Jellium and the Uniform Electron Gas in 2 Dimensions

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Abstract

We prove the 2-dimensional version of a result from [6], that the Jellium model and the Uniform Electron Gas are equivalent in 3 dimensions. Moreover, we consider the Jellium energy of different lattice configurations and compare these to known lower bounds. The energy of the triangular lattice is within 1 ‰ of the known lower bound.

Contents

1 The Models

The Jellium functional is

$$\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N) = -\sum_{j<k} \log|x_j - x_k| + \sum_{j=1}^{N} \int_{\Omega_N} \log|x_j - y| \, \mathrm{d}y - \frac{1}{2} \iint_{\Omega_N \times \Omega_N} \log|x - y| \, \mathrm{d}x \, \mathrm{d}y$$

for a domain Ω_N of size $|\Omega_N| = N$. The electrons are thought of as discrete classical particles in a uniform (positive) background, such that the entire system is neutral. The electrons and background all interact through Coulomb interaction, in 2 dimensions given by $-\log|x|$. The long range behaviour of the logarithm means that this setting is somewhat different from the 3-dimensional case.

In [11] it is shown that the thermodynamical limit

$$e_{\text{Jel}} = \lim_{\Omega_N \nearrow \mathbb{R}^2} \min_{x_1,\ldots,x_N \in \mathbb{R}^2} \frac{\mathcal{E}_{\text{Jel}}(\Omega_N, x_1, \ldots, x_N)}{|\Omega_N|}$$

exists under fairly non-restrictive conditions on the domain Ω_N.

The other important functional, which we study is that of the indirect energy. Given an N-particle probability density $\mathbb{P}$ (meaning $\mathbb{P}$ is a probability measure on $\mathbb{R}^{2N}$) we define the indirect energy as

$$\mathcal{E}_{\text{Ind}}(\mathbb{P}) = -\int \sum_{j<k} \log |x_j - x_k| \, \mathrm{d}\mathbb{P}(x_1, \ldots, x_N) + \frac{1}{2} \iint \log |x - y| \rho_{\mathbb{P}}(x) \rho_{\mathbb{P}}(y) \, \mathrm{d}x \, \mathrm{d}y,$$

where $\rho_{\mathbb{P}}$ is the one-particle density associated to $\mathbb{P}$, i.e. the sum of all the marginals

$$\rho_{\mathbb{P}} = \sum_{j=1}^{N} \int_{\mathbb{R}^{2(N-1)}} \mathrm{d}\mathbb{P}(x_1, \ldots, \hat{x}_j, \ldots, x_N).$$

We are interested in keeping the density fixed, and so, for any density ρ with $\int \rho \, \mathrm{d}x = N$ we define

$$\mathcal{E}_{\text{Ind}}(\rho) = \min_{\mathbb{P}: \rho_{\mathbb{P}} = \rho} \mathcal{E}_{\text{Ind}}(\mathbb{P})$$

Again, we are interested in the thermodynamic limit, and for a system of uniform density, i.e.

$$e_{\text{UEG}} = \lim_{\Omega_N \nearrow \mathbb{R}^2} \frac{\mathcal{E}_{\text{Ind}}(\mathbb{1}_{\Omega_N})}{|\Omega_N|}.$$

By a slight modification of the argument in [5] we show in section 5 that indeed this limit exists. (We in fact show a slightly stronger version.) One would imagine that the following is true.

Conjecture 1.1. *Suppose ρ_N is a sequence of densities with $\int \rho_N \, \mathrm{d}x = N$ and Ω_N is a sequence of sufficiently regular domains with $|\Omega_N| = N$. Moreover, suppose ρ_N satisfies*

$$\rho_N \equiv 1 \textit{ well inside } \Omega_N, \qquad \rho_N \equiv 0 \textit{ well outside } \Omega_N, \qquad \rho_N \textit{ bounded uniformly in } N.$$

Then

$$e_{\text{UEG}} = \lim_{\Omega_N \nearrow \mathbb{R}^2} \frac{\mathcal{E}_{\text{Ind}}(\rho_N)}{|\Omega_N|}$$

exists and is independent of the exact sequences ρ_N and Ω_N.

This, however, we have been unable to prove. What we do prove in section 5, however, is the following slightly weaker statement.

Proposition 1.2. *Suppose ρ_N is a sequence of densities with $\int \rho_N \, \mathrm{d}x = N$ and Ω_N is a sequence of sufficiently regular (explained in detail in the proof) domains with $|\Omega_N| = N$. Moreover, suppose ρ_N satisfies*

$$\rho_N \equiv 1 \textit{ well inside } \Omega_N, \qquad \rho_N \equiv 0 \textit{ well outside } \Omega_N, \qquad 0 \leq \rho_N \leq 1.$$

Then

$$e_{\text{UEG}} = \lim_{\Omega_N \nearrow \mathbb{R}^2} \frac{\mathcal{E}_{\text{Ind}}(\rho_N)}{|\Omega_N|}$$

exists and is independent of the exact sequences ρ_N and Ω_N.

Here "well in-/outside" means at a distance more than $\ell \ll |\Omega_N|^{1/2}$ from the boundary.

Our main theorem is

Theorem 1.3. *We have* $e_{\text{Jel}} = e_{\text{UEG}}$.

The first few sections deals with proving this theorem.

The inequality one way is the following argument. Let $\mathbb{P}$ be any N-particle probability measure with $\rho_{\mathbb{P}} = \mathbb{1}_{\Omega_N}$. Then,

$$-\int \sum_{j<k} \log|x_j - x_k| \, \mathrm{d}\mathbb{P}(x_1, \ldots, x_N) + \frac{1}{2} \iint_{\Omega_N \times \Omega_N} \log|x-y| \, \mathrm{d}x \, \mathrm{d}y$$
$$= \int \mathcal{E}_{\text{Jel}}(\Omega_N, x_1, \ldots, x_N) \, \mathrm{d}\mathbb{P}(x_1, \ldots, x_N) \geq \min \mathcal{E}_{\text{Jel}}(\Omega_N, x_1, \ldots, x_N).$$

Optimising over $\mathbb{P}$ and taking the thermodynamical limit we thus get

$$e_{\text{EUG}} \geq e_{\text{Jel}}.$$

In order to get the reverse inequality we will superficially introduce a crystal structure to the Jellium configuration. This is similar to (and inspired by) the floating crystal argument from [6].

2 Upper Bound of the Indirect Energy - Simple Argument

We give here a simple argument assuming conjecture 1.1 based on [6] to show that

$$e_{\text{UEG}} \leq \frac{\mathcal{E}_{\text{per},\ell}(x_1, \ldots, x_n)}{n}$$

for some appropriate functional $\mathcal{E}_{\text{per},\ell}$ and any n points $x_1, \ldots, x_n$.

In the next section we give the more involved argument using only proposition 1.2.

Hence, consider any arrangement of n points $x_1, \ldots, x_n$ in the cube C_ℓ of side length $\ell = n^{1/2}$ (centered at 0). Adding a background shifted by the center of mass $\tau = \frac{1}{n}\sum_{j=1}^n x_j$ we get an arrangement with no dipole moment:

$$\int y \left(\sum_{j=1}^n \delta_{x_j}(y) - \mathbb{1}_{C_\ell + \tau}(y) \right) \mathrm{d}y = 0$$

We copy this arrangement periodically in the larger cube

$$\Omega_N = \bigcup_{\substack{k \in \mathbb{Z}^2 \\ |k_1|, |k_2| \leq K}} C_\ell + \ell k$$

of volume $N = \ell^2(2K+1)^2$. We want the "crystal" to float, so we find a slightly larger cube C with $\Omega_N + 2C_\ell \subset C$ and $|C \setminus \Omega_N| = M = O\left(N^{1/2}\right)$ an integer.

We consider the following trial state of a floating crystal

$$\mathbb{P} = \frac{1}{\ell^2} \int_{C_\ell} \bigotimes_{\substack{j=1,\ldots,n \\ k \in \mathbb{Z}^2 \\ |k_1|, |k_2| \leq K}} \delta_{x_j + \ell k + a} \otimes \left(\frac{\mathbb{1}_{C \setminus (\Omega_N + a + \tau)}}{M} \right)^{\otimes M} \mathrm{d}a.$$

That is, we shift the "crystal" around, so that we get a uniform density, but we also include to uniform charge outside the crystal (in $C \setminus \Omega_N$) in order to cancel the boundary effects of building up charge in one end. The associated density is

$$\rho_{\mathbb{P}} = \ldots = \mathbb{1}_C + \frac{1}{n}\sum_{j=1}^{n} \mathbb{1}_{\Omega_N + x_j} - \mathbb{1}_{\Omega_N+\tau} * \frac{\mathbb{1}_{C_\ell}}{\ell^2}.$$

This density is 1 well inside Ω_N, is 0 well outside and bounded in the region in between. In order to ease notation define

$$D(f,g) := -\frac{1}{2}\iint \log|x-y| f(x)g(y)\,\mathrm{d}x\,\mathrm{d}y, \qquad D(f) := D(f,f).$$

We have that

Proposition 2.1. *Suppose f has $\int f\,\mathrm{d}x = 0$. Then $D(f) \geq 0$.*

Proof. By density we may assume that $f \in \mathcal{S}$, i.e. that f is rapidly decreasing. Define $f^{\#}(x) = f(-x)$. Note that $\widehat{f^{\#}} = \overline{\hat{f}}$. First we show that $\frac{\widehat{f^{\#}}\hat{f}}{p^2} = \frac{|\hat{f}(p)|}{p^2}$ is the Fourier transform of some function. Define $g := \frac{-1}{2\pi}\log * f^{\#} * f$. Then by [7, Theorem 6.21] we have that $g \in L^1_{\mathrm{loc}}$ and $-\Delta g = f^{\#} * f$ in $\mathcal{D}'$. Since $\log \in \mathcal{S}'$ we have that $g \in \mathcal{S}'$ and so $p^2\hat{g} = \widehat{f^{\#} * f}$ in $\mathcal{S}'$. Hence $\hat{g}(p) = 2\pi\frac{|\hat{f}(p)|^2}{p^2}$ as functions. By the assumption $\int f\,\mathrm{d}x = 0$ we have that the right-hand-side actually stays bounded (and smooth) as $p \to 0$. We conclude that $\hat{g} \in \mathcal{S}$ and so $g \in \mathcal{S}$ has a Fourier transform as a function.

Now,

$$\langle f | -\log * f\rangle = \left\langle \widehat{f^{\#} * f} \middle| \widehat{-\log} \right\rangle = 2\pi \left\langle \frac{|\hat{f}(p)|^2}{p^2} \middle| p^2 \cdot \widehat{-\log} \right\rangle = 2\pi \int \frac{|\hat{f}(p)|^2}{p^2}\,\mathrm{d}p \geq 0,$$

since by [7, Theorem 6.20] we have $-\Delta(-\log|\cdot|) = 2\pi\delta$ in $\mathcal{D}'$. □

Remark 2.2. In dimension $d = 1$ the (suitably modified) statement of the above also holds.

In fact we have the following characterisation, which holds for all f.

Proposition 2.3. *For any f we have the following characterisation of $D(f)$.*

$$D(f) = \pi \int_{|p|\leq 1} \frac{|\hat{f}(p)|^2 - |\hat{f}(0)|^2}{p^2}\,\mathrm{d}p + \pi\int_{|p|>1} \frac{|\hat{f}(p)|^2}{p^2}\,\mathrm{d}p + c|\hat{f}(0)|^2,$$

where $c = 2\pi^2(\gamma - \log 2) \approx -2.29$ and $\gamma \approx 0.577$ is the Euler-Mascheroni constant.

Proof. By density we may assume that $f \in \mathcal{S}$. Let $\eta_N \in C_c^\infty$ be a smooth radial function with

$$\eta_N(x) = 1 \text{ if } |x| \leq N, \quad \eta_N(x) = 0 \text{ if } |x| \geq 2N, \quad |\nabla\eta_N| \leq 2/N, \quad |\Delta\eta_N| \leq 2/N^2.$$

Then $\eta_N \log \in L^1$ and so has a Fourier transform as a function, $F_N := \widehat{-\log\cdot\eta_N}$. Now, for any $\psi \in \mathcal{S}$ we have $-\Delta(\psi\eta_N) = -\Delta\psi\eta_N - 2\nabla\psi\cdot\nabla\eta_N - \psi\Delta\eta_N$. Thus

$$\begin{aligned}
\left\langle p^2 F_N \middle| \hat{\psi}\right\rangle &= \langle -\log | -\Delta\psi\eta_N\rangle \\
&= \langle -\log|-\Delta(\psi\eta_N) + 2\nabla\psi\cdot\nabla\eta_N + \psi\Delta\eta_N\rangle \\
&= \langle -\Delta(-\log)|\eta_N\psi\rangle + \langle -\log|2\nabla\psi\cdot\nabla\eta_N + \psi\Delta\eta_N\rangle \\
&= 2\pi\psi(0) + \langle -\log|2\nabla\psi\cdot\nabla\eta_N + \psi\Delta\eta_N\rangle \\
&= \left\langle 1 + R_N \middle| \hat{\psi}\right\rangle
\end{aligned}$$

Where the error term R_N may be computed to be

$$R_N = -2\widehat{\frac{x}{|x|^2} \cdot \nabla\eta_N} + \widehat{\log \Delta\eta_N} \in \mathcal{S}'.$$

This is in fact a (rapidly decaying) function. Moreover, if $1 < q \le 2$ then by the Hausdorff-Young inequality

$$\|R_N\|_{L^{q'}} \le C \left\| \frac{|\nabla\eta_N|}{|x|} \right\|_{L^q} + C \,\|| \log ||\Delta\eta_N|\||_{L^q} = O\left(N^{\frac{2(1-q)}{q}}\right) + O\left(N^{\frac{2(1-q)}{q}} \log N\right) = o(1).$$

Thus for any $\phi \in L^1 \cap L^q$ we have that $\left\langle p^2 F_N \middle| \phi \right\rangle = \langle 1|\phi\rangle + o(1)$.

Since pointwise $\check{F_N} \nearrow -\log$ we have that

$$2D(f) = \langle f|-\log * f\rangle = \lim_{N\to\infty} \left\langle f \middle| \check{F_N} * f \right\rangle = 2\pi \lim_{N\to\infty} \left\langle |\hat{f}|^2 \middle| F_N \right\rangle.$$

Now, we may compute this as

$$\left\langle |\hat{f}|^2 \middle| F_N \right\rangle = \int_{|p|\ge 1} \frac{|\hat{f}(p)|^2}{p^2} p^2 F_N(p)\,\mathrm{d}p + \int_{|p|\le 1} \frac{|\hat{f}(p)|^2 - |\hat{f}(0)|^2}{p^2} p^2 F_N(p)\,\mathrm{d}p + |\hat{f}(0)|^2 \int_{|p|\le 1} F_N(p)\,\mathrm{d}p.$$

In the limit $N \to \infty$ we have that the first two summands converge, since both $\frac{|\hat{f}(p)|^2}{p^2}\mathbb{1}_{\{|p|\ge 1\}}$ and $\frac{|\hat{f}(p)|^2 - |\hat{f}(0)|^2}{p^2}\mathbb{1}_{\{|p|\le 1\}}$ are $L^1 \cap L^q$-functions for any $q < 2$. Hence the last summand also converges. We conclude that

$$D(f) = \pi \lim_{N\to\infty} \left\langle |\hat{f}|^2 \middle| F_N \right\rangle = \pi \int_{|p|\ge 1} \frac{|\hat{f}(p)|^2}{p^2}\,\mathrm{d}p + \pi \int_{|p|\le 1} \frac{|\hat{f}(p)|^2 - |\hat{f}(0)|^2}{p^2}\,\mathrm{d}p + c|\hat{f}(0)|^2$$

for some constant $c = \pi \lim_{N\to\infty} \int_{|p|\le 1} F_N(p)\,\mathrm{d}p$. In order to find this constant we consider a specific function f, namely a Gaussian. Hence, let $f(x) = e^{-x^2/2}$. Then $\hat{f}(p) = e^{-p^2/2}$ and $f * f(x) = \pi e^{-x^2/4}$. Thus

$$\begin{aligned}
D(f) &= \frac{1}{2}\langle f|-\log * f\rangle \\
&= \frac{-1}{2}\int_{\mathbb{R}^2} f * f(x) \log|x|\,\mathrm{d}x \\
&= -\frac{\pi}{2}\int_{\mathbb{R}^2} e^{-x^2/4} \log|x|\,\mathrm{d}x \\
&= -4\pi^2 \int_0^\infty e^{-y^2} \log(2y) y\,\mathrm{d}y \\
&= -2\pi^2 \log 2 - 4\pi^2 \int_0^\infty y e^{-y^2} \log y\,\mathrm{d}y \\
&= -2\pi^2 \log 2 - \pi^2 \int_0^\infty e^{-u} \log u\,\mathrm{d}u \\
&= -2\pi^2 \log 2 + \pi^2 \gamma.
\end{aligned}$$

The last integral here may be found in any integral table, $-\int_0^\infty e^{-u} \log u \, \mathrm{d}u = \gamma$ is the Euler-Mascheroni constant. For the right-hand-side we compute

$$
\begin{aligned}
&\pi \int_{|p|\geq 1} \frac{|\hat{f}(p)|^2}{p^2} \, \mathrm{d}p + \pi \int_{|p|\leq 1} \frac{|\hat{f}(p)|^2 - |\hat{f}(0)|^2}{p^2} \, \mathrm{d}p \\
&\quad = \pi \int_{|p|\geq 1} \frac{1}{p^2} e^{-p^2} \, \mathrm{d}p + \pi \int_{|p|\leq 1} \frac{e^{-p^2} - 1}{p^2} \, \mathrm{d}p \\
&\quad = 2\pi^2 \left[\int_1^\infty \frac{1}{p} e^{-p^2} \, \mathrm{d}p + \int_0^1 \frac{1}{p} \left(e^{-p^2} - 1 \right) \, \mathrm{d}p \right] \\
&\quad = 2\pi^2 \left[-\int_1^\infty \log p \cdot (-2p) e^{-p^2} \, \mathrm{d}p - \int_0^1 \log p \cdot (-2p) e^{-p^2} \, \mathrm{d}p \right] \\
&\quad = 4\pi^2 \int_0^\infty p e^{-p^2} \log p \, \mathrm{d}p \\
&\quad = \pi^2 \int_0^\infty e^{-u} \log u \, \mathrm{d}u \\
&\quad = -\pi^2 \gamma.
\end{aligned}
$$

Thus the constant c is

$$
c = D(f) - \left[\pi \int_{|p|\geq 1} \frac{|\hat{f}(p)|^2}{p^2} \, \mathrm{d}p + \pi \int_{|p|\leq 1} \frac{|\hat{f}(p)|^2 - |\hat{f}(0)|^2}{p^2} \, \mathrm{d}p \right] = 2\pi^2(\gamma - \log 2). \qquad \square
$$

We can compute the indirect energy of our trial state as

$$
\begin{aligned}
\mathcal{E}_{\mathrm{Ind}}(\mathbb{P}) &= -\int \sum_{j<k} \log |x_j - x_k| \, \mathrm{d}\mathbb{P}(x_1, \ldots, x_N) - D\left(\rho_{\mathbb{P}}\right) \\
&= \ldots \\
&= \mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N) - D\left(\frac{1}{n} \sum_{j=1}^n \mathbb{1}_{\Omega_N + x_j} - \mathbb{1}_{\Omega_N + \tau} * \frac{\mathbb{1}_{C_\ell}}{\ell^2} \right) - \frac{1}{M\ell^2} \int_{C_\ell} D(\mathbb{1}_{C \setminus (\Omega_N + \tau + a)}) \, \mathrm{d}a \\
&\leq \mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N) - \frac{1}{M\ell^2} \int_{C_\ell} D(\mathbb{1}_{C \setminus (\Omega_N + \tau + a)}) \, \mathrm{d}a.
\end{aligned}
$$

Here $x_{n+1}, \ldots, x_N$ are the points $x_j + \ell k$ for $k \neq 0$ ordered in some fashion.

We now bound the term $\frac{1}{M\ell^2} \int_{C_\ell} D(\mathbb{1}_{C \setminus (\Omega_N + \tau + a)}) \, \mathrm{d}a$. For any a denote by $A = C \setminus (\Omega_N + \tau + a)$. Then we have $|A| = M \ll N$ and $\operatorname{diam} A = O(L) = O\left(N^{1/2}\right)$. Thus

$$
D(\mathbb{1}_A) = \frac{1}{2} \iint_{A \times A} -\log |x - y| \, \mathrm{d}x \, \mathrm{d}y \geq \frac{1}{2} \iint_{A \times A} -\log \operatorname{diam} A \, \mathrm{d}x \, \mathrm{d}y = O(M^2 \log N).
$$

Hence

$$
-\frac{1}{M\ell^2} \int_{C_\ell} D(\mathbb{1}_{C \setminus (\Omega_N + \tau + a)}) \, \mathrm{d}a \leq O(M \log N) = o(N).
$$

Remark 2.4. In dimension $d = 1$ one may calculate that the analogous term $\frac{1}{M\ell} \int_{C_\ell} D(\mathbb{1}_{C \setminus (\Omega_N + \tau + a)}) \, \mathrm{d}a$ is in fact of order N, hence this leads to a non-vanishing shift of the energy.

We conclude that

$$\frac{\mathcal{E}_{\mathrm{Ind}}(\rho_{\mathbb{P}})}{N} \leq \frac{\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N)}{N} + o(1).$$

Taking $N \to \infty$ we thus get $e_{\mathrm{UEG}} \leq \liminf_{N\to\infty} \frac{\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N)}{N}$. We claim that the right hand side converges to

$$\frac{\mathcal{E}_{\mathrm{per},\ell}(x_1, \ldots, x_n)}{n},$$

for some appropriate functional $\mathcal{E}_{\mathrm{per},\ell}$, which we now describe.

Define the periodic Coulomb potential G_ℓ as follows. $G_\ell(x) = G_1(x/\ell)$, where G_1 is the one-periodic Coulomb potential, satisfying $-\Delta G_1 = 2\pi \left(\sum_{z\in\mathbb{Z}^2} \delta_z - 1\right)$ and $\int_{C_1} G_1 \, \mathrm{d}x = 0$, where $C_1 = (-1/2, 1/2)^2$. It corresponds to the potential generated by a point charge and all its images together with a uniform oppositely charged background. The background must be included for this not to diverge. One computes

$$G_\ell(x) = G_1(x/\ell) = \frac{2\pi}{\ell^2} \sum_{\substack{k \in \frac{2\pi}{\ell}\mathbb{Z}^2 \\ k \neq 0}} \frac{1}{k^2} e^{ikx}.$$

To explore the behaviour at G_ℓ near 0 define the function $V_1(x) := \frac{\pi}{2}x^2$ and note that then $-\Delta(G_1 + \log|x| - V_1) = 0$ in the ball B_1 and thus $G_1 + \log|x| - V_1$ has a limit C_{mad} as $x \to 0$. It follows that as $x \to 0$ we have

$$G_\ell(x) = -\log|x| + \log\ell + C_{\mathrm{mad}} + o(1).$$

The constant C_{mad} is the Madelung constant, i.e twice the energy of the configuration with 1 particle in the unit cell - i.e. a square lattice configuration (these are discussed in section 7).

The functional $\mathcal{E}_{\mathrm{per},\ell}$ may now be defined

$$\mathcal{E}_{\mathrm{per},\ell}(x_1, \ldots, x_n) = \sum_{j<k} G_\ell(x_j - x_k) + \frac{n}{2}\left(\log\ell + C_{\mathrm{mad}}\right).$$

The first term is what one gets if one just naively replaces the Coulomb interaction in the Jellium functional by the periodic version G_ℓ. Note that then the particle-background and background-background terms vanish due to the fact that $\int_{C_\ell} G_\ell \, \mathrm{d}x = 0$.

We now prove that indeed,

$$\lim_{N\to\infty} \frac{\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N)}{N} = \frac{\mathcal{E}_{\mathrm{per},\ell}(x_1, \ldots, x_n)}{n}.$$

We first give an inequality one way.

Note that the inter-particle distance is bounded uniformly from below (since there are only finitely many particles in the "unit cell" C_ℓ). Hence, by replacing the point charges by smeared out charges of some small radius η smaller than all the inter-particle distances Newton's theorem says that all the particle-particle energies are preserved, but the particle-background interaction only increases (decreases in numerical size, but this energy is negative). Writing $\chi_\eta = \frac{1}{\pi\eta^2}\mathbb{1}_{B(0,\eta)}$ we thus have

$$\begin{aligned}
\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N) &= -\sum_{j<k} \log|x_j - x_k| + \sum_{j=1}^N \int_{\Omega_N+\tau} \log|x_j - y|\,\mathrm{d}y \\
&\quad -\frac{1}{2}\iint_{(\Omega_N+\tau)\times(\Omega_N+\tau)} \log|x-y|\,\mathrm{d}x\,\mathrm{d}y \\
&\le -\sum_{j<k}\iint \log|(x_j+y)-(x_k+z)|\chi_\eta(y)\chi_\eta(z)\,\mathrm{d}y\,\mathrm{d}z \\
&\quad +\sum_{j=1}^N \int_{\Omega_N+\tau}\int \log|(x_j+z)-y|\chi_\eta(z)\,\mathrm{d}z\,\mathrm{d}y \\
&\quad -\frac{1}{2}\iint_{(\Omega_N+\tau)\times(\Omega_N+\tau)} \log|x-y|\,\mathrm{d}x\,\mathrm{d}y \\
&= \sum_{j<k} 2D(\chi_\eta(\cdot - x_j), \chi_\eta(\cdot - x_k)) - \sum_{j=1}^N 2D(\chi_\eta(\cdot - x_j), \mathbb{1}_{\Omega+\tau}) + D(\mathbb{1}_{\Omega_N+\tau}) \\
&= D\left(\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_N+\tau}\right) - \sum_{j=1}^N D(\chi_\eta) \\
&= D\left(\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_N+\tau}\right) - N\left(D(\chi_1) - \frac{1}{2}\log\eta\right).
\end{aligned}$$

We now investigate the first term more closely. We may write

$$\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_N+\tau} = \sum_{\substack{k\in\mathbb{Z}^2 \\ |k_1|,|k_2|\le K}} f(\cdot + \ell k),$$

where $f = \sum_{j=1}^n \chi_\eta(\cdot - x_j) - \mathbb{1}_{C_\ell+\tau}$. Thus

$$\begin{aligned}
D\left(\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_N+\tau}\right) &= D\left(\sum_k f(\cdot + \ell k)\right) \\
&= \pi \int \frac{1}{p^2}\left|\sum_k \widehat{f(\cdot + \ell k)}\right|^2 \mathrm{d}p \\
&= \pi \int \frac{|\hat f(p)|^2}{p^2}\left|\sum_k e^{ipk\ell}\right|^2 \mathrm{d}p
\end{aligned}$$

Since f is of compact support and satisfies $\int f\,\mathrm{d}x = 0$ and $\int x f(x)\,\mathrm{d}x = 0$ (this is where the zero dipole moment is used) we have that $\hat f$ is smooth and satisfies $\hat f(p) = o(p)$ as $p \to 0$, thus $\frac{|\hat f(p)|^2}{p^2}$ vanishes at zero. Thus, we need to consider the behaviour of $\left|\sum_k e^{ipk\ell}\right|^2$ in the limit $K \to \infty$ (i.e. $N \to \infty$).

We have

$$\frac{1}{(2K+1)^2}\left|\sum_{\substack{k\in\mathbb{Z}^2 \\ |k_1|,|k_2|\le K}} e^{ipk\ell}\right| = \prod_{\nu=1}^2 \frac{\sin^2(\ell p_\nu(K+1/2))}{\sin^2(\ell p_\nu/2)} \rightharpoonup \left(\frac{2\pi}{\ell}\right)^2 \sum_{p\in\frac{2\pi}{\ell}\mathbb{Z}^2} \delta_p$$

weakly, and so

$$
\begin{aligned}
\frac{1}{N} D\left(\sum_k f(\cdot+\ell k)\right) &= \frac{\pi}{\ell^2(2K+1)^2}\int \frac{|\hat f(p)|^2}{p^2}\left|\sum_k e^{ipk\ell}\right|^2 \mathrm{d}p \\
&\overset{N\to\infty}{\longrightarrow} \frac{\pi}{\ell^2}\int \frac{|\hat f(p)|^2}{p^2}\left(\frac{2\pi}{\ell}\right)^2 \sum_{p\in\frac{2\pi}{\ell}\mathbb{Z}^2}\delta_p \,\mathrm{d}p \\
&= \frac{4\pi^3}{\ell^4}\sum_{\substack{p\in\frac{2\pi}{\ell}\mathbb{Z}^2\\ p\neq 0}} \frac{|\hat f(p)|^2}{p^2} \\
&= \frac{\pi}{\ell^4}\sum_p \int_{C_\ell+\tau}\int_{C_\ell+\tau} f(x)e^{ipx} f(y) e^{-ipy}\frac{1}{p^2}\,\mathrm{d}x\,\mathrm{d}y \\
&= \frac{1}{2n}\int_{C_\ell+\tau}\int_{C_\ell+\tau}\frac{2\pi}{\ell^2}\sum_p \frac{1}{p^2}e^{ip(x-y)} f(x)f(y)\,\mathrm{d}x\,\mathrm{d}y \\
&= \frac{1}{2n}\int_{C_\ell+\tau}\int_{C_\ell+\tau} G_\ell(x-y)f(x)f(y)\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned}
$$

Plugging in the definition of f and using that $\int_{C_\ell} G_\ell \,\mathrm{d}x = 0$ we thus have

$$
\begin{aligned}
&\frac{1}{2n}\int_{C_\ell+\tau}\int_{C_\ell+\tau} G_\ell(x-y)f(x)f(y)\,\mathrm{d}x\,\mathrm{d}y \\
&\quad = \frac{1}{2}\iint G_\ell(x-y)\chi_\eta(x)\chi_\eta(y)\,\mathrm{d}x\,\mathrm{d}y + \frac{1}{n}\sum_{j<k}\iint G_\ell(x-y)\chi_\eta(x-x_j)\chi_\eta(y-x_k)\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned}
$$

Since $\chi_\eta \rightharpoonup \delta$ as $\eta \to 0$ the second term converges to $\frac{1}{n}\sum_{j<k} G_\ell(x_j-x_k)$, that is exactly the first term in the functional $\mathcal{E}_{\mathrm{per},\ell}$ as desired.

We now deal with the other term in the limit $\eta \to 0$.

$$
\begin{aligned}
&\frac{1}{2}\iint G_\ell(x-y)\chi_\eta(x)\chi_\eta(y)\,\mathrm{d}x\,\mathrm{d}y \\
&\quad = \frac{1}{2}\iint G_\ell(\eta(x-y))\chi_1(x)\chi_1(y)\,\mathrm{d}x\,\mathrm{d}y \\
&\quad = \frac{1}{2}\iint \left(-\log\eta - \log|x-y| + \log\ell + C_{\mathrm{mad}} + o_{\eta\to 0}(1)\right)\chi_1(x)\chi_1(y)\,\mathrm{d}x\,\mathrm{d}y \\
&\quad = -\frac{1}{2}\log\eta + D(\chi_1) + \frac{1}{2}\log\ell + \frac{C_{\mathrm{mad}}}{2} + o_{\eta\to 0}(1).
\end{aligned}
$$

Putting everything together we now conclude

$$
\begin{aligned}
&\frac{1}{N} D\left(\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_N+\tau}\right) - \left(D(\chi_1) - \frac{1}{2}\log\eta\right) \\
&\quad \overset{N\to\infty}{\longrightarrow} \frac{1}{n}\sum_{j<k} G_\ell(x_j-x_k) + \frac{1}{2}\iint G_\ell(x-y)\chi_\eta(x)\chi_\eta(y)\,\mathrm{d}x\,\mathrm{d}y - D(\chi_1) + \frac{1}{2}\log\eta \\
&\quad \overset{\eta\to 0}{\longrightarrow} \frac{1}{n}\sum_{j<k} G_\ell(x_j-x_k) + \frac{1}{2}\log\ell + \frac{1}{2}C_{\mathrm{mad}}.
\end{aligned}
$$

This proves the one inequality. In order to conclude the other inequality note that the error we made in replacing the point charges with smeared out ones can by Newton's theorem be bounded by $\int -\log|y|\chi_\eta(y)\,\mathrm{d}y = O(-\eta^2\log\eta)$ per particle. This vanishes as $\eta \to 0$ and thus we conclude the equality

$$\lim_{N\to\infty} \frac{\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N)}{N} = \frac{\mathcal{E}_{\mathrm{per},\ell}(x_1, \ldots, x_n)}{n}.$$

This proves that $e_{\mathrm{UEG}} \leq \frac{\mathcal{E}_{\mathrm{per},\ell}(x_1,\ldots,x_n)}{n}$ under the assumption of conjecture 1.1. We now give the argument based on proposition 1.2 instead.

3 Upper Bound of the Indirect Energy - Correct Argument

We now give the proof that

$$e_{\mathrm{UEG}} \leq \frac{\mathcal{E}_{\mathrm{per},\ell}(x_1, \ldots, x_n)}{n}$$

without using conjecture 1.1, but instead refer to proposition 1.2. The difficulty here lies in choosing a different test distribution $\mathbb{P}$ with $\rho_{\mathbb{P}} \leq 1$ and showing that the energy of this state is in fact very close to the desired. We want our density to satisfy $\rho_{\mathbb{P}} \leq 1$. In particular, we do not allow for the fluid to ever be where the crystal might also be (under different translations), i.e. we make a hole in the fluid which is larger than the crystal.

With $x_1, \ldots, x_n, \tau$ as before let C be a square with $C \supset \Omega_N + 5C_\ell$ and $|C \setminus \Omega_N| = M = O\left(N^{1/2}\right)$ and integer. Define $D = \Omega_N + 3C_\ell + \tau$ (the hole in the fluid) and β some density satisfying that $\mathbb{1}_C \leq \beta \leq \mathbb{1}_C + \mathbb{1}_D * \frac{\mathbb{1}_{C_\ell}}{\ell^2} - \frac{1}{n}\sum_{j=1}^n \mathbb{1}_{\Omega_N + x_j}$. Then define

$$\mathbb{P} = \frac{1}{\ell^2}\int_{C_\ell} \bigotimes_{\substack{j=1,\ldots,n \\ k\in\mathbb{Z}^2 \\ |k_1|,|k_2|\leq K}} \delta_{x_j + \ell k + a} \otimes \left(\frac{\beta - \mathbb{1}_{D+a}}{M}\right)^{\otimes M} \mathrm{d}a.$$

We choose D such that the fluid and the crystal never overlap. The crystal when shifted around, gives some density in the region $\Omega_N + C_\ell$. We thus want that any shift $D + a$ of D doesn't overlap with this. Since τ is in general just some vector $\tau \in C_\ell$, this leads to our definition of $D = \Omega_N + 3C_\ell + \tau$. We need $\beta \geq \mathbb{1}_{D+a}$ for any shift a, and so this leads to $\beta \geq \mathbb{1}_C$, with $C \supset \Omega_N + 5C_\ell$. Thus, for any such β the test distribution $\mathbb{P}$ is valid.

The same computation as before shows that

$$\rho_{\mathbb{P}} = \beta + \frac{1}{n}\sum_{j=1}^n \mathbb{1}_{\Omega_N + x_j} - \mathbb{1}_D * \frac{\mathbb{1}_{C_\ell}}{\ell^2}.$$

In order for this to be bounded by 1 we see that we need $\beta \leq \mathbb{1}_C + \mathbb{1}_D * \frac{\mathbb{1}_{C_\ell}}{\ell^2} - \frac{1}{n}\sum_{j=1}^n \mathbb{1}_{\Omega_N + x_j}$. By our construction of D we see that, indeed $\mathbb{1}_D * \frac{\mathbb{1}_{C_\ell}}{\ell^2} - \frac{1}{n}\sum_{j=1}^n \mathbb{1}_{\Omega_N + x_j} \geq 0$, so that it is possible to choose β satisfying the constraints. In fact, choosing β to equal this upper bound, we get $\rho_{\mathbb{P}} = \mathbb{1}_C$. This corresponds to adding some constant charge density to the regions we "hollowed" out, when we made the hole in the fluid D. Thus, we don't really need the generalised thermodynamic limit of proposition 1.2, but it is in fact enough to have the limit for ρ an indicator function. We prove it in section 5 anyway since it is trivial to extend the result to $0 \leq \rho \leq 1$.

To compute the energy $\mathcal{E}_{\mathrm{Ind}}(\mathbb{P})$ we first (re)introduce the notation

$$D(\mu,\nu)=\frac{1}{2}\iint_{x\neq y}-\log|x-y|\,\mathrm{d}\mu(x)\,\mathrm{d}\nu(y)$$

for two (signed) measures μ,ν. This clearly just extends the previous definition of D. Only we remove the diagonal so δ-measures don't have infinite self-energy. This doesn't matter for measures which are given by functions. With this we now simply compute (with x_j, for $j>n$ again denoting the points $x_j+\ell k$ for $k\neq 0$)

$$\begin{aligned}
\mathcal{E}_{\mathrm{Ind}}(\mathbb{P}) &= \sum_{1\leq j<k\leq N}-\log|x_j-x_k|+\sum_{j=1}^{N}\frac{1}{\ell^2}\int_{C_\ell}\int-\log|x_j+a-y|\left(\beta(y)-\mathbb{1}_{D+a}(y)\right)\,\mathrm{d}y\,\mathrm{d}a\\
&\quad+\left(1-\frac{1}{M}\right)\frac{1}{\ell^2}\int_{C_\ell}D\left(\beta-\mathbb{1}_{D+a}\right)\,\mathrm{d}a-D(\rho_{\mathbb{P}})\\
&= \sum_{j<k}-\log|x_j-x_k|+\frac{1}{n}\sum_{j=1}^{n}2D\left(\mathbb{1}_{\Omega_N+x_j},\beta\right)-2D\left(\sum_{j=1}^{N}\delta_{x_j},\mathbb{1}_D\right)\\
&\quad+D(\beta)+D\left(\mathbb{1}_D\right)-2D\left(\beta,\mathbb{1}_D*\frac{\mathbb{1}_{C_\ell}}{\ell^2}\right)-D\left(\rho_{\mathbb{P}}\right)-\frac{1}{M\ell^2}\int_{C_\ell}D\left(\beta-\mathbb{1}_{D+1}\right)\,\mathrm{d}a\\
&= \mathcal{E}_{\mathrm{Jel}}\left(\Omega_N+\tau,x_1,\ldots,x_N\right)+2D\left(\sum_{j=1}^{N}\delta_{x_j},\mathbb{1}_{\Omega_N+\tau}-\mathbb{1}_D\right)-D\left(\mathbb{1}_{\Omega_N+\tau}\right)\\
&\quad+2D\left(\beta,\frac{1}{n}\sum_{j=1}^{n}\mathbb{1}_{\Omega_N+x_j}-\mathbb{1}_D*\frac{\mathbb{1}_{C_\ell}}{\ell^2}\right)+D(\beta)+D\left(\mathbb{1}_D\right)-D\left(\rho_P\right)\\
&\quad-\frac{1}{M\ell^2}\int_{C_\ell}D\left(\beta-\mathbb{1}_{D+a}\right)\,\mathrm{d}a
\end{aligned}$$

Similarly as in the previous section we have that

$$-\frac{1}{M\ell^2}\int_{C_\ell}D\left(\beta-\mathbb{1}_{D+a}\right)\,\mathrm{d}a\leq o(N).$$

We thus want to consider the other error term

$$\begin{aligned}
2D\left(\sum_{j=1}^{N}\delta_{x_j},\mathbb{1}_{\Omega_N+\tau}-\mathbb{1}_D\right)+2D\left(\beta,\frac{1}{n}\sum_{j=1}^{n}\mathbb{1}_{\Omega_N+x_j}-\mathbb{1}_D*\frac{\mathbb{1}_{C_\ell}}{\ell^2}\right)&\\
-D\left(\mathbb{1}_{\Omega_N+\tau}\right)+D(\beta)+D\left(\mathbb{1}_D\right)-D\left(\rho_P\right)&
\end{aligned}$$

Plugging in the value of $\rho_{\mathbb{P}}$ we may calculate this term as

$$-\;2D\left(\sum_{j=1}^{N}\delta_{x_j}-\mathbb{1}_{\Omega_N+\tau},f\right)\;+\;D\left(\mathbb{1}_D-\mathbb{1}_D*\frac{\mathbb{1}_{C_\ell}}{\ell^2},g\right)\;+\;D\left(\frac{1}{n}\sum_{j=1}^{n}\mathbb{1}_{\Omega_N+x_j}-\mathbb{1}_{\Omega_N+\tau},g\right),\tag{3.1}$$

where

$$f=\mathbb{1}_D-\mathbb{1}_{\Omega_N+\tau},\qquad g=\mathbb{1}_D+\mathbb{1}_D*\frac{\mathbb{1}_{C_\ell}}{\ell^2}-\mathbb{1}_{\Omega_N+\tau}-\frac{1}{n}\sum_{j=1}^{n}\mathbb{1}_{\Omega_N+x_j}.$$

We claim that this term is $O(N^{1/2}\log N)$ and thus vanishes in the desired limit.

This will follow from appropriate Taylor expansions of $-\log|\cdot|$ and the following two propositions

Proposition 3.1. *Let A be a square of size $|A| = O(N)$. Let μ be a measure satisfying $\mu(A') = O(|A'|)$ for any nice set A' (squares and/or balls would suffice). Let B be the boundary region of A, meaning $B = \{x \in \mathbb{R}^2 : \mathrm{d}(x, \partial A) \le \ell\}$ for some fixed $\ell > 0$. Then*

$$\int_A \int_{B\cap\{|x-y|>1\}} \frac{1}{|x-y|^2}\,\mathrm{d}y\,\mathrm{d}\mu(x) = O\left(N^{1/2}\log N\right).$$

One should think that μ is either Lebesgue measure or a sum of appropriately distributed δ-measures.

To show this, note that for any fixed $y \in B$ we can bound the x-integral by the integral over a ball of radius $L = O\left(N^{1/2}\right)$ centered at y (removing the ball of radius 1). Thus

$$\int_A \int_{B\cap\{|x-y|>1\}} \frac{1}{|x-y|^2}\,\mathrm{d}y\,\mathrm{d}\mu(x) \le \int_B \int_{B_L\setminus B_1} \frac{1}{|z|^2}\,\mathrm{d}\mu(z)\,\mathrm{d}y \le C\int_B \log L\,\mathrm{d}y = O\left(N^{1/2}\log N\right).$$

Proposition 3.2. *Let A, B be as in proposition 3.1 and μ be a probability measure supported in B_ℓ. Denote by τ the first moment of μ, i.e. $\tau = \int a\,\mathrm{d}\mu(a)$. Let b be function supported in B, which is bounded uniformly in N. Then*

$$D\left(\mathbb{1}_{A+\tau} - \mathbb{1}_A * \mu, b\right) = O\left(N^{1/2}\log N\right).$$

Remark 3.3. In dimension $d \ge 2$ we similarly have

$$\int_A \int_{B\cap\{|x-y|>1\}} \frac{1}{|x-y|^d}\,\mathrm{d}y\,\mathrm{d}\mu(x) = O\left(N^{\frac{d-1}{d}}\log N\right),$$
$$D\left(\mathbb{1}_{A+\tau} - \mathbb{1}_A * \mu, b\right) = O\left(N^{\frac{d-1}{d}}\log N\right).$$

Thus our argument also works in higher dimensions.

Proposition 3.2 immediately gives that the second two terms of equation (3.1) are $O(N^{1/2}\log N)$. For the first term we use that by Taylor expansion

$$\begin{aligned} -\log|z+a| &= -\log|z| - \frac{z\cdot a}{|z|^2} + \int_0^1 (1-t)\left[\frac{|a|^2}{|z+ta|^2} - \frac{2((z+ta)\cdot a)^2}{|z+ta|^4}\right]\mathrm{d}t \\ &= -\log|z| - \frac{z\cdot a}{|z|^2} + O\left(\frac{1}{|z|^2}\right). \end{aligned}$$

Thus for the term

$$2D\left(\sum_{j=1}^N \delta_{x_j} - \mathbb{1}_{\Omega_N+\tau}, f\right) = \iint f(x)(-\log|x-y|)\left(\sum_{j=1}^N \delta_{x_j} - \mathbb{1}_{\Omega_N+\tau}\right)(y)\,\mathrm{d}y\,\mathrm{d}x$$

we have

$$
\begin{aligned}
&= \sum_{\substack{j=1,\dots,n\\ k\in\mathbb{Z}^2\\ |k_1|,|k_2|\le K}} \iint f(x)(-\log|x-y|)\left[\delta_{x_j+\ell k} - \frac{1}{\ell^2}\mathbb{1}_{C_\ell+\tau+\ell k}\right](y)\,\mathrm{d}y\,\mathrm{d}x \\
&= \sum_{j,k}\frac{1}{\ell^2}\int_{D\setminus(\Omega_N+\tau)}\int_{C_\ell} -\log|x-\ell k - x_j| - (-\log|x-\ell k-\tau+a)\,\mathrm{d}a\,\mathrm{d}x \\
&= \sum_{j,k}\int_{D\setminus(\Omega_N+\tau)}\left[-\log|x-\ell k-x_j| - (-\log|x-\ell k-\tau|)\right]\,\mathrm{d}x \\
&\quad + \sum_{j,k}\frac{1}{\ell^2}\int_{D\setminus(\Omega_N+\tau)}\int_{C_\ell} -\log|x-\ell k-\tau| - (-\log|x-\ell k-\tau+a|)\,\mathrm{d}a\,\mathrm{d}x \\
&= \int_{D\setminus(\Omega_N+\tau)} \underbrace{\sum_{j,k} -\frac{(x-\ell k-\tau)\cdot(\tau-x_j)}{|x-\ell k-\tau|^2}}_{=0\text{ by }\sum x_j=\sum\tau}\,\mathrm{d}x + \sum_{j,k}\int_{D\setminus(\Omega_N+\tau)} O\left(\frac{1}{|x-\ell k|^2}\right)\,\mathrm{d}x \\
&\quad + \sum_{j,k}\frac{1}{\ell^2}\int_{D\setminus(\Omega_N+\tau)} \underbrace{\int_{C_\ell}\frac{(x-\ell k-\tau)\cdot a}{|x-\ell k-\tau|^2}\,\mathrm{d}a}_{=0\text{ by }\int a\,\mathrm{d}a=0}\,\mathrm{d}x + \sum_{j,k}\int_{D\setminus(\Omega_N+\tau)} O\left(\frac{1}{|x-\ell k|^2}\right)\,\mathrm{d}x \\
&= O(N^{1/2}\log N)
\end{aligned}
$$

by proposition 3.1. This gives the bound

$$
\mathcal{E}_{\mathrm{Ind}}(\rho_{\mathbb{P}}) \le \mathcal{E}_{\mathrm{Ind}}(\mathbb{P}) \le \mathcal{E}_{\mathrm{Jel}}\left(\Omega_N+\tau, x_1,\dots,x_N\right) + o(N).
$$

Thus by proposition 1.2 and the computation of $\lim_N \frac{\mathcal{E}_{\mathrm{Jel}}(\Omega_N+\tau,x_1,\dots,x_N)}{N} = \frac{\mathcal{E}_{\mathrm{per},\ell}(x_1,\dots,x_n)}{n}$ in section 2 we have

$$
e_{\mathrm{UEG}} = \lim_{N\to\infty}\frac{\mathcal{E}_{\mathrm{Ind}}(\rho_{\mathbb{P}})}{N} \le \lim_{N\to\infty}\frac{\mathcal{E}_{\mathrm{Jel}}\left(\Omega_N+\tau,x_1,\dots,x_N\right)+o(N)}{N} = \frac{\mathcal{E}_{\mathrm{per},\ell}(x_1,\dots,x_n)}{n}.
$$

It remains to prove propositions 3.1 and 3.2.

Proof of proposition 3.2. Let $L = |A|^{1/2}$ be the side length of A, find an $\ell' \ge 4\ell$ of order 1 such that L/ℓ' is an integer. Let Q denote the square of side length ℓ' centered at zero. Tile the plane with translates of Q such that, for the relevant translates, the centers y_j lie on the boundary ∂A. That is, $\mathbb{R}^2 = \bigcup_j (y_j+Q)$ and if y_j+Q intersect both A and A^c, then $y_j \in \partial A$. Now, for any $x\in B$ we have that $x \in y_j+Q$ for some (unique) $y_j\in\partial A$, see figure 3.1. Thus

$$
D\left(\mathbb{1}_{A+\tau} - \mathbb{1}_A * \mu, b\right) = \frac{1}{2}\sum_{j:y_j\in\partial A}\int_{y_j+Q} b(x)\int -\log|x-y|\left(\mathbb{1}_{A+\tau} - \mathbb{1}_A*\mu\right)(y)\,\mathrm{d}y\,\mathrm{d}x
$$

We now split the y-integral in two according to whether y is “close” to x, namely if $y\in y_j+2Q$ or if y is “far” from x, namely if $y\notin y_j+2Q$. For the close y's we get the contribution

$$
\frac{1}{2}\sum_{j:y_j\in\partial A}\int_{y_j+Q} b(x)\int_{y_j+2Q} -\log|x-y|\left(\mathbb{1}_{A+\tau}-\mathbb{1}_A*\mu\right)(y)\,\mathrm{d}y\,\mathrm{d}x = O\left(N^{1/2}\right)
$$

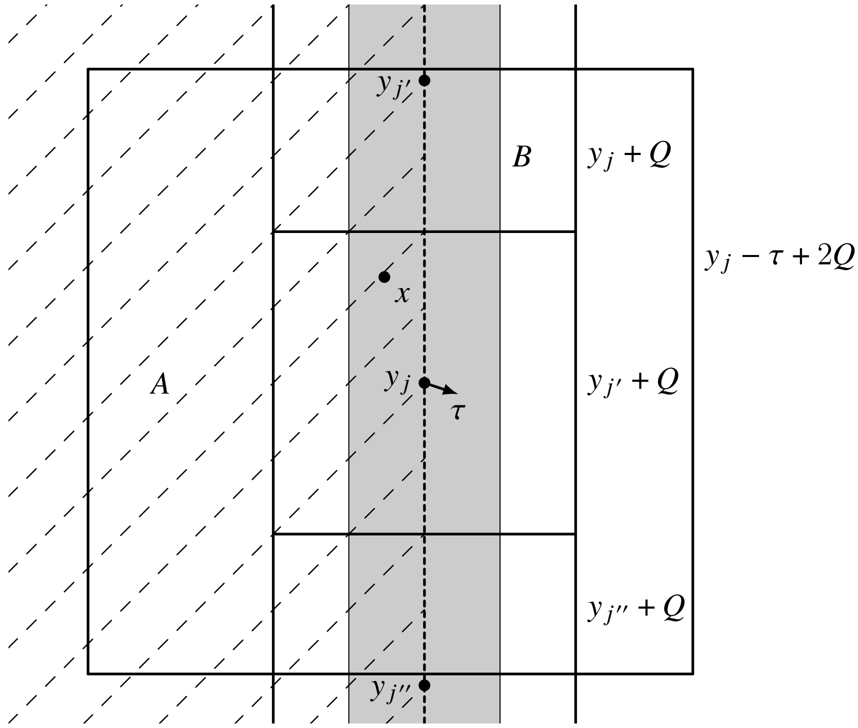

Figure 3.1: Picture of the boundary region B (in grey) with the relevant translates of Q.

since there are $O(N^{1/2})$ many such j's, with each some order 1 contribution. For the y's far away we get the contribution

$$\frac{1}{2}\sum_{j:y_j\in\partial A}\int_{y_j+Q} b(x)\int_{(y_j+2Q)^c} -\log|x-y|\left[\mathbb{1}_{A+\tau}(y)-\int \mathbb{1}_A(y-a)\,\mathrm{d}\mu(a)\right]\mathrm{d}y\,\mathrm{d}x$$

we compute

$$\begin{aligned}
=\ & \frac{1}{2}\sum_j\int_{y_j+Q} b(x)\int\Bigg[\int_{(y_j-\tau+2Q)^c\cap A} -\log|x-y-\tau|\,\mathrm{d}y \\
&\qquad -\int_{(y_j-a+2Q)^c\cap A} -\log|x-z-a|\,\mathrm{d}z\Bigg]\,\mathrm{d}\mu(a)\,\mathrm{d}x \\
=\ & \frac{1}{2}\sum_j\int_{y_j+Q} b(x)\int\int_{(y_j-\tau+2Q)^c\cap A} -\log|x-y-\tau|-(-\log|x-y-a|)\,\mathrm{d}y\,\mathrm{d}\mu(a)\,\mathrm{d}x \\
& +\frac{1}{2}\sum_j\int_{y_j+Q} b(x)\int\left[\int_{(y_j-\tau+2Q)^c\cap A}-\int_{(y_j-a+2Q)^c\cap A}\right] -\log|x-y-a|\,\mathrm{d}y\,\mathrm{d}\mu(a)\,\mathrm{d}x.
\end{aligned}$$

The first term here, we again use the Taylor expansion of $-\log$. we thus get for the integrand in the x-integral

$$\begin{aligned}
b(x)\int\int_{(y_j-\tau+2Q)^c\cap A} \frac{(x-y-\tau)\cdot(\tau-a)}{|x-y-\tau|^2}+O\left(\frac{1}{|x-y|^2}\right)\mathrm{d}y\,\mathrm{d}\mu(a) \\
= O\left(\int_{(y_j-\tau+2Q)^c\cap A}\frac{1}{|x-y|^2}\,\mathrm{d}y\right).
\end{aligned}$$

Thus, computing the x-integral of this we get a term which is $O(N^{1/2}\log N)$ by proposition 3.1 (note that for $y \in (y_j - \tau + 2Q)^c \cap A$ and $x \in y_j + Q$ we have that $|x-y| \geq \ell$). For the second term, the x-integrand is

$$b(x)\int\int_{(y_j-\tau+2Q)^c\cap A} - \int_{(y_j-a+2Q)^c\cap A} - \log|x-y-a|\,\mathrm{d}y\,\mathrm{d}\mu(a)$$
$$= b(x)\int\int_{(y_j-a+2Q)\cap A} - \int_{(y_j-\tau+2Q)\cap A} - \log|x-y-a|\,\mathrm{d}y\,\mathrm{d}\mu(a)$$

This is only an integral of y's "close" to x, and so a similar argument as above gives that when we integrate this over all x we get a term which is $O(N^{1/2})$. We conclude the desired

$$D\left(\mathbb{1}_{A+\tau} - \mathbb{1}_A * \mu, b\right) = O\left(N^{1/2}\log N\right). \qquad \square$$

4 Upper Bound for the Periodic Energy

We show that

$$\limsup_{N\to\infty}\min_{x_1,\ldots,x_N\in C_L}\frac{\mathcal{E}_{\mathrm{per},L}(x_1,\ldots,x_N)}{N} \leq e_{\mathrm{Jel}}.$$

This (together with the above arguments) proves our main theorem.

First, we show that a version of Newton's theorem hold for the periodic potential G_ℓ. Namely that separated neutral radial charge densities have zero total interaction. More precisely, let ρ be any compactly supported radial neutral charge distribution, i.e. $\operatorname{supp}\rho \subset B(0,R)$ for some $R > 0$, ρ is radial and $\int \rho\,\mathrm{d}x = 0$. Let L be large enough so that $B(0,R) \subset C_L$. Then we have that $V = \sum_{k\in\mathbb{Z}^2}(\rho * -\log)(\cdot + Lk)$ satisfies

$$-\Delta V = 2\pi\sum_k \rho(\cdot + Lk) = \rho * \left(2\pi\left(\sum_k \delta_{Lk} - \frac{1}{L^2}\right)\right) = -\Delta(\rho * G_L).$$

(Note the importance of ρ being neutral, so $\rho * 1 = 0$.) Since both V and $\rho * G_L$ are C_L-periodic this shows that they differ by a periodic harmonic function, i.e. a constant. Moreover, by Newton's theorem we have that V vanish on $C_L \setminus B(0,R)$, thus we see that $\rho * G_L$ is constant on $C_L \setminus B(0,R)$, and so for another neutral radial charge distribution ρ' supported in this region we have $\iint G_L(x - y)\rho(x)\rho'(y)\,\mathrm{d}x\,\mathrm{d}y = 0$.

We use the Swiss cheese theorem [8, sect. 14.5] to fill (most) of the cube C_L with balls of integer volume ranging in sizes from some fixed ℓ_0 to a largest size of order ℓ. The ratio of the volume not covered by the balls is small in comparison to the volume of the cube, in the sense that if we take $\ell \to \infty$ after taking $L \to \infty$ this ratio vanishes.

We now construct a trial state using these balls. In each ball B_n we place $N_n = |B_n|$ particles in the optimal Jellium configuration for the ball B_n. The remaining $M = N - \sum_n |B_n|$ particles are placed uniformly in the remainder $S = C_L \setminus \bigcup_n B_n$, meaning that we smear the particles out in this region. This gives us the bound

$$\begin{aligned}\min \mathcal{E}_{\mathrm{per},L}(x_1,\dots,x_N) \leq & \sum_{1\leq j<k\leq N-M} G_L(x_j-x_k)+\sum_{j=1}^{N-M}\int_S G_L(x_j-y)\,\mathrm{d}y \\ & +\frac{1}{2}\left(1-\frac{1}{M}\right)\iint_{S\times S} G_L(x-y)\,\mathrm{d}x\,\mathrm{d}y+\frac{N}{2}(\log L+C_{\mathrm{mad}}) \\ = & \sum_{1\leq j<k\leq N-M} G_L(x_j-x_k)-\sum_n\sum_{j=1}^{N-M}\int_{B_n} G_L(x_j-y)\,\mathrm{d}y \\ & +\frac{1}{2}\left(1-\frac{1}{M}\right)\sum_{n,m}\iint_{B_n\times B_m} G_L(x-y)\,\mathrm{d}x\,\mathrm{d}y+\frac{N}{2}(\log L+C_{\mathrm{mad}})\end{aligned}$$

where $x_1,\dots,x_{N-M}$ denote the points in $\bigcup_n B_n$ and we used that $\int_{C_L} G_L\,\mathrm{d}x=0$. Now, by rotating the charges inside each of the balls separately and taking the average over all such rotations we may use the modified Newton's theorem above to conclude that the balls don't interact with each other. Discarding the $1/M$-term and writing $\tilde{G}_L$ for the rotational average of G_L we thus get the upper bound

$$\sum_n\left(\sum_{1\leq j<k\leq|B_n|}\tilde{G}_L\left(x_j^{(n)}-x_k^{(n)}\right)-\sum_{j=1}^{|B_n|}\int_{B_n}\tilde{G}_L\left(x_j^{(n)}-y\right)\,\mathrm{d}y\right.$$
$$\left.+\frac{1}{2}\iint_{B_n\times B_n}\tilde{G}_L(x-y)\,\mathrm{d}x\,\mathrm{d}y+\frac{|B_n|}{2}(\log L+C_{\mathrm{mad}})\right).$$

As $L\longrightarrow\infty$ we have that $G_L(x)=-\log|x|+\log L+C_{\mathrm{mad}}+o(1)$. Plugging this into the bound above all the $\log L$ and C_{mad}-terms cancel. What we are left with is the bound

$$\sum_n\left(\mathcal{E}_{\mathrm{Jel}}\left(B_n,x_1^{(n)},\dots,x_{|B_n|}^{(n)}\right)+o_{L\to\infty}(1)\right).$$

Dividing by $N=L^2$ and taking the consecutive limit $L\longrightarrow\infty$, $\ell\longrightarrow\infty$ and $\ell_0\longrightarrow\infty$ this gives e_{Jel}, by the existence of the thermodynamic limit for Jellium [11]. We conclude that also in 2 dimensions we have $e_{\mathrm{UEG}}=e_{\mathrm{Jel}}$.

5 The Thermodynamic limit for the Uniform Electron Gas

In this section we prove proposition 1.2 that if ρ_N satisfies

$$\rho_N\equiv 1 \text{ well inside } \Omega_N,\qquad \rho_N\equiv 0 \text{ well outside } \Omega_N,\qquad 0\leq\rho_N\leq 1$$

And Ω_N satisfies that there exists a function $\eta:[0,t_0)\longrightarrow[0,\infty)$ (independent of N) such that $\eta(t)$ vanishes as $t\longrightarrow 0$ and $\left|\{x:\ \mathrm{d}(x,\partial\Omega_N)\leq|\Omega_N|^{1/2}t\}\right|\leq|\Omega_N|\eta(t)$ for all t. Then,

$$e_{\mathrm{UEG}}=\lim_{\Omega_N\nearrow\mathbb{R}^2}\frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|}.$$

This is a slight modification of the analogous result [5, Theorem 2.6].

Proof of proposition 1.2. Exactly as in [5, Lemma 2.5] we see that the indirect energy is subadditive $\mathcal{E}_{\mathrm{Ind}}(\rho_1+\rho_2) \le \mathcal{E}_{\mathrm{Ind}}(\rho_1)+\mathcal{E}_{\mathrm{Ind}}(\rho_2)$. In section 6 the following stability result is proved

$$\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1,\ldots,x_N) \ge -\left(\frac{3}{8}+\frac{1}{4}\log\pi\right)N = -CN.$$

This immediately gives that

$$\frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|} \ge \frac{\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1,\ldots,x_N)}{|\Omega_N|} \ge -C.$$

First we show that for $\rho_N = \mathbb{1}_{\Omega_N}$ we have the thermodynamic limit. Then we show it for the more general ρ_N discussed above. For simplicity write $\mathcal{E}_{\mathrm{Ind}}(\Omega_N) = \mathcal{E}_{\mathrm{Ind}}(\mathbb{1}_{\Omega_N})$.

Consider first a sequence of cubes C_n of side length 2^n, then, as we can just glue 4 smaller cubes C_n together to form the cube C_{n+1} we immediately get that

$$\frac{\mathcal{E}_{\mathrm{Ind}}(C_{n+1})}{|C_{n+1}|} \le \frac{2^d\mathcal{E}_{\mathrm{Ind}}(C_n)}{|C_{n+1}|} = \frac{\mathcal{E}_{\mathrm{Ind}}(C_n)}{|C_n|}.$$

Thus the limit $e_{\mathrm{UEG}} := \lim \frac{\mathcal{E}_{\mathrm{Ind}}(C_n)}{|C_n|}$ exists. We now approximate our general sequence of sets Ω_N by squares in order to show the general limit.

Let n be arbitrary and consider the tiling of $\mathbb{R}^2$ by cubes D_j of side length $\ell = 2^n$, $\mathbb{R}^2 = \bigcup D_j$. Let $\tilde{\Omega}_N = \bigcup_{D_j\subset\Omega_N} D_j$ be the union of all interior cubes. Then

$$|\tilde{\Omega}_N| = |\Omega_N| - \sum_{D_j\cap\Omega_N\neq\emptyset} |D_J\cap\Omega_N| \ge |\Omega_N| - \left|\left\{x : d(x,\partial\Omega_N) \le \sqrt{2}\ell\right\}\right| \ge |\Omega_N|\left(1-\eta(\sqrt{2}\ell|\Omega_N|^{-1/2})\right)$$

since points in the cubes intersecting the boundary of Ω_N are within a distance $\sqrt{2}\ell$ of the boundary. Since $\tilde{\Omega}_N$ is a disjoint union of cubes we have $\mathcal{E}_{\mathrm{Ind}}(\tilde{\Omega}_N) \le \frac{|\tilde{\Omega}_N|}{|C_n|}\mathcal{E}_{\mathrm{Ind}}(C_n)$ by the subadditivity. Now, since $\mathcal{E}_{\mathrm{Ind}}(\rho) \le 0$ for any ρ we have (using $\mathcal{E}_{\mathrm{Ind}}(\Omega_N\setminus\tilde{\Omega}_N) \le 0$)

$$\frac{\mathcal{E}_{\mathrm{Ind}}(\Omega_N)}{|\Omega_N|} \le \frac{\mathcal{E}_{\mathrm{Ind}}(\tilde{\Omega}_N)+\mathcal{E}_{\mathrm{Ind}}(\Omega_N\setminus\tilde{\Omega}_N)}{|\Omega_N|} \le \frac{\mathcal{E}_{\mathrm{Ind}}(C_n)}{|C_n|}\left(1-\eta(\sqrt{2}\ell|\Omega_N|^{-1/2})\right),$$

where we used the bound on $|\tilde{\Omega}_N|$ above. Taking $N\to\infty$ and then $n\to\infty$ we get that

$$\limsup_{N\to\infty}\frac{\mathcal{E}_{\mathrm{Ind}}(\Omega_N)}{|\Omega_N|} \le e_{\mathrm{UEG}}.$$

Similarly (exactly as in [5]) one may prove that

$$\liminf_{N\to\infty}\frac{\mathcal{E}_{\mathrm{Ind}}(\Omega_N)}{|\Omega_N|} \ge e_{\mathrm{UEG}}.$$

Now, let ρ_N be a general sequence of densities satisfying the assumptions. Define the sets $\Omega_N^- \subset \Omega_N \subset \Omega_N^+$ such that

$$\rho_N \equiv 1 \text{ on } \Omega_N^-, \qquad \rho_N \equiv 0 \text{ outside } \Omega_N^+$$

and

$$|\Omega_N^-| = |\Omega_N|(1+o(1)), \qquad |\Omega_N^+| = |\Omega_N|(1+o(1)).$$

One should think that $\Omega_N^\pm$ are the set Ω_N expanded/shrunk by a length of order $\ell \ll |\Omega_N|^{1/2}$.

First, write $\rho_N = \mathbb{1}_{\Omega_N^-} + \delta\rho_N^-$, where $\delta\rho_N^-$ is supported in $\Omega_N^+ \setminus \Omega_N^-$ and satisfies $0 \le \delta\rho_N^- \le 1$. Then, since $\mathcal{E}_{\mathrm{Ind}}(\delta\rho_N^-) \le 0$ we have

$$\frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|} \le \frac{\mathcal{E}_{\mathrm{Ind}}(\mathbb{1}_{\Omega_N^-})}{|\Omega_N^-|}\frac{|\Omega_N^-|}{|\Omega_N|} + \frac{\mathcal{E}_{\mathrm{Ind}}(\delta\rho_N^-)}{|\Omega_N|} \le \frac{\mathcal{E}_{\mathrm{Ind}}(\mathbb{1}_{\Omega_N^-})}{|\Omega_N^-|}(1+o(1)),$$

so $\limsup \frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|} \le e_{\mathrm{UEG}}$.

For the other inequality write $\mathbb{1}_{\Omega_N^+} = \rho_N + \delta\rho_N^+$ where $\delta\rho_N^+$ is supported in $\Omega_N^+ \setminus \Omega_N^-$ and satisfies $0 \le \delta\rho_N^+ \le 1$. (Note here how we critically use $\rho_N \le 1$.) Then

$$\frac{\mathcal{E}_{\mathrm{Ind}}(\mathbb{1}_{\Omega_N^+})}{|\Omega_N^+|} \le \frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|}\frac{|\Omega_N|}{|\Omega_N^+|} + \frac{\mathcal{E}_{\mathrm{Ind}}(\delta\rho_N^+)}{|\Omega_N^+|} \le \frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|}(1+o(1)),$$

so $\liminf \frac{\mathcal{E}_{\mathrm{Ind}}(\rho_N)}{|\Omega_N|} \ge e_{\mathrm{UEG}}$. □

6 Stability of Jellium

In this section we prove that the Jellium model is stable, i.e. that for any configuration of N electrons we have

$$\mathcal{E}_{\mathrm{Jel}} \ge -CN$$

For some explicit value of the constant C. We do this argument in dimension d with the Coulomb potential

$$V_{d-2}(x) = \begin{cases} -|x| & \text{if } d = 1, \\ -\log|x| & \text{if } d = 2, \\ |x|^{2-d} & \text{if } d \ge 3. \end{cases}$$

This argument is from [9]. We adopt the notation from there. The idea is to smear out the electrons to a ball of radius a of uniform charge. We then optimise the result over the radius a. We will denote by $B_a = B(0,a)$ the ball of radius a. Define

$$U_{BB} := \frac{1}{2}\iint_{\Omega_N\times\Omega_N} V_{d-2}(x-y)\,\mathrm{d}x\,\mathrm{d}y, \qquad \text{the background self-energy,}$$

$$U_j := -\int_{\Omega_N} V_{d-2}(x_j - y)\,\mathrm{d}y, \qquad \text{particle } j\text{-background interaction,}$$

$$U_{jk} := V_{d-2}(x_j - x_k), \qquad \text{particle } j \text{ - particle } k \text{ interaction,}$$

$$\hat{U}_j := -\frac{1}{|B_a|}\int_{B(x_j,a)}\int_{\Omega_N} V_{d-2}(x-y)\,\mathrm{d}x\,\mathrm{d}y, \qquad \text{ball } j \text{ - background interaction,}$$

$$\hat{U}_{jk} := \frac{1}{|B_a|^2}\int_{B(x_j,a)}\int_{B(x_k,a)} V_{d-2}(x-y)\,\mathrm{d}x\,\mathrm{d}y, \qquad \text{ball } j \text{ - ball } k \text{ interaction.}$$

Then $\hat{U}_{jj}$ is twice the self-energy of ball j.

We then write

$$\mathcal{E}_{\mathrm{Jel}}(\Omega_N, x_1, \ldots, x_N) = \underbrace{U_{BB} + \sum_{j=1}^N \hat{U}_j + \frac{1}{2}\sum_{j,k}\hat{U}_{jk}}_{(\alpha)} + \underbrace{\sum_{j=1}^N U_j - \hat{U}_j}_{(\beta)} + \underbrace{\frac{-1}{2}\sum_{j=1}^N \hat{U}_{jj}}_{(\gamma)} + \underbrace{\sum_{j<k} U_{jk} - \hat{U}_{jk}}_{(\delta)}.$$

Here (α) is the "Jellium"-like functional, where the electrons are no longer particles, but instead are a cloud of charge density. Such a cloud has lowest energy when it perfectly cancels the background, i.e. $(\alpha) \geq 0$.

Also $(\delta) \geq 0$, since if the balls are not overlapping, then this term is 0, but if they are overlapping, then by Newton's theorem this term is positive.

For (β) we have by Newton's theorem

$$\begin{aligned} U_j - \hat{U}_j &= \int_{\Omega_N} -V_{d-2}(x_j - z) + \frac{1}{|B_a|}\int_{B(x_j,a)} V_{d-2}(x-z)\,\mathrm{d}x\,\mathrm{d}z \\ &\geq \frac{1}{|B_a|}\int_{B(x_j,a)}\int_{B(x_j,a)} V_{d-2}(x-z) - V_{d-2}(x_j - z)\,\mathrm{d}x\,\mathrm{d}z \\ &= \frac{1}{|B_a|}\iint_{B_a\times B_a} V_{d-2}(x-z) - V_{d-2}(z)\,\mathrm{d}x\,\mathrm{d}z. \end{aligned}$$

We have equality if $B(x_j, a) \subset \Omega_N$, but in general always the stated inequality.

For (γ) we have $(\gamma) = -\frac{N}{2|B_a|^2}\iint_{B_a\times B_a} V_{d-2}(x-y)\,\mathrm{d}x\,\mathrm{d}y$.

These we can just compute (this is done for $d = 2$ in [11] and for $d = 3$ in [9]). For $d \geq 3$ we get the bound

$$\frac{1}{N}\mathcal{E}_{\mathrm{Jel},d} \geq -\frac{d}{d+2}a^{2-d} + \frac{2-d}{2(d+2)}\left|S^{d-1}\right| a^2. \quad \text{Thus} \quad \frac{1}{N}\mathcal{E}_{\mathrm{Jel},d} \geq -\frac{d^{1+d/2}}{2(d+2)}\left|S^{d-1}\right|^{1-2/d}$$

by optimising over a. This gives for $d = 3$ the bound

$$\frac{1}{N}\mathcal{E}_{\mathrm{Jel},d=3} \geq -\frac{9}{10}\left(\frac{4\pi}{3}\right)^{1/3} \simeq -1.4508.$$

In $d = 1, 2$ we similarly get the bounds

$$\frac{1}{N}\mathcal{E}_{\mathrm{Jel},d=2} \geq \frac{1}{2}\log a - \frac{1}{8} - \frac{\pi}{4}a^2, \qquad \frac{1}{N}\mathcal{E}_{\mathrm{Jel},d=2} \geq -\left(\frac{3}{8} + \frac{1}{4}\log\pi\right) \simeq -0.66118,$$

and

$$\frac{1}{N}\mathcal{E}_{\mathrm{Jel},d=1} \geq \frac{1}{3}\left(a - a^2\right), \qquad \frac{1}{N}\mathcal{E}_{\mathrm{Jel},d=1} \geq \frac{1}{12}.$$

7 Lattice Configurations and ζ-functions

Define for $s \in \mathbb{R}$ the Riesz potentials V_s on $\mathbb{R}^d$ by

$$V_s(x) = \begin{cases} |x|^{-s} & \text{if } s > 0, \\ -\log|x| & \text{if } s = 0, \\ -|x|^{-s} & \text{if } s < 0. \end{cases}$$

Then V_{d-2} is the Coulomb potential in d dimensions. With this we may define for $s < d$ the Jellium energy in d dimensions with potential V_s,

$$\mathcal{E}_{\mathrm{Jel},d,s}(\Omega_N, x_1, \ldots, x_N) = \sum_{j<k} V_s(x_j - x_k) - \sum_{j=1}^{N}\int_{\Omega_N} V_s(x_j - y)\,\mathrm{d}y + D_{d,s}\left(\mathbb{1}_{\Omega_N}\right),$$

where $D_{d,s}(f,g) = \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} f(x)g(y)V_s(x-y)\,\mathrm{d}x\,\mathrm{d}y$. Define for a lattice $\mathcal{L}\subset\mathbb{R}^d$ with Wigner-Seitz unit cell Q with $|Q| = 1$ and s satisfying $d-4 < s < d$ the energy

$$e^{\mathcal{L}}_{\mathrm{Jel},s} = \lim_{\Omega_N\nearrow\mathbb{R}^2} \frac{\mathcal{E}_{\mathrm{Jel},d,s}(\Omega_N, x_1,\ldots,x_N)}{|\Omega_N|}$$

as the thermodynamic limit of Jellium, when the electrons are placed on the lattice. (The existence of this thermodynamic limit follows from the proof of the theorem below.) Here $\Omega_N = \bigcup_{i=1}^N Q + x_i$.

Define for $\mathrm{Re}(s) > d$ the function

$$\zeta_{\mathcal{L}}(s) = \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0}\frac{1}{|x|^s}.$$

This function has a meromorphic continuation to all of $\mathbb{C}$ with a simple pole at $s = d$, see [2]. These more complicated ζ-functions can oftentimes be expressed in terms of simpler functions, see [12]. We prove the following.

Theorem 7.1. *Suppose s satisfies $d-4 < s < d$. Let $\mathcal{L}\subset\mathbb{R}^d$ be a lattice with Wigner-Seitz unit cell Q, $|Q| = 1$. Then the Jellium energy of the lattice configuration is*

$$e^{\mathcal{L}}_{\mathrm{Jel},s} = \begin{cases} \zeta_{\mathcal{L}}(s) & \text{if } s > 0,\\ \zeta'_{\mathcal{L}}(0) & \text{if } s = 0,\\ -\zeta_{\mathcal{L}}(s) & \text{if } s < 0.\end{cases}$$

As an application of this theorem, we compute the energy of Jellium in the triangular lattice (in 2 dimensions).

Example 7.2. The triangular lattice is given by $\mathcal{L} = c(1,0)\mathbb{Z}\oplus c\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)\mathbb{Z}$, where the constant c is such that $|Q| = 1$, i.e. $c^2 = \frac{2}{\sqrt{3}}$. Thus by [12] we have

$$\zeta_{\mathcal{L}}(s) = \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0}\frac{1}{|x|^s} = \frac{1}{2}\sum_{(n,m)\in\mathbb{Z}^2\setminus(0,0)}\frac{1}{(c^2n^2+c^2mn+c^2m^2)^{s/2}} = 3c^{-s}\zeta\left(\frac{s}{2}\right)L_3\left(\frac{s}{2}\right),$$

where ζ is the Riemann zeta-function and $L_3(s) = L(s,\chi)$ is the Dirichlet L-series for the nontrivial character mod 3, i.e.

$$L_3(s) = \sum_{n=1}^{\infty}\frac{\chi(n)}{n^s} = 1 - 2^{-s} + 4^{-s} - 5^{-s} + \ldots = 3^{-s}\left(\zeta\left(s,\frac{1}{3}\right) - \zeta\left(s,\frac{2}{3}\right)\right)$$

where $\zeta(s,a)$ is the Hurwitz ζ-function. The values of these functions and their derivatives can be found in [10]. We conclude that $e^{\mathcal{L}}_{\mathrm{Jel},s=0} = \zeta'_{\mathcal{L}}(0) = \frac{1}{8}\log\left(\frac{48\pi}{\Gamma(1/6)^6}\right) \simeq -0.66056$. In comparison, we proved in section 6 that $e_{\mathrm{Jel},s=0} \geq -\left(\frac{3}{8}+\log\pi\right) \simeq -0.66118$. The triangular lattice, which is what we expect to be the ground state, is remarkably close to this lower bound.

Example 7.3. In dimension $d = 1$, there is only one lattice, namely $\mathbb{Z}$. Thus

$$e^{\mathbb{Z}}_{\mathrm{Jel},s=-1} = -\zeta(-1) = \frac{1}{12}.$$

This is exactly the same as the lower bound found in section 6. It is in fact known that Jellium is crystalised in one dimension [1, 3, 4].

We now prove this theorem. This argument is (mostly) from Lorenzo's notes to the course "Mathematics of many-body quantum mechanics - spring 2020".

Proof. First consider any $s \in \mathbb{R}$. Define $W_s = V_s - 2V_s * \mathbb{1}_Q + V_s * \mathbb{1}_Q * \mathbb{1}_Q = V_s * (\delta - \mathbb{1}_Q) * (\delta - \mathbb{1}_Q)$. By a tedious but straightforward Taylor expansion one checks that $W_s(x) \sim |x|^{-s-4}$ as $|x| \to \infty$. Let $x_1, \ldots, x_N$ be N points on the lattice and set $\Omega_N = \bigcup_{j=1}^N Q + x_j$. Then

$$\begin{aligned}
\sum_{j<k} W_s(x_j - x_k) &= \sum_{j<k} V_s(x_j - x_k) - 2\sum_{j<k} \int_Q V_s(x_j - x_k - y)\,\mathrm{d}y \\
&\quad + \sum_{j<k} \iint_{Q\times Q} V_s(x_j - x_k - y - z)\,\mathrm{d}y\,\mathrm{d}z \\
&= \sum_{j<k} V_s(x_J - x_k) - \left(\sum_{j=1}^N \int_{\Omega_N} V_s(x_j - y)\,\mathrm{d}y - N\int_Q V_s(y)\,\mathrm{d}y \right) \\
&\quad + \left(\frac{1}{2} \iint_{\Omega_N\times\Omega_N} V_s(y-z)\,\mathrm{d}y\,\mathrm{d}z - \frac{1}{2}\sum_{j=1}^N \iint_{Q\times Q} V_s(y-z)\,\mathrm{d}y\,\mathrm{d}z \right) \\
&= \mathcal{E}_{\mathrm{Jel},d,s}(\Omega_N, x_1, \ldots, x_N) + N\int_Q V_s(y)\,\mathrm{d}y - \frac{N}{2}\iint_{Q\times Q} V_s(y-z)\,\mathrm{d}y\,\mathrm{d}z.
\end{aligned}$$

Taking the thermodynamic limit we thus have

$$e^{\mathcal{L}}_{\mathrm{Jel},s} = \lim_N \frac{1}{N}\sum_{j<k} W_s(x_j - x_k) - \int_Q V_s(y)\,\mathrm{d}y + D_{d,s}(\mathbb{1}_Q) = \sum_{x\in\mathcal{L}\setminus 0} W_s(x) - \int_Q V_s(y)\,\mathrm{d}y + D_{d,s}(\mathbb{1}_Q).$$

This is valid for $s > d-4$ since then the sum $\sum_{x\in\mathcal{L}\setminus 0} W_s(x)$ converges (recall that $W_s(x) \sim |x|^{-s-4}$). Let now $s \in \mathbb{C}$, $\mathrm{Re}(s) > d$. We may then write (where $V_s = |\cdot|^{-s}$ and $W_s = |\cdot|^{-s} * (\delta - \mathbb{1}_Q) * (\delta - \mathbb{1}_Q)$)

$$\begin{aligned}
\zeta_{\mathcal{L}}(s) &= \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0} \frac{1}{|x|^s} \\
&= \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0} W_s(x) + \sum_{x\in\mathcal{L}\setminus 0} \int_Q V_s(x-y)\,\mathrm{d}y - \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0} \iint_{Q\times Q} V_s(x-y-z)\,\mathrm{d}y\,\mathrm{d}z \\
&= \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0} W_s(x) + \int_{\mathbb{R}\setminus Q} V_s(y)\,\mathrm{d}y - \frac{1}{2}\int_{\mathbb{R}\setminus Q}\int_Q V_s(y-z)\,\mathrm{d}y\,\mathrm{d}z.
\end{aligned}$$

We now want to write this in a form, that makes sense for all $s \neq d$ satisfying $\mathrm{Re}(s) > d-4$.

For any fixed $\varepsilon > 0$ such that $B_\varepsilon \subset Q$ we have

$$\begin{aligned}
\int_{\mathbb{R}\setminus Q} V_s(y)\,\mathrm{d}y &= \int_{|y|>\varepsilon} V_s(y)\,\mathrm{d}y - \int_{Q\setminus B_\varepsilon} V_s(y)\,\mathrm{d}y \\
&= \left|S^{d-1}\right| \varepsilon^{d-s}\frac{1}{s-d} - \int_{Q\setminus B_\varepsilon} \frac{1}{|y|^s}\,\mathrm{d}y.
\end{aligned}$$

Both of these terms are holomorphic for $s \neq d$ for any such fixed $\varepsilon > 0$. For $\mathrm{Re}(s) < d$ we may take $\varepsilon \to 0$. Hence the analytic continuation of this term is $-\int_Q |y|^{-s}\,\mathrm{d}y$ when $\mathrm{Re}(s) < d$.

For the second term we write

$$\int_{\mathbb{R}\setminus Q}\int_Q \frac{1}{|y-z|^s}\,\mathrm{d}y\,\mathrm{d}z = \int_Q \int_{\mathbb{R}\setminus(Q+z)} \frac{1}{|w|^s}\,\mathrm{d}w\,\mathrm{d}z.$$

We now split this integral according to

$$\begin{aligned}\int_Q\int_{\mathbb{R}\setminus(Q+z)} &= \int_Q\int_{|w|>\varepsilon|z|} - \int_Q\int_{(Q+z)\setminus B_{\varepsilon|z|}}\\ &= \int_{Q\setminus B_\delta}\int_{|w|>\varepsilon|z|} + \int_{B_\delta}\int_{|w|>\varepsilon|z|} - \int_{Q\setminus B_\delta}\int_{(Q+z)\setminus B_{\varepsilon|z|}} - \int_{B_\delta}\int_{(Q+z)\setminus B_\rho} - \int_{B_\delta}\int_{B_\rho\setminus B_{\varepsilon|z|}}\end{aligned}$$

where $\varepsilon, \delta, \rho, > 0$ are all sufficiently small. The terms

$$\int_{Q\setminus B_\delta}\int_{(Q+z)\setminus B_{\varepsilon|z|}} |w|^{-s}\,\mathrm{d}w\,\mathrm{d}z, \qquad \int_{B_\delta}\int_{(Q+z)\setminus B_\rho} |w|^{-s}\,\mathrm{d}w\,\mathrm{d}z$$

are analytic in s. For the remaining terms we calculate. The term

$$\int_{Q\setminus B_\delta}\int_{|w|>\varepsilon|z|} |w|^{-s}\,\mathrm{d}w\,\mathrm{d}z = \left|S^{d-1}\right| \frac{1}{s-d}\varepsilon^{d-s}\int_{Q\setminus B_\delta} |z|^{d-s}\,\mathrm{d}z$$

makes sense for $\mathrm{Re}(s) > d$ and extends analytically to $s \neq d$. The term

$$\int_{B_\delta}\int_{|w|>\varepsilon|z|} |w|^{-s}\,\mathrm{d}w\,\mathrm{d}z = \left|S^{d-1}\right|^2 \frac{1}{s-d}\frac{1}{2d-s}\varepsilon^{d-s}\delta^{2d-s}$$

makes sense for $d < \mathrm{Re}(s) < 2d$ and extends analytically to $s \neq d, 2d$. The term

$$\int_{B_\delta}\int_{B_\rho\setminus B_{\varepsilon|z|}} |w|^{-s}\,\mathrm{d}w\,\mathrm{d}z = \left|S^{d-1}\right| |B_1| \frac{1}{d-s}\delta^d\rho^{d-s} - \left|S^{d-1}\right|^2 \frac{1}{d-s}\varepsilon^{d-s}\frac{1}{2d-s}\delta^{2d-s}$$

makes sense for $d < \mathrm{Re}(s) < 2d$ and extends analytically to $s \neq d, 2d$. The "poles" at $s = 2d$ in fact cancel out, so $2d$ is not a pole of $\zeta_{\mathcal{L}}(s)$.

For $\mathrm{Re}(s) < d$ we may take $\varepsilon, \delta, \rho \to 0$ in a suitable order. All these terms combined then give the limit

$$-\int_Q\int_{Q+z} |w|^{-s}\,\mathrm{d}w\,\mathrm{d}z = -\iint_{Q\times Q} \frac{1}{|w-z|^s}\,\mathrm{d}w\,\mathrm{d}z.$$

Thus, for $d-4 < \mathrm{Re}(s) < d$ we have that (for the analytic continuation)

$$\zeta_{\mathcal{L}}(s) = \frac{1}{2}\sum_{x\in\mathcal{L}\setminus 0} \tilde{W}_s(x) - \int_Q \frac{1}{|y|^s} + \frac{1}{2}\iint_{Q\times Q} \frac{1}{|y-z|^s}\,\mathrm{d}y\,\mathrm{d}z$$

where $\tilde{W}_s(x) = |\cdot|^{-s} * \left(\delta - \mathbb{1}_Q\right) * \left(\delta - \mathbb{1}_Q\right)$. Thus for real $d-4 < s < d$ with $s \neq 0$ we have

$$\zeta_{\mathcal{L}}(s) = \begin{cases} e^{\mathcal{L}}_{\mathrm{Jel},s} & \text{if } s > 0,\\ -e^{\mathcal{L}}_{\mathrm{Jel},s} & \text{if } s < 0.\end{cases}$$

For $s = 0$ we have

$$\begin{aligned} e^{\mathcal{L}}_{\mathrm{Jel},s=0} &= \sum_{x\in\mathcal{L}\setminus 0} W_{s=0}(x) - \int_Q V_{s=0}(y)\,\mathrm{d}y + D_{d,s=0}(\mathbb{1}_Q)\\ &= \frac{\mathrm{d}}{\mathrm{d}s}\left[\sum_{x\in\mathcal{L}\setminus 0} W_s(x) - \int_Q V_s(y)\,\mathrm{d}y + D_{d,s}(\mathbb{1}_Q)\right]_{s=0^+} = \zeta'_{\mathcal{L}}(0). \qquad \square\end{aligned}$$

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