \\ &= \frac{\sin\left(\pi\left(\rho + \frac{1}{2L}\right)(x-y)\right)}{2L \sin\left(\frac{\pi}{2L}(x-y)\right)} - \frac{\sin\left(\pi\left(\rho + \frac{1}{2L}\right)(x+y)\right)}{2L \sin\left(\frac{\pi}{2L}(x+y)\right)}\end{aligned}\tag{1.72}$$

Of course Wick's theorem still applies to compute a general n -particle reduced matrix.

1.2.2 Taylor's theorem

We notice now that

$$\gamma^{(1)}(x, y) = \frac{\pi}{L} \left(D_N\left(\pi \frac{x-y}{L}\right) + D_N\left(\pi \frac{x+y}{L}\right) \right), \tag{1.73}$$

where $D_N(x) = \frac{1}{2\pi} \sum_{k=-N}^N e^{ikx} = \frac{\sin((N+1/2)x)}{2\pi \sin(x/2)}$ is the Dirichlet kernel. One obvious consequence is that $|\partial_x^{k_1} \partial_y^{k_2} \gamma^{(1)}(x, y)| \leq \frac{1}{\pi} (2N)^{k_1+k_2+1} \left(\frac{\pi}{L}\right)^{k_1+k_2+1} = \pi^{k_1+k_2} (2\rho)^{k_1+k_2+1}$. This bound will allow us to Taylor expand any $\gamma^{(k)}$, as all derivatives are uniformly bounded by a constant times some power of ρ . In fact the relevant power of ρ can be directly obtained from dimensional analysis. Alternatively Taylor expanding may be thought of as using the mean value theorem multiple times.

1.2.3 Estimating E_1

Recall the definition

$$E_1 = \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N |\nabla_i \tilde{\Psi}|^2 + \sum_{i < j} v_{ij} |\tilde{\Psi}|^2 - \sum_{i=1}^N |\nabla_i \tilde{\Psi}_F|^2 \tag{1.74}$$

As with periodic b.c., we estimate E_1 by splitting it in three terms. First we have

$$\begin{aligned}E_1^{(1)} &= 2 \binom{N}{2} \int_{A_{12}} |\nabla_1 \tilde{\Psi}|^2 \\ &= 2 \binom{N}{2} \int_{A_{12}} \tilde{\Psi} (-\Delta_1 \tilde{\Psi}) + 2 \binom{N}{2} \int \left[\tilde{\Psi} \nabla_1 \tilde{\Psi} \right]_{x_1=x_2-b}^{x_1=x_2+b}.\end{aligned}\tag{1.75}$$

The boundary term can be explicitly calculated, and to lowest order in b we find

$$2 \binom{N}{2} \int \left[\bar{\Psi} \nabla_1 \tilde{\Psi} \right]_{x_1=x_2-b}^{x_1=x_2+b} = \int \left[\frac{\omega(x_1-x_2)}{(x_1-x_2)} \partial_{x_1} \left(\frac{\omega(x_1-x_2)}{(x_1-x_2)} \right) \rho^{(2)}(x_1, x_2) \right]_{x_2-b}^{x_2+b} dx_2 \\ + \int \left[\left(\frac{\omega(x_1-x_2)}{(x_1-x_2)} \right)^2 \partial_{x_1} \left(\gamma^{(2)}(x_1, x_2; y, x_2) \right) \right]_{y=x_1} \Big|_{x_2-b}^{x_2+b} dx_2. \quad (1.76)$$

Since the continuously differentiable function $\frac{\omega(x)}{(x_1-x_2)} = \frac{|x_1-x_2|-a}{b-a} \frac{b}{(x_1-x_2)}$ for $|x_1-x_2| > b$, we see that

$$\partial_{x_1} \left(\frac{\omega(x_1-x_2)}{(x_1-x_2)} \right) \Big|_{x=x_2 \pm b} \approx \pm b \frac{\frac{1}{b-a} - 1}{b} = \pm \frac{a}{b^2} \quad (1.77)$$

and we know that to leading order in L and $|x_1-x_2|$ we have $\rho^{(2)}(x_1, x_2) = (\frac{\pi^2}{3} \rho^4 + f(x_2, \rho, L))(x_1-x_2)^2$. The following lemma, will be of use in estimating E_1

Lemma 1. $\rho^{(2)}(x_1, x_2) \leq \left(\frac{\pi^2}{3} \rho^4 + f(x_2) \right) (x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4)$ with $\int f(x_2) dx_2 \leq \text{const. } \rho^3 \log(N)$.

Proof. Notice that with periodic b.c. we have by translation invariance $\rho_{\text{per}}^{(2)}(x_1-x_2) = \frac{\pi^2}{3} \rho^4 (x_1-x_2)^2 + \mathcal{O}(\rho^4(x_1-x_2)^4)$. Furthermore, we have $\gamma^{(1)}(x_1, x_2) - \rho^{(1)}((x_1+x_2)/2) = \gamma_{\text{per}, (\rho+1/(2L))}^{(1)}(x_1, x_2) - \rho$. Now by Wick's theorem we have

$$\rho^{(2)}(x_1, x_2) = \rho^{(1)}(x_1) \rho^{(1)}(x_2) - \gamma^{(1)}(x_1, x_2) \gamma^{(1)}(x_2, x_1). \quad (1.78)$$

Using that $\gamma^{(1)}$ is symmetric, and that

$$\rho^{(1)}(x_1) = \rho^{(1)}((x_1+x_2)/2) + \rho^{(1)'}((x_1+x_2)/2) \frac{x_1-x_2}{2} + \frac{1}{2} \rho^{(1)''}((x_1+x_2)/2) \left(\frac{x_1-x_2}{2} \right)^2 \\ + \mathcal{O}(\rho^4(x_1-x_2)^3) \quad (1.79)$$

$$\rho^{(1)}(x_2) = \rho^{(1)}((x_1+x_2)/2) + \rho^{(1)'}((x_1+x_2)/2) \frac{x_2-x_1}{2} + \frac{1}{2} \rho^{(1)''}((x_1+x_2)/2) \left(\frac{x_1-x_2}{2} \right)^2 \\ + \mathcal{O}(\rho^4(x_1-x_2)^3) \quad (1.80)$$

we see that

$$\rho^{(2)}(x_1, x_2) \leq \rho^{(1)}((x_1+x_2)/2)^2 - \gamma^{(1)}(x_1, x_2)^2 - \left[\rho^{(1)'}((x_1+x_2)/2) \right]^2 \left(\frac{x_1-x_2}{2} \right)^2 \\ + \rho^{(1)}((x_1+x_2)/2) \frac{1}{2} \rho^{(1)''}((x_1+x_2)/2) \left(\frac{x_1-x_2}{2} \right)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4) \quad (1.81)$$

Notice that $\mathcal{O}(\rho^5(x_1-x_2)^3)$ terms must cancel due to symmetry.

Now use the fact that $0 \leq \rho^{(1)} \leq \rho$ and that $\int_{[0,L]} |\rho^{(1)''}| \leq \text{const. } \rho^2 \log(N)$, which follows from

the bound on Dirichlet's kernel $\|D_N^{(k)}\|_{L^1([0,2\pi])} \leq \text{const. } N^k \log(N)$, to conclude that

$$\rho^{(2)}(x_1, x_2) \leq \rho^{(1)}((x_1 + x_2)/2)^2 - \gamma^{(1)}(x_1, x_2)^2 + g_1(x_1 + x_2)(x_1 - x_2)^2 + \mathcal{O}(\rho^6(x_1 - x_2)^4), \quad (1.82)$$

for some function g_1 satisfying $\int_{[0,L]} g_1 \leq \text{const. } \rho^3 \log(N)$. Furthermore, notice that

$$\begin{aligned} \rho^{(1)}((x_1 + x_2)/2)^2 - \gamma^{(1)}(x_1, x_2)^2 &= (\rho^{(1)}((x_1 + x_2)/2) - \gamma^{(1)}(x_1, x_2))(\rho^{(1)}((x_1 + x_2)/2) + \gamma^{(1)}(x_1, x_2)) \\ &= (\rho - \gamma_{\text{per}, (\rho+1/(2L))}^{(1)}(x_1, x_2))(\rho - \gamma_{\text{per}, (\rho+1/(2L))}^{(1)}(x_1, x_2) + 2\rho^{(1)}((x_1 + x_2)/2)) \\ &= (\rho - \gamma_{\text{per}, (\rho+1/(2L))}^{(1)}(x_1, x_2))^2 + 2(\rho - \gamma_{\text{per}, (\rho+1/(2L))}^{(1)}(x_1, x_2))\rho^{(1)}((x_1 + x_2)/2) \\ &= \mathcal{O}(\rho^6(x_1 - x_2)^4) + 2 \left(\frac{\pi^2}{6} \rho^3(x_1 - x_2)^2 + \mathcal{O}(\rho^5(x_1 - x_2)^4) \right) \left(\rho + \frac{1}{2L} - \frac{\pi}{L} D_N((x_1 + x_2)/(2L)) \right) \\ &\leq \frac{\pi^2}{3} \rho^4(x_1 - x_2)^2 + g_2(x_1 - x_2)(x_1 - x_2)^2 + \mathcal{O}(\rho^6(x_1 - x_2)^4) \end{aligned} \quad (1.83)$$

where we have choosen $g_2(x) = \frac{\pi^2}{3} \rho^3 \left(\frac{1}{2L} + \left| \frac{\pi}{L} D_N(x/(2L)) \right| \right)$ which clearly satisfies $\int_{[0,L]} g_2 \leq \text{const. } \rho^3 \log(N)$. Thus we conclude that

$$\rho^{(2)}(x_1, x_2) \leq \left(\frac{\pi^2}{3} \rho^4 + f(x_2) \right) (x_1 - x_2)^2 + \mathcal{O}(\rho^6(x_1 - x_2)^4) \quad (1.84)$$

with $f = g_1 + g_2$, satifying $\int_{[0,L]} f \leq \text{const. } \rho^3 \log(N)$ □

Using lemma 1, we see that

$$\int \left[\frac{\omega(x_1 - x_2)}{(x_1 - x_2)} \partial_{x_1} \left(\frac{\omega(x_1 - x_2)}{(x_1 - x_2)} \right) \gamma^{(2)}(x_1, x_2) \right]_{x_2-b}^{x_2+b} dx_2 \leq 2aN \frac{\pi^2}{3} \rho^3 \left(1 + \text{const. } \frac{\log(N)}{N} \right) \quad (1.85)$$

Furthermore, we denote

$$\begin{aligned} &\int \left[\left(\frac{\omega(x_1 - x_2)}{(x_1 - x_2)} \right)^2 \partial_{x_1} \left(\gamma^{(2)}(x_1, x_2; y, x_2) \right) \right]_{y=x_1}^{x_2+b} dx_2 \\ &= \int \left[\partial_{x_1} \left(\gamma^{(2)}(x_1, x_2; y, x_2) \right) \right]_{y=x_1}^{x_2+b} dx_2 =: \kappa_1 \end{aligned} \quad (1.86)$$

Thus we have

$$E_1^{(1)} = \frac{\pi^2}{3} N \rho^3 (2a) + \kappa_1 + 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi}(-\Delta_1 \tilde{\Psi}) \quad (1.87)$$

Another contribution to E_1 is

$$\begin{aligned}
E_1^{(2)} &= -\binom{N}{2} \int_{A_{12}} 2 |\nabla_1 \Psi_F|^2 + \sum_{i=3}^N |\nabla_i \Psi_F|^2 = \\
&= -\binom{N}{2} \int_{A_{12}} \sum_{i=1}^N \overline{\Psi_F} (-\Delta_i \Psi_F) - 2 \binom{N}{2} \int [\overline{\Psi_F} \nabla_1 \Psi_F]_{x_1=x_2-b}^{x_1=x_2+b} \\
&= -E_0 \binom{N}{2} \int_{A_{12}} |\Psi_F|^2 - \underbrace{\int [\partial_y \gamma^{(2)}(x_1, x_2; y, x_2)|_{y=x_1}]_{x_2-b}^{x_2+b} dx_2}_{\kappa_1}
\end{aligned} \tag{1.88}$$

Again using the bound on $\rho^{(2)}$ we find to leading order in L and b

$$E_1^{(2)} = -E_0 \frac{1}{2} \frac{\pi^2}{9} N \rho^3 b^3 - \kappa_1. \tag{1.89}$$

The last contributions are $E_1^{(3)} = \binom{N}{2} \int_{A_{12}} \sum_{i < j}^N v_{ij} |\tilde{\Psi}|^2 = \binom{N}{2} \int_{A_{12}} v_{12} |\tilde{\Psi}|^2 + \binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} |\tilde{\Psi}|^2$ and $E_1^{(4)} = \int_{A_{12}} \sum_{i=3}^N |\nabla_i \tilde{\Psi}|^2$. First we notice that

$$\begin{aligned}
&\binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} |\tilde{\Psi}|^2 \\
&\leq C'_1 \int_{A_{12} \cap \text{supp}(v_{34})} v(x_3 - x_4) \rho^{(4)}(x_1, x_2, x_3, x_4) + C'_2 \int_{A_{12} \cap \text{supp}(v_{23})} v(x_2 - x_3) \rho^{(3)}(x_1, x_2, x_3).
\end{aligned} \tag{1.90}$$

To leading order in L , $|x_3 - x_4|$ and $|x_1 - x_2|$ we find that

$$\rho^{(4)}(x_1, x_2, x_3, x_4) = \text{const. } \rho^8 (x_1 - x_2)^2 (x_3 - x_4)^2 \tag{1.91}$$

and to leading order in L , $|x_1 - x_2|$ and $|x_2 - x_3|$ we find

$$\rho^{(3)}(x_1, x_2, x_3) = \text{const. } \rho^9 \underbrace{(x_1 - x_3)^2}_{=[(x_1-x_2)+(x_2-x_3)]^2} (x_1 - x_2)^2 (x_2 - x_3)^2. \tag{1.92}$$

Therefore we have

$$\begin{aligned}
&\binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N v_{ij} |\tilde{\Psi}|^2 \\
&\leq C' \left(N^2 (\rho b)^3 \rho^3 \int x^2 v(x) dx + N (\rho b)^3 \rho^5 \int x^4 v(x) dx + N (\rho b)^4 \rho^4 \int x^3 v(x) dx \right. \\
&\quad \left. + N (\rho b)^5 \rho^3 \int x^2 v(x) dx \right) \\
&\leq C' N^2 (\rho b)^5 \rho \int v = \text{const. } E_0 N (\rho b)^3 \left(b \int v \right)
\end{aligned} \tag{1.93}$$

and then we find that

$$\begin{aligned}
E_1 &= E_1^{(1)} + E_1^{(2)} + E_1^{(3)} + E_1^{(4)} \\
&\leq \frac{2\pi^2}{3} N \rho^3 a + 2 \binom{N}{2} \int_{A_{12}} \left(\bar{\Psi}(-\Delta_1) \tilde{\Psi} + \frac{1}{2} \sum_{i=3}^N \left| \nabla_i \tilde{\Psi} \right|^2 + \frac{1}{2} v_{12} \left| \tilde{\Psi} \right|^2 \right) + E_0 N (\rho b)^3 \text{const.} \left(1 + b \int v \right)
\end{aligned} \tag{1.94}$$

Using the two body scattering equation this implies

$$\begin{aligned}
E_1 &\leq \frac{2\pi^2}{3} N \rho^3 a + 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \omega(-\Delta_1) \frac{\Psi_F}{(x_1 - x_2)} \\
&\quad + 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} (\nabla_1 \omega) \nabla_1 \frac{\Psi_F}{(x_1 - x_2)} \\
&\quad + \binom{N}{2} \int_{A_{12}} \sum_{i=3}^N \bar{\Psi} \frac{\omega}{(x_1 - x_2)} (-\Delta_i) \Psi_F \\
&\quad - E_0 \frac{1}{2} \frac{\pi^2}{9} N \rho^3 b^3 + \text{const.} \quad E_0 N (\rho b)^3 \left(b \int v \right)
\end{aligned} \tag{1.95}$$

Now using that to leading order in L and b we have

$$\begin{aligned}
&\binom{N}{2} \int_{A_{12}} \sum_{i=3}^N \bar{\Psi} \frac{\omega}{(x_1 - x_2)} (-\Delta_i) \Psi_F \\
&= E_0 \binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{(x_1 - x_2)} \Psi_F \right|^2 - 2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \frac{\omega}{(x_1 - x_2)} (-\Delta_1) \Psi_F,
\end{aligned} \tag{1.96}$$

$$\binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{(x_1 - x_2)} \tilde{\Psi} \right|^2 \leq C_1 b^2 \pi^2 \rho^4 L b = C_1 N \rho^3 b^3 \tag{1.97}$$

and that

$$2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \frac{\omega}{(x_1 - x_2)} (-\Delta_1) \Psi_F \leq C_2 N \rho^2 (\rho b)^3 \tag{1.98}$$

we find that

$$\binom{N}{2} \int_{A_{12}} \sum_{i=3}^N \bar{\Psi} \frac{\omega}{(x_1 - x_2)} (-\Delta_i) \Psi_F \leq C E_0 N (\rho b)^3. \tag{1.99}$$

Furthermore we find to leading order in N and ρb that

$$2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} \omega(-\Delta_1) \frac{\Psi_F}{(x_1 - x_2)} = \frac{\pi^2}{15} N \rho^2 (\rho b)^3, \tag{1.100}$$

and that

$$2 \binom{N}{2} \int_{A_{12}} \bar{\Psi} (\nabla_1 \omega) \nabla_1 \frac{\Psi_F}{(x_1 - x_2)} = \frac{\pi^2}{45} N \rho^2 (\rho b)^3. \tag{1.101}$$

Combining everything we find

$$E_1 \leq E_0 \left(2 \rho a + \text{const.} \quad N (\rho b)^3 \left[1 + b \int v \right] \right) \tag{1.102}$$

1.2.4 Calculating E_2

Recall that $E_2 = E_2^{(1)} + E_2^{(2)}$ with

$$\begin{aligned} E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \Psi_F|^2 \\ E_2^{(2)} &= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^N |\nabla_i \Psi_F|^2 \end{aligned} \quad (1.103)$$

To estimate these, we first split them in two terms each and use partial integration. Consider first $E_2^{(1)}$:

$$\begin{aligned} E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\nabla_i \Psi_F|^2 \\ &= \binom{N}{2} 2N \left(\int_{A_{12} \cap A_{13}} |\nabla_1 \Psi_F|^2 + 2 \int_{A_{12} \cap A_{13}} |\nabla_2 \Psi_F|^2 \right) + \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=4}^N |\nabla_i \Psi_F|^2 \end{aligned} \quad (1.104)$$

For the second term, we can perform partial integration directly, in order to obtain

$$\begin{aligned} \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=3}^N |\nabla_i \Psi_F|^2 &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=3}^N \overline{\Psi_F} (-\Delta_i \Psi_F) \\ &\leq E_0 N^3 \int_{A_{12} \cap A_{23}} |\Psi_F|^2 - N^3 \int_{A_{12} \cap A_{23}} \sum_{i=1}^3 \overline{\Psi_F} (-\Delta_i \Psi_F) \\ &\leq 2E_0 \int_{[0,L]} \int_{[x_2-b, x_2+b]} \int_{x_2-b, x_2+b} \rho^{(3)}(x_1, x_2, x_3) dx_3 dx_1 dx_2 - N^3 \int_{A_{12} \cap A_{23}} \sum_{i=1}^3 \overline{\Psi_F} (-\Delta_i \Psi_F) \end{aligned} \quad (1.105)$$

Changing variable $y_1 = x_1 - x_2$, $y_3 = x_3 - x_2$ and using translational invariance, we find

$$\begin{aligned} 2E_0 L \int_{[-b,b]} \int_{[-b,b]} \gamma^{(3)}(y_1, 0, y_3) dy_1 dy_3 &\approx \text{const.} \quad E_0 L \rho^9 \int_{[-b,b]} \int_{[-b,b]} y_1^4 y_3^2 dy_1 dy_3 \\ &= \text{const.} \quad E_0 N (b\rho)^8. \end{aligned} \quad (1.106)$$

Using Wick's theorem, we find that to leading order in $L\rho$, $|x_1 - x_2|$, $\rho|x_2 - x_3|$, and $\rho|x_1 - x_3|$ we have

$$\left(\partial_{x_1} \partial_{y_1} \gamma^{(3)}(x_1, x_2, x_3; y_1, y_2, y_3) \right) \Big|_{y=x} = \text{const.} \quad \rho^9 (x_2 - x_3)^2 ((x_1 - x_3) + (x_1 - x_2))^2 \quad (1.107)$$

and

$$\left(\partial_{y_1}^2 \gamma^{(3)}(x_1, x_2, x_3; y_1, y_2, y_3) \right) \Big|_{y=x} = \text{const.} \quad \rho^9 (x_1 - x_2)(x_1 - x_3)(x_2 - x_3)^2 \quad (1.108)$$

Thus we find

$$\binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^3 \left(|\nabla_i \Psi_F|^2 - \overline{\Psi_F}(-\Delta_i \Psi_F) \right) \leq \tilde{C}_1 \frac{\pi^2}{3} \rho^9 L b^6 = \tilde{C}_1 E_0 (b\rho)^6. \quad (1.109)$$

Collecting everything we find

$$E_2^{(1)} \leq \text{const. } E_0 (\rho b)^6 (1 + N(\rho b)^2). \quad (1.110)$$

To estimate $E_2^{(2)}$ use integration by parts

$$\begin{aligned} E_2^{(2)} &= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \left(4 |\nabla_1 \Psi_F|^2 + \sum_{i=5}^N |\nabla_i \Psi_F|^2 \right) \\ &= \binom{N}{2} \binom{N-2}{2} \left(4 \int_{|x_3-x_4|<b} [\overline{\Psi_F} \nabla_1 \Psi_F]_{x_1=x_2-b}^{x_1=x_2+b} + \int_{A_{12} \cap A_{34}} \sum_{i=1}^N \overline{\Psi_F}(-\Delta_i \Psi_F) \right) \\ &= 4 \int_{x_2 \in [0, L]} \int_{|x_3-x_4|<b} \left[\partial_{y_1} \gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, x_2, x_3, x_4) \Big|_{y_1=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} + E_0 \int_{A_{12} \cap A_{34}} \rho^{(4)}(x_1, \dots, x_4). \end{aligned} \quad (1.111)$$

We find by straightforward computation that to leading order in ρL and $|x_3 - x_4|$ we have

$$\left| \left[\partial_y \gamma^{(4)}(x_1, x_2, x_3, x_4; y, x_2, x_3, x_4) \Big|_{y=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} \right| \leq \text{const. } \rho^8 b (x_3 - x_4)^2 \quad (1.112)$$

and we therefore get

$$4 \int_{x_2 \in [0, L]} \int_{|x_3-x_4|<b} \left[\partial_{y_1} \gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, y_2, y_3, y_4) \Big|_{y_1=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} = \text{const. } E_0 N (\rho b)^4 \quad (1.113)$$

Furthermore we find that to leading order in L , $|x_1 - x_2|$, and $|x_3 - x_4|$ we have

$$\rho^{(4)}(x_1, x_2, x_3, x_4) \leq \text{const. } \rho^8 (x_1 - x_2)^2 (x_3 - x_4)^2 \quad (1.114)$$

from which it follows that

$$E_0 \int_{A_{12} \cap A_{34}} \rho^{(4)}(x_1, \dots, x_4) \leq \text{const. } E_0 N^2 (\rho b)^6. \quad (1.115)$$

Collecting all terms we find the upper bound

$$E \leq E_0 \left(1 + 2\rho a + \text{const. } N(\rho b)^3 \left(1 + b \int v \right) \right) \quad (1.116)$$

1.3 Localization with Dirichlet b.c.

We will in this section localize in smaller boxes, in order to have better control on the error. The localization is straightforward with Dirichlet boundary conditions, as gluing the wavefunctions for each box together is simple, since the wavefunctions vanish at the boundaries. This we consider the state $\Psi_{\text{full}} = \sum_{i=1}^M \Psi_\ell(x_1^i, \dots, x_{\tilde{N}}^i)$, where $(x_1^i, \dots, x_{\tilde{N}}^i)$ are the particles in box i and ℓ is the length of each box. Of course $\cup_{i=1}^M \{x_1^i, \dots, x_{\tilde{N}}^i\} = \{x_1, \dots, x_N\}$ and $\{x_1^i, \dots, x_{\tilde{N}}^i\} \cap \{x_1^j, \dots, x_{\tilde{N}}^j\} = \emptyset$ for $i \neq j$, such that $M\tilde{N} = N$. The boxes are of length $\ell = L/M - b$, and are equally spaced through out $[0, L]$ such that they are a distance of b from each other. This is to make sure that no particle interact between boxes. The full energy is then given by

$$E \leq M e_0 \left(1 + 2\tilde{\rho}a + \text{const. } \tilde{N}(b\tilde{\rho})^3 \left(1 + b \int v_{\text{reg}} \right) \right) \quad (1.117)$$

with $e_0 = \frac{\pi^2}{3} \tilde{N} \tilde{\rho}^2 (1 + \text{const. } \frac{1}{\tilde{N}})$ and $\tilde{\rho} = \tilde{N}/\ell = \rho/(1 - \frac{bM}{L}) \simeq \rho(1 + bM/L)$. Thus, choosing M such that $bM/L \ll 1$ we have

$$E \leq E_0 \left(1 + 2\rho a + \text{const. } \frac{M}{N} + \text{const. } 2\rho abM/L + \text{const. } \tilde{N}(b\rho)^3 \left(1 + b \int v_{\text{reg}} \right) \right). \quad (1.118)$$

Now in fact, we would choose $\tilde{N} = N/M = \rho L/M \gg 1$, *i.e.* $M/L \ll \rho$. It is clear that we minimize the error, by choosing $b = R_0$ the range of the potential. Furthermore, setting $x = M/N$ we see that the error is

$$\text{const. } \left[(1 + 2\rho^2 ab)x + x^{-1}(b\rho)^3 \left(1 + b \int v_{\text{reg}} \right) \right] \quad (1.119)$$

Optimizing in x we find $x = M/N = \frac{(b\rho)^{3/2}(1+b \int v_{\text{reg}})^{1/2}}{1+2\rho^2 ab} \simeq (b\rho)^{3/2} (1 + b \int v_{\text{reg}})^{1/2}$, which gives the error

$$\text{const. } (R_0\rho)^{3/2} \left(1 + R_0 \int v_{\text{reg}} \right)^{1/2} \quad (1.120)$$

Thus we arrive at the following result

Theorem 1. *Let the two-body potential $v \in L^1([0, L]) + \text{h.c.p.}$ be fixed, with two-body s -wave scattering length a . Then bosonic N -body groundstate energy satisfies the upper bound*

$$E \leq E_0 \left(1 + 2\rho a + \mathcal{O} \left((R\rho)^{3/2} \left(1 + R \int v_{\text{reg}} \right)^{1/2} \right) \right) \quad (1.121)$$

where E_0 is the free fermionic groundstate energy.

here h.c.p denotes the space of hard core potentials

1.4 Periodic boundary conditions revised

Another approach, would be to prove the result with periodic boundary conditions, then use the bound [[2], lemma 4 or [3] lemma 2.1.12]

$$\langle \Psi_D | H_L^D | \Psi_D \rangle \leq \langle \Psi_P | H_{L-2d}^P | \Psi_P \rangle + \frac{4N}{d^2} \|\Psi\|^2. \quad (1.122)$$

In this case, we get errors from the periodic b.c. calculation plus errors $4N/d^2 + E_0 \frac{d}{L}$, where the last one comes from change in the density assuming that $d/L \ll 1$. Optimizing in d this gives an error of const. $E_0 \frac{1}{N^{2/3}}$. Thus the total result after localization is

$$E \leq E_0 \left(1 + 2\rho a + \text{const.} \left(\frac{M}{N} \right)^{2/3} + \text{const.} 2\rho abM/L + \text{const.} \tilde{N}(b\rho)^3 \left(1 + b \int v_{\text{reg}} \right) \right). \quad (1.123)$$

And optimizing in M and setting $b = R_0$ we find

$$E_0 \left(1 + 2\rho a + \mathcal{O} \left((R\rho)^{6/5} \left(1 + R \int v_{\text{reg}} \right)^{1/2} \right) \right) \quad (1.124)$$

which is not quite as good, as the bound computed directly with Dirichlet b.c.

2 Lower bound

We will in this section, prove a matching lower bound to the upper bound found above. To begin with, we prove the weaker result that the dilute Bose gas with repulsive two-body potentials, is lower bounded to leading order, by the free Fermi energy.

Let Ψ be the groundstate of \mathcal{E} , we then define $\psi \in L^2([0, \ell - (n-1)R]^n)$ by $\psi(x_1, x_2, \dots, x_n) = \Psi(x_1, R + x_2, \dots, (n-1)R + x_n)$ for $x_1 \leq x_2 \leq \dots \leq x_n$ and symmetrically extended.

Lemma 2. *For any function $\psi \in H^1(\mathbb{R})$ such that $\psi(0) = 0$ then we have*

$$\int_{[0,R]} |\partial\psi|^2 \geq \max_{[0,R]} |\psi|^2 / R \quad (2.1)$$

Proof. write $\psi(x) = \int_0^x \psi'(t) dt$, and find that

$$|\psi(x)| \leq \int_0^x |\psi'(t)| dt. \quad (2.2)$$

Hence $\max_{x \in [0,R]} |\psi(x)| \leq \int_0^R |\psi'(t)| dt \leq \sqrt{R} \left(\int |\psi'(t)|^2 dt \right)^{1/2}$ □

In the Fermi case, we can estimate the norm loss in the following way

$$\langle \psi | \psi \rangle = 1 - \int_B |\Psi|^2 \geq 1 - \sum_{i < j} \int_{B_{ij}} |\Psi|^2 \quad (2.3)$$

where $B = \{x \in \mathbb{R}^n \mid \min_{i,j} |x_i - x_j| < R\}$, and $B_{ij} = \{x \in \mathbb{R}^n \mid \mathbf{r}_i(x) = |x_i - x_j| < R\}$. Hence by the Sobolev inequality above we have

$$\langle \psi | \psi \rangle \geq 1 - \sum_{i < j} \int R \max_{\mathbf{r}_i(x)=|x_i-x_j|<R} |\Psi|^2 d\bar{x}^i \geq 1 - R^2 \sum_{i < j} \int_{B_{ij}} |\partial_i \Psi|^2 \geq 1 - R^2 E \geq 1 - \text{const. } n(\rho R)^2. \quad (2.4)$$

For bosons we need to following lemma

Lemma 3. *Let ψ be defined as above, then*

$$1 - \langle \psi | \psi \rangle \leq \text{const.} \left(R^2 \sum_{i < j} \int_{B_{ij}} |\partial_i \Psi|^2 + R(R-a) \sum_{i < j} \int v_{ij} |\Psi|^2 \right) \quad (2.5)$$

Proof. Notice that by (2.1) we have for any $\phi \in H^1$,

$$||\phi(x)| - |\phi(x')||^2 \leq |\phi - \phi(x')|^2 \leq R \left(\int_{[0,R]} |\partial \phi|^2 \right), \quad (2.6)$$

for $x, x' \in [0, R]$. Furhtermore,

$$|\phi(x)|^2 - |\phi(x')|^2 = (|\phi(x)| - |\phi(x')|)^2 + 2(|\phi(x)| - |\phi(x')|) |\phi(x')| \leq 2(|\phi(x)| - |\phi(x')|)^2 + |\phi(x')|^2 \quad (2.7)$$

So for It follows that

$$\max_{x \in [0,R]} |\phi|^2 \leq 2R \int_{[0,R]} |\partial \phi|^2 + 2 \min_{x \in [0,R]} |\phi(x')|^2 \quad (2.8)$$

Viewing Ψ as a function of x_i we have

$$2 \min_{\mathbf{r}_i(x)=|x_i-x_j|<R} |\Psi|^2 \geq \max_{\mathbf{r}_i(x)=|x_i-x_j|<R} |\Psi|^2 - 4R \left(\int_{\mathbf{r}_i(x)=|x_i-x_j|<R} |\partial_i \Psi|^2 \right). \quad (2.9)$$

Hence we find

$$\begin{aligned} 2 \sum_{i < j} \int v_{ij} |\Psi|^2 &\geq 2 \sum_{i < j} \int_{B_{ij}} v_{ij} |\Psi|^2 \\ &\geq \left(\int v \right) \sum_{i < j} \int \left(\max_{B'_{ij}} |\Psi|^2 - 4R \left(\int_{B'_{ij}} |\partial_i \Psi|^2 dx_i \right) \right) d\bar{x}^i \\ &\geq \frac{4}{R-a} \sum_{i < j} \left(\frac{1}{2R} \int_{B_{ij}} |\Psi|^2 - 4R \int_{B_{ij}} |\partial_i \Psi|^2 \right) d\bar{x}^i \end{aligned} \quad (2.10)$$

where $B_{ij} = \{x \in \mathbb{R}^n \mid \mathbf{r}_i(x) = |x_i - x_j| < R\}$ and $B'_{ij} = \{x_i \in \mathbb{R} \mid \mathbf{r}_i(x) = |x_i - x_j| < R\}$. Now noticing that $\sum_{i < j} \int_{B_{ij}} |\Psi|^2 \geq 1 - \langle \psi | \psi \rangle$ we see that

$$1 - \langle \psi | \psi \rangle \leq \text{const.} \left(R^2 \sum_{i < j} \int_{B_{ij}} |\partial_i \Psi|^2 + R(R-a) \int \sum_{i < j} v_{ij} |\Psi|^2 \right) \quad (2.11)$$

□

Choosing $R \geq 2|a|$ we clearly see that $\langle \psi | \psi \rangle \geq 1 - \text{const. } R^2 E$.

The following lemma will also be useful

Lemma 4 (Dyson). *Let $R > R_0 = \text{range}(v)$, then*

$$\int_{[0,R]} |\partial \varphi|^2 + \frac{1}{2} v |\varphi|^2 \geq \frac{2}{R-a} \varphi(R) \quad (2.12)$$

where a is the s -wave scattering length.

Proof. This follows from the variational scattering problem, by comparing left-hand side to the minimizer of the scattering functional. □

This lemma will essentially allows us to replace the potential by a shell potential of range R and strength $\frac{2}{R-a}$, where

2.1 Bootstrapping

We have seen in the previous section that the free Fermi energy provides a lower bound to the ground state energy of the dilute Bose gas with a repulsive pair potential. Now this bound can be further improved, by noticing that the computation we did also reveals that most of the energy comes from the region where particles are distance at least R from each other. The energy contribution coming from the region where at least one pair is within distance R can be bounded by a bootstrapping method. To do that we reduce to a Lieb-Liniger type model, in the same way as above, but keeping some of the energy. By doing this, we can bound the mass thrown away by comparing the already established upper bound, and the lower bound achieved by this Lieb-Liniger reduction.

Lemma 5. *We have for any $\epsilon > 0$*

$$1 - \langle \psi | \psi \rangle \leq \text{const. } \frac{1}{(1-\epsilon)} \frac{1}{\epsilon} n \rho^2 R^2 ((\rho R) + \rho(R-a)) = \text{const. } n \rho^2 R^2 \left(\rho R + n(\rho R)^2 + \frac{1}{n} \right) \quad (2.13)$$

Proof. By splitting $\int_{[-R,R]} |\partial \phi|^2 + \frac{1}{2} v |\phi|^2$, and use Dyson's lemma on one term and lemma 3 on

the other, we get

$$\begin{aligned}
& \int \sum_i |\partial_i \Psi|^2 + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq \\
& \int \sum_i |\partial_i \Psi|^2 \chi_{\mathbf{r}_i(x) > R} + \epsilon \sum_i \frac{2}{R-a} (\delta(\mathbf{r}_i(x) + R) + \delta(\mathbf{r}_i(x) - R)) |\Psi|^2 \\
& \quad + \sum_{i < j} (1 - \epsilon) \left(\sum_{i < j} \int_{B_{ij}} |\partial_i \Psi|^2 + \int \sum_{i < j} v_{ij} |\Psi|^2 \right) \\
& \geq E_{LL}^{\tilde{\rho}, \tilde{\ell}, \tilde{c} = \frac{2\epsilon}{R-a}} \langle \psi | \psi \rangle + \frac{(1 - \epsilon)}{R^2} (1 - \langle \psi | \psi \rangle) \\
& \geq n \rho^2 \left(1 + \frac{2}{\epsilon} \rho(R-a) + 2\rho R - \text{const.} \left(n(\rho R)^2 + \frac{1}{n} \right) \right) + \frac{1 - \epsilon}{R^2} (1 - \langle \psi | \psi \rangle)
\end{aligned} \tag{2.14}$$

From this and the known upper bound, it follows that

$$1 - \langle \psi | \psi \rangle \leq \text{const.} \cdot \frac{1}{(1 - \epsilon)} \frac{1}{\epsilon} n \rho^2 R^2 ((\rho R) + \rho(R-a)) = \text{const.} \cdot n \rho^2 R^2 \left(\rho R + n(\rho R)^2 + \frac{1}{n} \right) \tag{2.15}$$

□

Hence we get

Theorem 2. *We have*

$$E \geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + \text{const.} (\rho R)^{4/3} \right) \tag{2.16}$$

Proof. By using Dyson's lemma, we reduce as above to a Lieb-Liniger model with volume $\tilde{\ell}$, density $\tilde{\rho}$, and coupling c , and we have $\tilde{\ell} = \ell - (n-1)R$, $\tilde{\rho} = \frac{n}{\tilde{\ell}} \approx \rho(1 + \rho R)$ and $c = \frac{2}{R-a}$. Hence we have

$$\begin{aligned}
E & \geq \mathcal{E}_{LL}^{\tilde{\rho}, \tilde{\ell}, c}(\psi) \geq E_{LL}^{\tilde{\rho}, \tilde{\ell}, c} \langle \psi | \psi \rangle \\
& \geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + \text{const.} \frac{1}{n} \right) (1 - \text{const.} (n^2(\rho R)^4 + n(\rho R)^3 + (\rho R)^2)) \\
& \geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + \text{const.} \frac{1}{n} + n^2(\rho R)^4 + n(\rho R)^3 + (\rho R)^2 \right)
\end{aligned} \tag{2.17}$$

Choosing $n = (\rho R)^{-4/3}$ we have

$$E \geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + \text{const.} (\rho R)^{4/3} \right) \tag{2.18}$$

□

By a localization argument, this proves that $E \geq N \frac{\pi^2}{3} \rho^2 (1 + 2\rho a + \mathcal{O}((\rho R)^{4/3}))$ for any N with $N \gg (\rho R)^{-4/3} \gg N^{-1}$.

2.2 Lieb-Liniger model lower bound

In the proof above, we use that the Lieb Liniger energy is lower bounded by $E_{LL}^{\rho,\ell,c} \geq \frac{\pi^2}{3}\rho^2(1 + 4\rho/c)$. This we will show in this subsection we show this lower bound.

We use that the energy in the Lieb Liniger model, is determined by the sytem of equation ((3.3) and (3.18)–(3.20) in [1])

$$E_{LL}^{\rho,\ell,c=\gamma\rho} = N\rho^2 e(\gamma), \quad (2.19)$$

$$e(\gamma) = \frac{\gamma^3}{\lambda^3} \int_{-1}^1 g(x)x^2 dx, \quad (2.20)$$

$$2\pi g(y) = 1 + 2\lambda \int_{-1}^1 \frac{g(x) dx}{\lambda^2 + (x-y)^2}, \quad (2.21)$$

$$\lambda = \gamma \int_{-1}^1 g(x) dx. \quad (2.22)$$

Neglecting $(x-y)^2$ in the denominator of (2.21), we see that $g \leq \frac{1}{2\pi} + 2\frac{1}{\lambda} \int_{-1}^1 g(x) dx$. On the other hand (2.22) shows that $e(\gamma) = \frac{\int_{-1}^1 g(x)x^2 dx}{(\int_{-1}^1 g(x) dx)^3}$. Hence we denote $\int_{-1}^1 g(x) dx = M$, and notice that we have $g \leq \frac{1}{2\pi} (1 + \frac{2M}{\lambda})$. It is now easily verified that, $\int_{-1}^1 g(x)x^2 dx$ with M and $g \leq \frac{1}{2\pi} (1 + \frac{2M}{\lambda}) = \frac{1}{2\pi} (1 + 2\gamma^{-1})$ is mininmized by $g = K\chi_{[-M/(2K), M/(2K)]}$, with $K = \frac{1}{2\pi} (1 + \frac{2}{\gamma})$. This gives us $\int_{-1}^1 g(x)x^2 dx = \frac{M^3}{3K^2}$ so that we have $e(\gamma) \geq \frac{1}{3K^2} = \frac{\pi^2}{3} \left(\frac{\gamma}{\gamma+2} \right)^2 \geq \frac{\pi^2}{3} (1 - \frac{4}{\gamma})$ for $\gamma > 0$.

References

- [1] Elliott H. Lieb and Werner Liniger, *Exact analysis of an interacting bose gas. i. the general solution and the ground state*, Phys. Rev. **130** (1963), 1605–1616.
- [2] Simon Mayer and Robert Seiringer, *The free energy of the two-dimensional dilute Bose gas. II. Upper bound*, Journal of Mathematical Physics **61** (2020), no. 6, 061901.
- [3] D.W. Robinson, *The thermodynamic pressure in quantum statistical mechanics*, Lecture Notes in Physics, Springer Berlin Heidelberg, 2014.