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 Asbjørn Bækgaard Lauritsen



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Asbjørn Bækgaard Lauritsen^{a)} 

AFFILIATIONS

IST Austria (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria

^{a)} Author to whom correspondence should be addressed: asbjornbaekgaard.lauritsen@ist.ac.at

ABSTRACT

Extending on ideas of Lewin, Lieb, and Seiringer [Phys. Rev. B **100**, 035127 (2019)], we present a modified “floating crystal” trial state for jellium (also known as the classical homogeneous electron gas) with density equal to a characteristic function. This allows us to show that three definitions of the jellium energy coincide in dimensions $d \geq 2$, thus extending the result of Cotar and Petrache [“Equality of the Jellium and uniform electron gas next-order asymptotic terms for Coulomb and Riesz potentials,” arXiv: 1707.07664 (2019)] and Lewin, Lieb, and Seiringer [Phys. Rev. B **100**, 035127 (2019)] that the three definitions coincide in dimension $d \geq 3$. We show that the jellium energy is also equivalent to a “renormalized energy” studied in a series of papers by Serfaty and others, and thus, by the work of Bétermin and Sandier [Constr. Approximation **47**, 39–74 (2018)], we relate the jellium energy to the order n term in the logarithmic energy of n points on the unit 2-sphere. We improve upon known lower bounds for this renormalized energy. Additionally, we derive formulas for the jellium energy of periodic configurations.

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I. INTRODUCTION

The *jellium* model is an important and very simple model, which models electrons in a uniformly charged background interacting via Coulomb interaction. It was introduced by Wigner¹ who conjectured that the minimal energetic configuration was that of a lattice configuration (in two dimensions, the triangular lattice), called a *Wigner crystal*. The thermodynamic limit of jellium was established in dimension $d = 2$ in Ref. 2 building on Ref. 3.

Another important object is the *Uniform Electron Gas* (UEG).^{4–7} It appears naturally in the local density approximation of density functional theory and gives the correlation energy of the electrons (see Refs. 5 and 7). In this model, there is no background, and the density of the electrons is a constant. The jellium model and the UEG are nonetheless related. Indeed, jellium is expected to crystallize.¹ This crystal has no preferred position or orientation, and so one may take the average over all translations of such a crystal. This gives a state with constant density sometimes called the *floating crystal*.⁶ The energy of this floating crystal is the jellium energy of the crystal. This relation has been explored in dimensions $d \neq 2$.^{6,8–12} In dimensions $d \geq 3$, the UEG and jellium ground state energy densities are known to coincide.^{6,12} In dimension $d = 1$, they are known to differ.^{6,8–11} In dimension $d = 2$, Cotar and Petrache¹² (Remark 1.7) conjectured that they coincide.

In this paper, we show that the jellium and UEG energy densities coincide in dimensions $d \geq 2$, thus verifying the conjecture of Cotar and Petrache. For this analysis, we will study a third definition of the energy density, namely, that of periodic jellium, meaning that the electrons live on a torus and interact with all their periodic images. The thermodynamic limit of periodic jellium was established in Refs. 13–17 for both the Coulomb case and various generalizations to Riesz interactions. We will use a similar method as in Ref. 6 to show that the three energy densities are the same. This involves a modified “floating crystal” trial state for the UEG, for which the density is a characteristic function. This requirement of having density a characteristic function was not needed in the three-dimensional case.⁶ We will discuss why it is needed in the two-dimensional case and construct this trial state in Sec. V.

Additionally, we consider the question of periodic jellium configurations, where the electrons are confined to sites of a lattice. Here, we find that the energy is given by the Epstein (or lattice) ζ -function associated with the lattice, on which the electrons sit.

Finally, we relate the evaluation of the jellium energy to that of a “renormalized energy” W studied in Refs. 12 and 14–21. Here, we show that $\min_{A_1} W = 2\pi e_{\text{jel}}$ (notation explained in Sec. IV). This gives another equivalent definition of the jellium energy. Bétermin and Sandier²¹ showed that the logarithmic energy on n points on \mathbb{S}^2 has a term of order n given by $c_{\log} = \frac{1}{\pi} \min_{A_1} W + \frac{\log 4\pi}{2}$ (see Remark IV.6). Hence, we get yet another equivalent definition of the jellium energy. The relation of e_{jel} and $\min_{A_1} W$ carries over the known bounds for the jellium energy. The lower bound of $e_{\text{jel}} \geq -0.66118$ by Lieb and Narnhofer³ and Sari and Merlini² has been known for many years. It improves upon known bounds for the constants c_{\log} and $\min_{A_1} W$. In particular, it gives the bound $-0.0569 \leq c_{\log} \leq -0.0556$ improving on the best-known lower bound of $c_{\log} \geq -0.0954$ due to Steinerberger.²² Since the proof of the lower bound in Ref. 2 is not very detailed, we give the proof in Appendix B.

II. THREE DEFINITIONS OF THE JELLIUM ENERGY

We now introduce the three models. We will give the argument only in dimension $d = 2$, partly because this case is where the argument is most complicated and partly because the physically interesting cases are dimensions $d = 1, 2, 3$, and the cases $d \geq 3$ are solved.^{6,12} For dimensions $d \geq 3$, the argument is the same, and only one should replace every occurrence of $-\log$ with $|\cdot|^{-d}$.

The first model is what we will call jellium. By scaling, we may assume that the density of the background is $\rho = 1$. Then, the jellium energy of N particles in a domain Ω_N of size $|\Omega_N| = N$ is

$$\mathcal{E}_{\text{jel}}(\Omega_N, x_1, \dots, x_N) = -\sum_{j < k} \log|x_j - x_k| + \sum_{j=1}^N \int_{\Omega_N} \log|x_j - y| dy - \frac{1}{2} \iint_{\Omega_N \times \Omega_N} \log|x - y| dx dy.$$

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 two dimensions given by $-\log|x|$. The long range behavior of the logarithm means that this setting is somewhat different from the three-dimensional case. In Ref. 2, it is shown that the thermodynamic limit

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

exists under fairly non-restrictive conditions on the sequence of domains Ω_N . For instance, $\Omega_N = N^{1/2}\Omega$ for a fixed convex set Ω of size $|\Omega| = 1$.

The second model is that of periodic jellium. Here, the $n = \ell^2$ electrons live on a torus of side length ℓ in a uniform background of opposite charge. The Coulomb potential between the electrons is replaced by the periodic Coulomb potential, where the electrons interact with all the periodic images of the other electrons and the uniform background. The functional is defined as follows.

First, we 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 $-\Delta G_1 = 2\pi(\sum_{z \in \mathbb{Z}^2} \delta_z - 1)$ and $\int_{C_1} G_1 dx = 0$, 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. Then,

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

Now, $G_1(x) + \log|x|$ has a limit as $x \rightarrow 0$, which we call C_{mad} . It is the Madelung constant, i.e., twice the energy per particle of the configuration with one particle in the unit cell, i.e., a square lattice configuration. The functional $\mathcal{E}_{\text{per},\ell}$ may now be defined as

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

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 $\int_{C_\ell} G_\ell dx = 0$. We then define

$$e_{\text{per}} = \lim_{\ell \rightarrow \infty} \min_{x_1, \dots, x_n} \frac{\mathcal{E}_{\text{per},\ell}(x_1, \dots, x_n)}{\ell^2}.$$

The existence of this limit was established in Refs. 13–17. It will also follow from the Proof of Theorem II.1 that indeed this limit exists.

The third model is what has been called the uniform electron gas (UEG) in Refs. 5–7. For a complete description of this model, see Ref. 5. Here, there is no background charge, and the electrons are no longer point particles. Instead, the electrons are distributed according to

a probability density \mathbb{P} (meaning \mathbb{P} is a probability measure on \mathbb{R}^{2N}), which we require to give a constant density $\rho_{\mathbb{P}} = \mathbb{1}_{\Omega_N}$, where $\rho_{\mathbb{P}}$ is the sum of all the marginals. The indirect energy of the distribution is then

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

We are interested in keeping the density fixed, and so, for any density ρ with $\int \rho dx = N$, we define

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

Since the electrons are indistinguishable, we should, in principle, restrict to symmetric \mathbb{P} 's. This, however, gives the same minimum. Again, we are interested in the thermodynamic limit, and for a system of uniform density, i.e.,

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

The existence of this limit was established in Ref. 5 (Theorem 2.6). Their proof is done in dimensions $d \geq 3$ but works without change also in dimensions $d = 1, 2$. Now, our main theorem is

Theorem II.1. *We have $e_{\text{Jel}} = e_{\text{per}} = e_{\text{UEG}}$.*

The analogous result in dimensions $d \geq 3$ was proven by Cotar and Petrache¹² using methods of optimal transport and later in dimension $d = 3$ by Lewin, Lieb, and Seiringer⁶ using a “floating crystal” trial state, which our method builds on. Cotar and Petrache¹² (Remark 1.7) note that the case of $d = 2$ is an open problem. Our findings here thus solve this open problem.

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

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

Optimizing over \mathbb{P} and taking the thermodynamical limit, we thus get $e_{\text{UEG}} \geq e_{\text{Jel}}$. In order to get the inequality $e_{\text{UEG}} \leq e_{\text{per}} \leq e_{\text{Jel}}$, we will superficially introduce a crystal structure to the jellium configuration. This is similar to (and inspired by) the floating crystal argument from Ref. 6. We give the proof in Secs. V and VI.

III. LATTICE CONFIGURATIONS

We now consider the jellium energies of periodic configurations when the electrons are positioned on a lattice. We will consider these configurations in any dimension d and for general Riesz interactions. These we first define. For $s \in \mathbb{R}$, the Riesz potential V_s on \mathbb{R}^d is given 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 ,

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

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

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

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 III.1.) Here, $\Omega_N = \cup_{i=1}^N (Q + x_i)$. Define for $\text{Re}(s) > d$ the Epstein (or lattice) ζ -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 Ref. 23). These more complicated ζ -functions can oftentimes be expressed in terms of simpler functions (see Ref. 24). We prove the following theorem:

Theorem III.1. *Let s satisfy $d - 4 < s < d$, and let $\mathcal{L} \subset \mathbb{R}^d$ be a lattice with the Wigner–Seitz unit cell Q , $|Q| = 1$. Then, the jellium energy of the lattice configuration is*

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

Many similar results exist in the literature. In Refs. 23 and 25, a similar result is shown for a slightly different energy functional in the case $d - 2 < s < d$ via analytic continuation of the Epstein ζ -function. Extending upon these ideas, a partial result for the jellium energy is shown in Ref. 4 (Appendix B). Other formulations also exist (see, for instance, Refs. 21, 26, and 27 for the case of logarithmically interacting points on the unit two-sphere and Refs. 18 and 21 for the case of logarithmically interacting points on the plane). As we have not found a complete proof of Theorem III.1 in the literature, we give a straightforward proof in Sec. VII. As an application of the theorem, we compute the energy density of jellium in the triangular lattice (in two dimensions).

Example III.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 Ref. 24, we have

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

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.,

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

where $\zeta(s, a)$ is the Hurwitz ζ -function. The values of these functions and their derivatives can be found in Ref. 28. We conclude that $e_{\text{jel},s=0}^{\mathcal{L}} = \zeta'_{\mathcal{L}}(0) = \frac{1}{8} \log\left(\frac{48\pi}{\Gamma(1/6)^6}\right) \simeq -0.66056$. In comparison, the best-known lower bound^{2,3} is $e_{\text{jel},s=0} \geq -\left(\frac{3}{8} + \frac{1}{4} \log \pi\right) \simeq -0.66118$. The triangular lattice, which is what we expect to be the ground state, is remarkably close to this lower bound.

Example III.3. In dimension $d = 1$, there is only one lattice, namely, \mathbb{Z} . Thus, $e_{\text{jel},s=-1}^{\mathbb{Z}} = -\zeta(-1) = \frac{1}{12}$. It is, in fact, known that jellium is crystallized in one dimension.⁸⁻¹⁰

IV. RELATION TO THE RENORMALIZED ENERGY

We now relate the jellium energy to the renormalized energy studied in Refs. 12 and 14–20, where it has been used in both the study of Ginzburg–Landau theory and Coulomb gases. We give here the definition from Ref. 14.

Definition IV.1. Let E be a vector-field on \mathbb{R}^2 . Let $m > 0$. We say that $E \in \mathcal{A}_m$ if

$$\text{div } E = 2\pi(v - m), \quad \text{curl } E = 0, \quad \sup_{R>1} \frac{v(B_R)}{|B_R|} < \infty, \tag{1}$$

where $v = \sum_{p \in \Lambda} \delta_p$ for a discrete set $\Lambda \subset \mathbb{R}^2$.

Then, for any function χ , we define

$$W(E, \chi) = \lim_{\eta \rightarrow 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \bigcup_{p \in \Lambda} B(p, \eta)} \chi |E|^2 + \pi \log \eta \sum_{p \in \Lambda} \chi(p) \right).$$

The renormalized energy is then defined as follows:

Definition IV.2. The renormalized energy of E is

$$W(E) := \limsup_{R \rightarrow \infty} \frac{W(E, \chi_R)}{|K_R|},$$

where χ_R denotes any cut-off functions satisfying

$$|\nabla \chi_R| \leq C, \quad \text{supp}(\chi_R) \subset K_R, \quad \chi_R(x) = 1 \text{ if } d(x, K_R^c) \geq 1,$$

where $K_R = [-R, R]^2$ is the square of sides $2R$.

We recall a few properties of W from Ref. 14. (These are proven in Ref. 18.)

- The renormalized energy $W(E)$ does not depend on the choice of cut-off functions χ_R , and these need not be defined in terms of squares either.
- If $E \in \mathcal{A}_m$, then $E' = \frac{1}{\sqrt{m}} E(\cdot/\sqrt{m}) \in \mathcal{A}_1$ and $W(E) = m(W(E') - \frac{\pi}{2} \log m)$. In particular, $\min_{\mathcal{A}_m} W = m(\min_{\mathcal{A}_1} W - \frac{\pi}{2} \log m)$.
- If $E \in \mathcal{A}_m$ with $W(E) < \infty$, then $\lim_{R \rightarrow \infty} \frac{v(B_R)}{|B_R|} = m$.
- $\min_{\mathcal{A}_1} W$ is the limit of a sequence of periodic configurations with period $n \rightarrow \infty$.

For periodic Λ , we have the following result:

Proposition IV.3 [Ref. 18 (Proposition 3.1) and Ref. 14 (p. 2044)]. Suppose Λ is periodic with respect to some lattice \mathcal{L} , and denote the points of Λ in the torus $\mathbb{T} = \mathbb{R}^2/\mathcal{L}$ by $\{x_1, \dots, x_n\}$. Define $H_{\{x_i\}}$ and $E_{\{x_i\}}$ on \mathbb{T} by

$$-\Delta H_{\{x_i\}} = 2\pi \left(\sum_{i=1}^n \delta_{x_i} - \frac{n}{|\mathbb{T}|} \right), \quad E_{\{x_i\}} := -\nabla H_{\{x_i\}}.$$

Then, $W(E) \geq W(E_{\{x_i\}})$ for any E satisfying Eq. (1).

Note that $H_{\{x_i\}}$ is defined uniquely up to a constant, and thus, $E_{\{x_i\}}$ is well-defined. Now, the relation of this renormalized energy to the jellium energy is the following corollary:

Corollary IV.4. The renormalized energy is given by

$$\min_{\mathcal{A}_1} W = 2\pi e_{\text{jel}}.$$

Cotar and Petrache¹² showed a similar result for more general Riesz interactions, but not including the $d = 2, s = 0$ case, which is the one considered here (see Remark IV.8). This relation between the renormalized energy and the jellium energy is also discussed in Ref. 18 for the Coulomb case and in Ref. 16 for the Riesz case.

Proof. Since $\min_{\mathcal{A}_1} W$ is the limit of periodic configurations¹⁸ (Theorem 1) and any such periodic configuration clearly has energy at least $\min_{\mathcal{A}_1} W$, we have

$$\min_{\mathcal{A}_1} W = \lim_{\ell \rightarrow \infty} \min_{\substack{E \in \mathcal{A}_1 \\ E \text{ is } \ell\text{-periodic}}} W(E).$$

Now, suppose E is ℓ -periodic. Denote the points of Λ in the torus $\mathbb{R}^2/\ell\mathbb{Z}^2$ by $\{x_1, \dots, x_n\}$. Then, $W(E) \geq W(E_{\{x_i\}})$ by Proposition IV.3. Now, by Ref. 19 (Lemma 2.7),

$$W(E_{\{x_i\}}) = \frac{2\pi}{n} \sum_{i < j} G_\ell(x_i - x_j) + \pi \lim_{x \rightarrow 0} (G_\ell(x) + \log|x|) = \frac{2\pi}{n} \mathcal{E}_{\text{per}, \ell}(x_1, \dots, x_n).$$

Hence, by Theorem II.1,

$$\min_{\mathcal{A}_1} W = 2\pi \lim_{n \rightarrow \infty} \min_{x_1, \dots, x_n} \frac{\mathcal{E}_{\text{per}, \ell}(x_1, \dots, x_n)}{n} = 2\pi e_{\text{per}} = 2\pi e_{\text{jel}}.$$

□

With this, the known bounds on e_{jel} carry over. The upper bound of

$$\min_{\mathcal{A}_1} W = 2\pi e_{\text{jel}} \leq 2\pi e_{\text{jel}}^{\mathcal{L}} \simeq -4.1504,$$

where \mathcal{L} is the triangular lattice, was previously known.^{18,21} It is, in fact, conjectured that we have equality.^{1,18} This is the famous “crystallization conjecture” (see Ref. 29 for a review). As shown in Ref. 30, this crystallization would follow from the Cohn–Kumar conjecture. The “crystallization conjecture” states roughly that the optimal configuration for the electrons is to arrange in a triangular lattice (at least in the bulk). Thus, the energy density would be the one given by a triangular lattice configuration. This problem is solved in one dimension,^{8–10} where crystallization has been shown. In dimensions $d \geq 2$, it is open. Partial results include the equidistribution of points.²⁰

The lower bound^{2,3} $e_{\text{jel}} \geq -\left(\frac{3}{8} + \frac{1}{4} \log \pi\right)$ gives the following corollary:

Corollary IV.5. We have $\min_{\mathcal{A}_1} W = 2\pi e_{\text{jel}} \geq -\pi\left(\frac{3}{4} + \frac{1}{2} \log \pi\right) \simeq -4.1543$.

This is an improvement on previously known lower bounds. The previously known lower bound by Steinerberger,²² translated to this setting using the results of Ref. 21, is $\min_{\mathcal{A}_1} W \geq -\frac{\pi}{2}(1 + \gamma + \log \pi) \simeq -4.2756$, where $\gamma \simeq 0.577$ is the Euler–Mascheroni constant.

Remark IV.6. The renormalized energy has also been used by Bétermin and Sandier²¹ in the problem of optimal point-configurations on the sphere \mathbb{S}^2 with a logarithmic energy functional, i.e., points $x_1, \dots, x_n \in \mathbb{S}^2$ minimizing $E(x_1, \dots, x_n) = -\sum_{i \neq j} \log|x_i - x_j|$. The problem of minimizing the logarithmic energy of points on the sphere has received much study (see Refs. 21, 22, 26, 27, and 31) and is linked to Smale’s seventh problem (see Ref. 32 for a review).

Let $\mathcal{E}_{\log}(n) = \min E(x_1, \dots, x_n)$ denote the minimal energy. Bétermin and Sandier²¹ showed that there exists a constant $c_{\log} = \frac{1}{\pi} \min_{\mathcal{A}_1} W + \frac{\log 4\pi}{2}$ such that

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2\right)n^2 - \frac{1}{2}n \log n + c_{\log}n + o(n)$$

as $n \rightarrow \infty$. The previously known lower bound of the constant c_{\log} due to Steinerberger²² is $c_{\log} \geq \frac{\log 4 - 1 - \gamma}{2} \simeq -0.0954$. Written in terms of the constant c_{\log} , the improved lower bound gives the following corollary:

Corollary IV.7. We have $c_{\log} = 2e_{\text{jel}} + \frac{\log 4\pi}{2} \geq \log 2 - \frac{3}{4} \simeq -0.0569$.

Remark IV.8. The renormalized energy has also been defined for general Riesz potentials in Ref. 16 and jellium and periodic jellium in Ref. 6. Let \mathcal{W} be as defined in Ref. 16 (Definition 1.3) (this differs from the W considered above by a factor of 2 in the case $d = 2, s = 0$) and $e_{\text{per}}(d, s)$ be the periodic jellium energy for the Riesz potential with parameter s and in dimension d as defined in Ref. 6. Exactly the same proof as above shows that $\min_{\mathcal{A}_1} \mathcal{W} = 2c_{d,s}e_{\text{per}}(d, s)$ for $\max(0, d - 2) \leq s < d$, where

$$c_{d,s} = \begin{cases} 2s \frac{2\pi^{d/2} \Gamma\left(\frac{s+2-d}{2}\right)}{\Gamma\left(\frac{s+2}{2}\right)} & \text{if } \max(0, d - 2) < s < d, \\ (d - 2) \frac{2\pi^{d/2}}{\Gamma(d/2)} & \text{if } s = d - 2 > 0, \\ 2\pi & \text{if } s = 0, d = 1, 2. \end{cases}$$

In Refs. 6, 12, 16, and 17 and Theorem II.1, it is proved that $e_{\text{jel}}(d, s) = e_{\text{per}}(d, s)$ for the relevant d, s . Thus, we have $\min_{\mathcal{A}_1} \mathcal{W} = 2c_{d,s}e_{\text{jel}}(d, s)$. This result was previously shown in Ref. 12 only not including the case $d = 2, s = 0$.

We now turn to the proofs of Theorems II.1 and III.1.

V. UPPER BOUND FOR THE UNIFORM ELECTRON GAS ENERGY

We first show that

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

The proof is very similar to the proof of the same result in dimension $d = 3$ presented in Ref. 6. The main difference is the different choice of trial state \mathbb{P} , which we will need to be a characteristic function. We now explain why we need this.

In dimension $d = 3$, the thermodynamic limit of the uniform electron gas exists under weaker conditions by the Graf–Schenker inequality,³³ as discussed in Refs. 5 and 6. There, it is only required that the density $\rho_{\mathbb{P}}$ is 1 in the bulk of Ω_N , 0 outside, and bounded close to the boundary. In dimension $d \neq 3$, we do not have this weaker formulation, so we need that the density is a characteristic function for the thermodynamic limit to exist. (Actually, if we have the stricter bound $\rho_{\mathbb{P}} \leq 1$, then the thermodynamic limit⁵ still holds. The modification of the argument in Ref. 5 to this case is trivial.) Additionally, due to the long range behavior of the logarithm, some error bounds are slightly more complicated in two dimensions.

The construction of the trial state \mathbb{P} is similar to that of Ref. 6. We consider a floating crystal immersed in a thin fluid layer (uncorrelated electrons). The fluid is needed to counteract the charge build-up from translating the crystal, exactly as in Ref. 6. We want the density $\rho_{\mathbb{P}}$ to be a characteristic function. In particular, we have to control the overlap of the fluid (under one translation) with the crystal (under a different translation). This amounts to making a “hole” in the fluid, which is larger than the crystal. Additionally, the fluid layer is not chosen to have constant density 1 but instead have some density profile β , which we describe below. The density profile β is chosen to fill out the gaps left by having a larger hole in the fluid than the crystal.

We now give the construction of the trial state (see also Fig. 1). For the intuition of the construction, it is perhaps easiest to consider the fluid layer to have constant density 1 (meaning $\beta = \mathbb{1}_C$ in the notation below) and then *a posteriori* update the density profile to the stated β to ensure that $\rho_{\mathbb{P}}$ is a characteristic function.

Consider any arrangement of n points x_1, \dots, x_n in the cube $C_\ell = [-\ell/2, \ell/2]^2$ of side length $\ell = n^{1/2}$. 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: $\int y (\sum_{j=1}^n \delta_{x_j}(y) - \mathbb{1}_{C_\ell + \tau}(y)) dy = 0$. 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 $N = \ell^2(2K + 1)^2$. The electrons are located at the points $x_j = x_{j_0} + \ell k$. Let C be a square with $C \supset \Omega_N + 5C_\ell$ and $|C \setminus \Omega_N| = M = O(N^{1/2})$ be an integer. Define $F = \Omega_N + 3C_\ell + \tau$ (the “hole in the fluid”) and $\beta = \mathbb{1}_C + \mathbb{1}_F * \frac{\mathbb{1}_{C_\ell}}{\ell^2} - \frac{1}{n} \sum_{j=1}^n \mathbb{1}_{\Omega_N + x_j}$. The trial state \mathbb{P} is then the average over all translations of the crystal, with the fluid moving opposite to counteract the build-up of charge (see Fig. 1). That is,

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

We choose $F = \Omega_N + 3C_\ell + \tau$ such that the fluid and the crystal have minimal overlap. (For the case of constant fluid density, there is no overlap.) The term $+\tau$ is there to ensure the vanishing dipole moment, and the term $+3C_\ell$ comes from the following considerations.

The crystal, when shifted around, gives some density in the region $\Omega_N + C_\ell$. We thus want that, for any shift $F + a$ of F , the region $C \setminus (F + a)$ does not overlap with the region $\Omega_N + C_\ell$. Since τ is, in general, just some vector $\tau \in C_\ell$, this leads to our definition of $F = \Omega_N + 3C_\ell + \tau$. In order for the fluid to have positive density, we need $\beta \geq \mathbb{1}_{F+a}$ for any shift a . This leads to $\beta \geq \mathbb{1}_C$, with $C \supset \Omega_N + 5C_\ell$. This is true by construction. Now, we compute that

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

Thus, $\rho_{\mathbb{P}}$ is a characteristic function as desired.

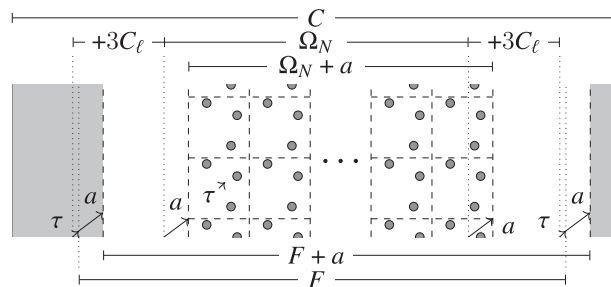


FIG. 1. Slice of the crystal and fluid in the construction of the trial state. The gray circles indicate the positions of the electrons, and each square tile is one copy of the n -point configuration. The gray areas at the left and right edges are the region $C \setminus (F + a)$. For the choice of a constant fluid density, this is exactly the region where the fluid is.

As mentioned, the thermodynamic limit⁵ (Theorem 2.6) also holds for densities $\rho_{\mathbb{P}} \leq 1$. Thus, we can actually choose β any function with $\mathbb{1}_C \leq \beta \leq \mathbb{1}_C + \mathbb{1}_F * \frac{\mathbb{1}_{C_\ell}}{\ell^2} - \frac{1}{n} \sum_{j=1}^n \mathbb{1}_{\Omega_N+x_j}$. This will not change the argument. In the computations below, we will use the description of $\rho_{\mathbb{P}}$ in terms of β , as this will make the computations slightly nicer.

We now use this trial state to show that

$$e_{\text{UEG}} \leq \liminf_{N \rightarrow \infty} \frac{\mathcal{E}_{\text{Jel}}(\Omega_N + \tau, x_1, \dots, x_N)}{N}.$$

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

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

for two (signed) measures μ, ν . This is the Coulomb interaction energy between charge distributions μ and ν . Mostly, we will use this in the case where the measures are given by functions. The analogous object in dimensions $d \geq 3$ has $D(f) \geq 0$ for any function. This is, however, not true in dimension $d = 2$. In general, it is only true for functions with zero mean.

Proposition V.1. Suppose f has $\int f dx = 0$. Then, $D(f) \geq 0$.

This is well-known. A proof may, for instance, be found in Ref. 34 (Lemma 3.2). For completeness, we provide a short proof here.

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 $\widehat{f^\#} = \widehat{f}$. First we show that $\frac{\widehat{f^\#}}{p^2} = \frac{|\widehat{f}(p)|}{p^2}$ is the Fourier transform of some function. Define $g := \frac{-1}{2\pi} \log * f^\# * f$. Then, by Ref. 35 (Theorem 6.21), we have that $g \in L^1_{\text{loc}}$ and $-\Delta g = f^\# * f$ in \mathcal{D}' . Since $\log \in \mathcal{S}'$, we have that $g \in \mathcal{S}'$ and so $p^2 \widehat{g} = \widehat{f^\# * f}$ in \mathcal{S}' . Hence, $\widehat{g}(p) = 2\pi \frac{|\widehat{f}(p)|^2}{p^2}$ as functions. By the assumption $\int f dx = 0$, we have that the right-hand-side actually stays bounded (and smooth) as $p \rightarrow 0$. We conclude that $\widehat{g} \in \mathcal{S}$ and so $g \in \mathcal{S}$ has a Fourier transform as a function.

Now, with $\langle \cdot | \cdot \rangle$ denoting application of a distribution, we have

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

since by Ref. 35 (Theorem 6.20), we have $-\Delta(-\log | \cdot |) = 2\pi \delta$ in \mathcal{D}' . □

Remark V.2. In dimension $d = 1$, an analogous statement also holds.

Now, we may calculate the energy (with x_j , for $j > n$ denoting the points $x_j + \ell k$ for $k \neq 0$)

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

First, we claim that

$$-\frac{1}{M\ell^2} \int_{C_\ell} D(\beta - \mathbb{1}_{F+a}) da \leq o(N).$$

Remark V.3. In dimensions $d \geq 3$, the analogous term is ≤ 0 since $D(f) \geq 0$ for any function f .

For any a , denote by $A = \text{supp}(\beta - \mathbb{1}_{F+a})$. Then, we have $|A| = O(N^{1/2})$ and $\text{diam}A = O(N^{1/2})$. Thus,

$$\begin{aligned} D(\beta - \mathbb{1}_{F+a}) &= \frac{1}{2} \iint_{A \times A} -\log|x-y|(\beta - \mathbb{1}_{F+a})(x)(\beta - \mathbb{1}_{F+a})(y) \, dx \, dy \\ &\geq C \iint_{A \times A} -\log \text{diam}A \, dx \, dy = O(N \log N). \end{aligned}$$

Hence,

$$-\frac{1}{M\ell^2} \int_{C_\ell} D(\beta - \mathbb{1}_{F+a}) \, da \leq O(N^{1/2} \log N) = o(N).$$

We are thus left with the error term

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

Plugging in the value of ρ_P , we may calculate this term as

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

where

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

We claim that Eq. (2) 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 V.4. Let A be a square of size $|A| = O(N)$. Let μ be a measure satisfying $\mu(B_R) = O(R^2)$ as $R \rightarrow \infty$. Let B be the boundary region of A , meaning $B = \{x \in \mathbb{R}^2 : d(x, \partial A) \leq \ell\}$ for some fixed $\ell > 0$. Then,

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

One should think that μ is either the 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 $L = O(N^{1/2})$ centered at y (removing the ball of radius 1). Thus,

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

Proposition V.5. Let A, B be as in Proposition V.4 and μ be a probability measure supported in B_ℓ . Denote by τ the first moment of μ , i.e., $\tau = \int a \, d\mu(a)$. Let b be a function supported in B , which is bounded uniformly in N . Then,

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

Remark V.6. In dimension $d \geq 1$, we similarly have

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

Thus, our argument also works in higher dimensions.

We postpone the Proof of Proposition V.5 to [Appendix A](#). Proposition V.5 immediately gives that the second and third terms of Eq. (2) are $O(N^{1/2} \log N)$. For the first term, we use that by Taylor expansion,

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

for a bounded and $|z|$ bounded from below. Thus, for the term

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

we have

$$\begin{aligned} &= \sum_{\substack{j=1, \dots, n \\ k \in \mathbb{Z}^2 \\ |k_1|, |k_2| \leq K}} \iint f(x)(-\log|x-y|) \left[\delta_{x_j+\ell k} - \frac{1}{\ell^2} \mathbb{1}_{C_\ell+\tau+\ell k}\right](y) dy dx \\ &= \sum_{j,k} \frac{1}{\ell^2} \int_{F \setminus (\Omega_N+\tau)} \int_{C_\ell} -\log|x-\ell k-x_j| + \log|x-\ell k-\tau+a| da dx \end{aligned}$$

Hence, since $|x-\ell k|$ is bounded from below on $F \setminus (\Omega_N+\tau)$, we have

$$\begin{aligned} &= \int_{F \setminus (\Omega_N+\tau)} \sum_{j,k} \underbrace{-\frac{(x-\ell k-\tau) \cdot (\tau-x_j)}{|x-\ell k-\tau|^2}}_{=0 \text{ by } \sum x_j = \sum \tau} dx + \sum_{j,k} \int_{F \setminus (\Omega_N+\tau)} O\left(\frac{1}{|x-\ell k|^2}\right) dx \\ &+ \sum_{j,k} \frac{1}{\ell^2} \int_{F \setminus (\Omega_N+\tau)} \int_{C_\ell} \underbrace{\frac{(x-\ell k-\tau) \cdot a}{|x-\ell k-\tau|^2}}_{=0 \text{ by } \int a da=0} da dx + \sum_{j,k} \int_{F \setminus (\Omega_N+\tau)} O\left(\frac{1}{|x-\ell k|^2}\right) dx \\ &= O(N^{1/2} \log N) \end{aligned}$$

by Proposition V.4. This gives the bound $\mathcal{E}_{\text{ind}}(\rho_{\mathbb{P}}) \leq \mathcal{E}_{\text{ind}}(\mathbb{P}) \leq \mathcal{E}_{\text{jel}}(\Omega_N+\tau, x_1, \dots, x_N) + o(N)$. Hence, by taking the thermodynamic limit, we get the desired.

We now show that

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}_{\text{jel}}(\Omega_N+\tau, x_1, \dots, x_N)}{N} = \frac{\mathcal{E}_{\text{per}, \ell}(x_1, \dots, x_n)}{n}.$$

This argument is more or less the same as in Ref. 6. There are slight differences in the case $d=2$ compared to the case $d \geq 3$, which is why we present the argument here. We really only need the bound \leq , and this is what we now show.

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

$$\begin{aligned} \mathcal{E}_{\text{jel}}(\Omega_N+\tau, x_1, \dots, x_N) &\leq -\sum_{j < k} \iint \log|(x_j+y)-(x_k+z)| \chi_\eta(y) \chi_\eta(z) dy dz \\ &+ \sum_{j=1}^N \int_{\Omega_N+\tau} \int \log|(x_j+z)-y| \chi_\eta(z) dz dy - \frac{1}{2} \iint_{(\Omega_N+\tau) \times (\Omega_N+\tau)} \log|x-y| dx dy \\ &= \sum_{j < k} 2D(\chi_\eta(\cdot-x_j), \chi_\eta(\cdot-x_k)) - \sum_{j=1}^N 2D(\chi_\eta(\cdot-x_j), \mathbb{1}_{\Omega_N+\tau}) + D(\mathbb{1}_{\Omega_N+\tau}) \\ &= D\left(\sum_{j=1}^N \chi_\eta(\cdot-x_j) - \mathbb{1}_{\Omega_N+\tau}\right) - N\left(D(\chi_1) - \frac{1}{2} \log \eta\right). \end{aligned}$$

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

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

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

$$D\left(\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_{N+\tau}}\right) = D\left(\sum_k f(\cdot + \ell k)\right) = \pi \int \frac{|\hat{f}(p)|^2}{p^2} \left| \sum_k e^{ipk\ell} \right|^2 dp.$$

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

We have

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

weakly, and so

$$\begin{aligned} \frac{1}{N} D\left(\sum_k f(\cdot + \ell k)\right) &\xrightarrow{N \rightarrow \infty} \frac{\pi}{\ell^2} \int \frac{|\hat{f}(p)|^2}{p^2} \left(\frac{2\pi}{\ell}\right)^2 \sum_{p \in \frac{2\pi}{\ell} \mathbb{Z}^2} \delta_p dp \\ &= \frac{\pi}{\ell^4} \sum_p \int_{C_{\ell+\tau}} \int_{C_{\ell+\tau}} f(x) e^{ipx} f(y) e^{-ipy} \frac{1}{p^2} dx dy \\ &= \frac{1}{2n} \int_{C_{\ell+\tau}} \int_{C_{\ell+\tau}} G_\ell(x-y) f(x) f(y) dx dy. \end{aligned}$$

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

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

Since $\chi_\eta \rightarrow \delta$ as $\eta \rightarrow 0$, the second term converges to $\frac{1}{n} \sum_{j < k} G_\ell(x_j - x_k)$. This is exactly the first term in the functional $\mathcal{E}_{\text{per}, \ell}$ as desired. We now deal with the other term in the limit $\eta \rightarrow 0$,

$$\frac{1}{2} \iint G_\ell(x-y) \chi_\eta(x) \chi_\eta(y) dx dy = \frac{1}{2} \iint (-\log \eta - \log|x-y| + \log \ell + C_{\text{mad}} + o_{\eta \rightarrow 0}(1)) \chi_1(x) \chi_1(y) dx dy,$$

where $o_{\eta \rightarrow 0}(1)$ vanishes as $\eta \rightarrow 0$ uniformly in x, y by the compact support of χ_1 . Hence,

$$\frac{1}{2} \iint G_\ell(x-y) \chi_\eta(x) \chi_\eta(y) dx dy = -\frac{1}{2} \log \eta + D(\chi_1) + \frac{1}{2} \log \ell + \frac{C_{\text{mad}}}{2} + o_{\eta \rightarrow 0}(1).$$

Putting everything together, we now conclude

$$\begin{aligned} &\frac{1}{N} D\left(\sum_{j=1}^N \chi_\eta(\cdot - x_j) - \mathbb{1}_{\Omega_{N+\tau}}\right) - \left(D(\chi_1) - \frac{1}{2} \log \eta\right) \\ &\xrightarrow{N \rightarrow \infty} \frac{1}{n} \sum_{j < k} G_\ell(x_j - x_k) + \frac{1}{2} \iint G_\ell(x-y) \chi_\eta(x) \chi_\eta(y) dx dy - D(\chi_1) + \frac{1}{2} \log \eta \\ &\xrightarrow{\eta \rightarrow 0} \frac{1}{n} \sum_{j < k} G_\ell(x_j - x_k) + \frac{1}{2} \log \ell + \frac{1}{2} C_{\text{mad}}. \end{aligned}$$

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

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

This proves that $e_{\text{UEG}} \leq \frac{\mathcal{E}_{\text{per}, \ell}(x_1, \dots, x_n)}{n}$.

VI. UPPER BOUND FOR THE PERIODIC ENERGY

We now show that

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

This finishes the Proof of Theorem II.1. This argument is again more or less the same as in Ref. 6. Again, there are some slight differences in the case $d = 2$, which is why we give the argument here.

First, we show that a version of Newton's theorem hold for the periodic potential G_ℓ . In particular, that separated neutral radial charge densities have zero total interaction. More precisely, let ρ be any compactly supported radial neutral charge distribution, i.e., $\text{supp } \rho \subset B_R$ for some $R > 0$, ρ is radial, and $\int \rho dx = 0$. Let L be large enough so that $B_R \subset C_L$. 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 vanishes on $C_L \setminus B_R$; thus, we see that $\rho * G_L$ is constant on $C_L \setminus B_R$, and so for another neutral radial charge distribution ρ' supported in this region, their interaction vanish, $\iint G_L(x-y)\rho(x)\rho'(y) dx dy = 0$.³⁶

We use the Swiss cheese theorem [Ref. 37 (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 $\ell \rightarrow \infty$ after taking $L \rightarrow \infty$, 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 . (Note that n refers to the index of the ball, and not its radius.) The remaining $M = N - \sum_n |B_n|$ particles are placed uniformly in the remainder $S = C_L \setminus \cup_n B_n$, meaning that we smear the particles out in this region. This yields

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

where x_1, \dots, x_{N-M} denote the points in $\cup_n B_n$ and we used that $\int_{C_L} G_L dx = 0$. 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 do not interact with each other. Writing \tilde{G}_L for the rotational average of G_L , we thus get the upper bound

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

As $L \rightarrow \infty$, we have that $G_L(x) = -\log|x| + \log L + C_{\text{mad}} + o(1)$. Plugging this into the bound above, the $\frac{1}{M}$ -term is $o(1)$ and the remaining $\log L$ and C_{mad} -terms cancel. What we are left with is the bound

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

where the term $o_{L \rightarrow \infty}(1)$ depends on ℓ but not on n . Dividing by $N = L^2$ and taking the consecutive limits $L \rightarrow \infty$, $\ell \rightarrow \infty$, and $\ell_0 \rightarrow \infty$, this gives e_{Jel} by the existence of the thermodynamic limit for jellium.² We conclude that

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

Hence, we have shown

$$e_{\text{UEG}} \leq \liminf_{N \rightarrow \infty} \min_{x_1, \dots, x_N \in C_L} \frac{\mathcal{E}_{\text{per},L}(x_1, \dots, x_N)}{N} \leq \limsup_{N \rightarrow \infty} \min_{x_1, \dots, x_N \in C_L} \frac{\mathcal{E}_{\text{per},L}(x_1, \dots, x_N)}{N} \leq e_{\text{Jel}}.$$

Thus, $e_{\text{UEG}} = e_{\text{per}} = e_{\text{Jel}}$.

VII. PROOF OF THEOREM III.1

We now give the Proof of Theorem III.1.

Proof of Theorem III.1. First, we extend V_s to complex-valued s as follows. For $s \in \mathbb{C} \setminus \mathbb{R}$, we define $V_s(x) = |x|^{-s}$. Now, define the functions W_s and \tilde{W}_s for any $s \in \mathbb{C}$ by

$$W_s = V_s - 2V_s * \mathbb{1}_Q + V_s * \mathbb{1}_Q * \mathbb{1}_Q = V_s * (\delta - \mathbb{1}_Q) * (\delta - \mathbb{1}_Q), \quad \text{and} \quad \tilde{W}_s = |\cdot|^{-s} * (\delta - \mathbb{1}_Q) * (\delta - \mathbb{1}_Q).$$

Note that $W_s = \tilde{W}_s$ if $s \in \mathbb{C} \setminus (-\infty, 0]$, that $W_s = -\tilde{W}_s$ if $s < 0$, and that $W_s = \frac{d}{ds} \tilde{W}_s|_{s=0}$ if $s = 0$.

By a tedious but straightforward Taylor expansion, one checks that $\tilde{W}_s(x)$, $W_s(x) \sim |x|^{-\text{Re}(s)-4}$ for large $|x|$. Let x_1, \dots, x_N be N points on the lattice, say, $\{x_1, \dots, x_N\} = \mathcal{L} \cap B_R$ for some R , and set $\Omega_N = \bigcup_{j=1}^N (Q + x_j)$. Consider now $s < d$. Then,

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

For $s > d - 4$, the sum $\sum_{x \in \mathcal{L} \setminus 0} W_s(x)$ converges, and so we may take the thermodynamic limit

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

Let now $s \in \mathbb{C}$, $\text{Re}(s) > d$. We may then write

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

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

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

$$\int_{\mathbb{R} \setminus Q} V_s(y) dy = \int_{|y| > \epsilon} V_s(y) dy - \int_{Q \setminus B_\epsilon} V_s(y) dy = |S^{d-1}| \epsilon^{d-s} \frac{1}{s-d} - \int_{Q \setminus B_\epsilon} \frac{1}{|y|^s} dy.$$

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

For the second term, we write

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

We now split this integral according to

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

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

$$\int_{Q \setminus B_\delta} \int_{(Q+z) \setminus B_{\epsilon|z|}} |w|^{-s} dw dz, \quad \int_{B_\delta} \int_{(Q+z) \setminus B_\rho} |w|^{-s} dw dz$$

are analytic in s . We calculate the remaining terms. The term

$$\int_{Q \setminus B_\delta} \int_{|w|>\epsilon|z|} |w|^{-s} dw dz = |S^{d-1}| \frac{1}{s-d} \epsilon^{d-s} \int_{Q \setminus B_\delta} |z|^{d-s} dz$$

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

$$\int_{B_\delta} \int_{|w|>\epsilon|z|} |w|^{-s} dw dz = |S^{d-1}|^2 \frac{1}{s-d} \frac{1}{2d-s} \epsilon^{d-s} \delta^{2d-s}$$

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

$$\int_{B_\delta} \int_{B_\rho \setminus B_{\epsilon|z|}} |w|^{-s} dw dz = |S^{d-1}| |B_1| \frac{1}{d-s} \delta^d \rho^{d-s} - |S^{d-1}|^2 \frac{1}{d-s} \epsilon^{d-s} \frac{1}{2d-s} \delta^{2d-s}$$

makes sense for $d < \text{Re}(s) < 2d$ 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 $\text{Re}(s) < d$, we may take $\epsilon, \delta, \rho \rightarrow 0$ in a suitable order. All these terms combined then give the limit

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

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

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

Thus, for real $d-4 < s < d$ with $s \neq 0$, we have

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

For $s = 0$, we have $W_{s=0} = \frac{d}{ds} \tilde{W}_s|_{s=0}$ and similarly $V_{s=0} = \frac{d}{ds} |\cdot|^{-s}|_{s=0}$. Thus,

$$\begin{aligned} e_{\text{rel},s=0}^{\mathcal{L}} &= \sum_{x \in \mathcal{L} \setminus 0} W_{s=0}(x) - \int_Q V_{s=0}(y) dy + D_{d,s=0}(\mathbb{1}_Q) \\ &= \frac{d}{ds} \left[\sum_{x \in \mathcal{L} \setminus 0} \tilde{W}_s(x) - \int_Q \frac{1}{|y|^s} dy + \frac{1}{2} \iint_{Q \times Q} \frac{1}{|y-z|^s} dy dz \right]_{s=0} = \zeta'_{\mathcal{L}}(0). \end{aligned}$$

This finishes the Proof of Theorem III.1. □

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APPENDIX A: PROOF OF PROPOSITION V.5

Proof of Proposition V.5. Let $L = |A|^{1/2}$ be the side length of A , and find an $\ell' \geq 4\ell$ 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, $\mathbb{R}^2 = \cup_j (y_j + Q)$ 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 Fig. 2). Thus,

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

We now split the y -integral into 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

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

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

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

We compute

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

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

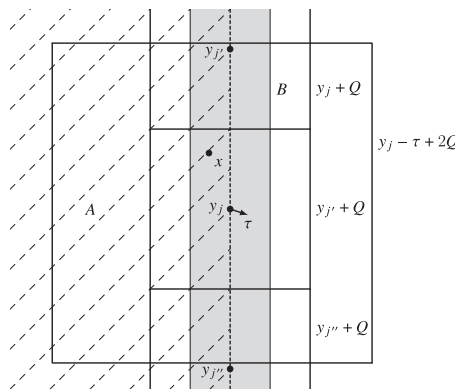


FIG. 2. Picture of the boundary region B (in gray) with the relevant translates of Q .

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

Thus, computing the x -integral of this, we get a term which is $O(N^{1/2} \log N)$ by Proposition V.4 (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

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

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

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

□

APPENDIX B: LOWER BOUND OF THE JELLIUM ENERGY

We here present the proof of the lower bound of the jellium energy from Refs. 2 and 3.

Proposition B.1 (Refs. 2 and 3). *Let Ω_N be any domain with $|\Omega_N| = N$, and let $x_1, \dots, x_N \in \Omega_N$ be any configuration of points. Then,*

$$\mathcal{E}_{\text{jel}}(\Omega_N, x_1, \dots, x_N) \geq -\left(\frac{3}{8} + \frac{1}{4} \log \pi\right) N \simeq -0.661 \, 18 \, N.$$

In particular, $e_{\text{jel}} \geq -\left(\frac{3}{8} + \frac{1}{4} \log \pi\right) \simeq -0.661 \, 18$.

Proof. The idea is to smear out the electrons to a ball of radius a of uniform charge. Then, optimize the result over the radius a . Define

$$\begin{aligned} U_{BB} &:= -\frac{1}{2} \iint_{\Omega_N \times \Omega_N} \log|x - y| dx dy, && \text{the background self - energy,} \\ U_j &:= \int_{\Omega_N} \log|x_j - y| dy, && \text{particle } j\text{-background interaction,} \\ U_{jk} &:= -\log|x_j - x_k|, && \text{particle } j\text{-particle } k \text{ interaction,} \\ \hat{U}_j &:= \frac{1}{|B_a|} \int_{B(x_j, a)} \int_{\Omega_N} \log|x - y| dx dy, && \text{ball } j\text{-background interaction,} \\ \hat{U}_{jk} &:= -\frac{1}{|B_a|^2} \int_{B(x_j, a)} \int_{B(x_k, a)} \log|x - y| dx dy, && \text{ball } j - \text{ball } k \text{ interaction.} \end{aligned}$$

Then, \hat{U}_{jj} is twice the self-energy of ball j . We then write

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

Now, (α) is the total electrostatic energy of the combined charge distribution of the smeared out electrons and the background, i.e., $(\alpha) = D\left(\sum_{j=1}^N \frac{1}{|B_a|} \mathbb{1}_{B(x_j, a)} - \mathbb{1}_\Omega\right)$. Since the entire configuration is neutral, we have $(\alpha) \geq 0$ by Proposition V.1. In addition, $(\delta) \geq 0$, 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. Now, (β) can be bounded by Newton's theorem

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

We have equality if $B(x_j, a) \subset \Omega_N$ but, in general, always the stated inequality. Finally, (γ) is given by $(\gamma) = \frac{N}{2|B_a|^2} \iint_{B_a \times B_a} \log|x-y| dx dy$.

Computing (γ) and the bound for (β) , we arrive at $\mathcal{E}_{\text{jel}} \geq \left(\frac{1}{2} \log a - \frac{1}{8} - \frac{\pi}{4} a^2\right)N$. By optimizing over a , we thus get $\mathcal{E}_{\text{jel}} \geq -\left(\frac{3}{8} + \frac{1}{4} \log \pi\right)N$ as desired. \square

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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