Floating Wigner Crystal and Periodic Jellium Configurations

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Quantissima in the Serenissima IV
Venice
2022-08-16

Definition (Jellium)

Domain $\Omega_N \subset \mathbb{R}^2$ of size $|\Omega_N| = N$ sufficiently regular. Jellium energy is

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

Thermodynamic limit exists (Sari–Merlini 1976),

$$\min \mathcal{E}_{\mathrm{Jel}} = N e_{\mathrm{Jel}}(1 + o(1)),$$

$e_{\mathrm{Jel}} \geq -0.66118.$

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Definition (UEG)

The indirect energy of a charge distribution ρ is

$$\mathcal{E}_{\mathrm{Ind}} = \inf_{\mathbb{P}:\rho_{\mathbb{P}}=\rho} \left[\int \sum_{j<k} -\log|x_j - x_k| \,\mathrm{d}\mathbb{P} + \frac{1}{2} \iint \log|x-y| \rho(x)\rho(y) \,\mathrm{d}x\,\mathrm{d}y \right],$$

$\rho_{\mathbb{P}}$ is one-particle density of $\mathbb{P}$,

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

Thermodynamic limit exists for $\rho = \mathbb{1}_{\Omega_N}$ (Lewin–Lieb–Seiringer 2018),

$$\mathcal{E}_{\mathrm{Ind}}(\mathbb{1}_{\Omega_N}) = N e_{\mathrm{UEG}}(1 + o(1)).$$

Connection: Take $\mathbb{P}$ average over translations of crystal configuration.

$$\mathcal{E}_{\mathsf{Ind}}(\mathbb{P}) = \int \mathcal{E}_{\mathsf{Jel}}(\Omega_N, x_1, \dots, x_N)\, \mathrm{d}\mathbb{P}(x_1, \dots, x_N) \geq \min \mathcal{E}_{\mathsf{Jel}}(\Omega_N, x_1, \dots, x_N),$$

if $\rho_{\mathbb{P}} = \mathbb{1}_{\Omega_N}$. Thus $e_{\mathsf{EUG}} \geq e_{\mathsf{Jel}}$.

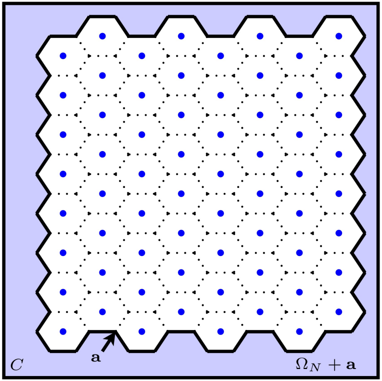

Figure: Hexagonal lattice trial state. From (Lewin–Lieb–Seiringer, 2019)

Trial state $\mathbb{P}$ of "floating crystal". Lattice $\mathcal{L}$ of sites. Take $\{x_1, \dots, x_N\} = [-L, L]^2 \cap \mathcal{L}$

$$\mathbb{P} = \int_Q \bigotimes_{j=1}^N \delta_{x_j + a}\, \mathrm{d}a, \quad \rho_{\mathbb{P}} = \mathbb{1}_{\Omega_N}$$

Q: Wigner-Seitz unit cell of lattice, $|Q| = 1$, $\Omega_N = \bigcup (x_j + Q)$.

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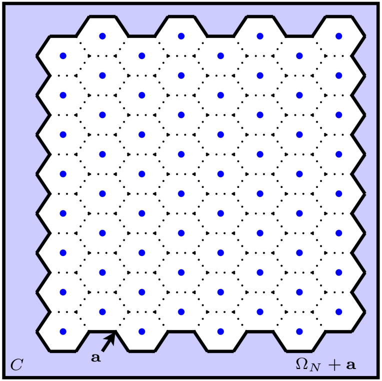

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Neglecting boundary terms

$$\mathcal{E}_{\mathrm{Ind}}(\mathbb{P}) \approx N e_{\mathrm{Jel}}^{\mathcal{L}}.$$

More particles in unit cell $\longrightarrow$ periodic jellium.

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Theorem (Lewin–Lieb–Seiringer 2019; Cotar–Petrache 2019)

$$e_{\mathrm{UEG}} = e_{\mathrm{Jel}} \qquad \text{in dimensions } d \geq 3.$$

False in $d = 1$,

$$e_{\mathrm{UEG},d=1} = \frac{1}{6}, \qquad e_{\mathrm{Jel},d=1} = \frac{1}{12}.$$

(Baxter 1963; Kunz 1974; Choquard 1975; Colombo–De Pascale–Di Marino 2015)

Theorem (L. 2021)

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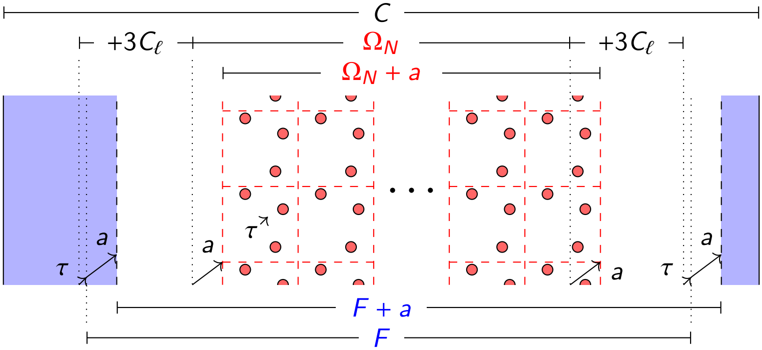
Trial state

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



Periodic configurations

In dimension d. Riesz interaction $V_s(x) = \mathrm{sgn}(s)|x|^{-s}$ instead of Coulomb $|x|^{2-d}$.

Theorem (L. 2021)

Let $d-4 < s < d$. Let $\mathcal{L} \subset \mathbb{R}^d$ be a lattice. Then the Jellium energy of the lattice configuration is

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

Lattice zeta-function $\zeta_{\mathcal{L}}$ for a lattice $\mathcal{L} \subset \mathbb{R}^d$ is (analytic continuation of)

$$\zeta_{\mathcal{L}}(s) = \frac{1}{2} \sum_{x \in \mathcal{L}\setminus 0} \frac{1}{|x|^s}, \qquad \mathrm{Re}(s) > d.$$

Compute for triangular lattice. Gives $-0.66056\ldots \geq e_{\mathrm{Jel},d=2} \geq -0.66118\ldots$