On infinite configurations of classical charges and their potential

Mathieu LEWIN

(CNRS & Paris-Dauphine University)

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Potential of infinite configurations

Goal

Renormalize the divergent series

$$\sum_{j\geq 1} \frac{1}{|x-x_j|}$$

- What is a natural renormalization procedure?
- Final result should ideally not depend on renormalization method
- Which configurations $\{x_j\}_{j\geq 1}$ have a renormalizable potential?
- Renormalized potential $\Phi(x)$ should appear in equilibrium equation for **infinite Gibbs equilibrium state of classical Jellium** (Dobrušin–Lanford–Ruelle equations)
- Infinite Gibbs point process should concentrate on configurations with a renormalizable potential

History of a conendrum

- **1934–35** (Wigner, Fuchs) computation of Jellium energy and potential of BCC lattice in a uniform background (Jellium)

- **1959:** unpublished notes by Plaskett

- **1979:** Hall found *"an error in Fuchs' calculation of the electrostatic energy of a Wigner solid"*

  $\rightsquigarrow$ De Wette (1980), Ihm–Cohen (1980), Hall–Rice (1980), Hall (1981), Alastuey–Jancovici (1981), Nijboer–Ruijgrok (1988)

- **1980:** Choquard–Favre–Gruber found at $T > 0$ that *"several definitions of the pressure"* were *"nonequivalent in the presence of a rigid neutralizing background"*

- **1988:** Borwein–Borwein–Shail–Zucker found *"jump discontinuities in Wigner limits"*

- **2015:** ML–Lieb had problems comparing Jellium with Uniform Electron Gas. Solved by Cotar–Petrache (2019) and ML–Lieb–Seiringer (2019)

Main message

Renormalization of Coulomb potential is **ambiguous** for infinite periodic lattice

Renormalization methods

- **Jellium:** if points have average density ρ, insert uniform background of same density

$$\Phi(x) := \lim_{R\to\infty}\left(\sum_{x_j\in B_R}\frac{1}{|x-x_j|}-\rho\int_{B_R}\frac{dy}{|x-y|}\right)$$

- **Cut-off long range:**

$$\Phi(x) := \lim_{m\to 0}\left(\sum_{j\geq 1}\frac{e^{-m|x-x_j|}}{|x-x_j|}-\rho\int_{\mathbb{R}^3}\frac{e^{-m|x-y|}dy}{|x-y|}\right)$$

- **Meromorphic continuation:**

$$\Phi(x) := \left\{\sum_{j\geq 1}\frac{1}{|x-x_j|^s}\quad\text{for } \{\Re(s)>3\}\right\}\Bigg|_{s=1}$$

- **PDE methods:**

$$-\Delta\Phi = 4\pi\left(\sum_{j\geq 1}\delta_{x_j}-\rho\right)$$

defines Φ up to a harmonic function (a constant under growth assumptions)

[Caffareli-Silvestre '07 for $|x|^{-s}$]

Jellium $\equiv$ analytic continuation

Lemma (ML '22)

Let $X = \{x_j\}_{j\geq 1} \subset \mathbb{R}^d$ with $\inf_{j\neq k}|x_j - x_k| > 0$. Let $x \in \mathbb{R}^d \setminus X$ and assume that

$$\left|\#X \cap B_R(x) - \rho\frac{|\mathbb{S}^{d-1}|R^d}{d}\right| \leq CR^{d-\alpha}, \qquad \forall R \geq C$$

for some $\rho, C > 0$ and $0 < \alpha \leq d$. Then the potential $\Phi_s(x) := \sum_{j\geq 1}|x - x_j|^{-s}$, initially defined on $\{\Re(s) > d\}$, admits a meromorphic extension to $\{\Re(s) > d - \alpha\}$ with a unique simple pole at $s = d$, of residue $\rho|\mathbb{S}^{d-1}|$. This extension satisfies

$$\Phi_s(x) = \lim_{R\to\infty}\left(\sum_{x_j\in B_R(x)}\frac{1}{|x - x_j|^s} - \rho\int_{B_R(x)}\frac{\mathrm{d}y}{|x - y|^s}\right) \qquad \forall d - \alpha < \Re(s) < d.$$

Borwein *et al* '88, Blanc–Le Bris–Lions '02, Ge–Sandier '21

- $Y = \{|k|^{\frac{\alpha}{d-\alpha}}k,\ k \in \mathbb{Z}^d\}$ has $O(R^{d-\alpha})$ points in B_R and yields a pole at $s = d - \alpha$. Adding it to nice X shows that range of extension is optimal
- For periodic systems, $\alpha = 2$ in $d \geq 5$ (Götze 2004), $\alpha < 2$ in $d = 4$, $\alpha < 2 - 2/(d+1)$ in $d \in \{2, 3\}$ (Landau, 1915–24), $\alpha = 1$ in $d = 1$.

Jellium $\equiv$ analytic continuation II

Lemma (Borwein *et al* '88, Lauritsen '21, ML '22)

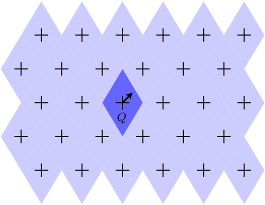
Let $X = \{x_j\}_{j\geq 1} \subset \mathbb{R}^d$ and assume that $\mathbb{R}^d = \cup_j \overline{\Omega_j}$ for disjoints sets Ω_j satisfying

$$|\Omega_j| = \rho^{-1}, \qquad \rho \int_{\Omega_j} x\, dx = x_j, \qquad B_r(x_j) \subset \Omega_j \subset B_{1/r}(x_j)$$

for some $0 < r < 1$ and all $j \geq 1$. The potential $\Phi_s(x) := \sum_{j\geq 1} |x - x_j|^{-s}$, initially defined for $\{\Re(s) > d\}$, admits a meromorphic extension to $\{\Re(s) > d-2\}$ with a unique simple pole at $s = d$, of residue $\rho|\mathbb{S}^{d-1}|$. We have

$$\Phi_s(x) = \lim_{R\to\infty} \left(\sum_{x_j \in B_R} \frac{1}{|x - x_j|^s} - \rho \int_{\cup_{x_j\in B_R} \Omega_j} \frac{dy}{|x-y|^s} \right) \qquad \text{for } \max(0, d-2) < \Re(s) < d.$$

- Now covers periodic lattices for $\Re(s) > d-2$ in all dimensions, with $\Omega_j = x_j + Q$ and symmetric unit cell $Q = \{x \in \mathbb{R}^d \ :\ |x| < |x - x_k|,\ x_k \neq 0\}$



Proof

Assume $x = 0$ for simplicity. Since no dipole, function

$$f(s) := \sum_j \underbrace{\left(\frac{1}{|x_j|^s} - \rho \int_{\Omega_j \setminus B_1} \frac{dy}{|y|^s} \right)}_{= O\left(\frac{1}{|x_j|^{s+2}}\right)}$$

is analytic on $\{\Re(s) > d - 2\}$

- For $\Re(s) > d$

$$f(s) = \Phi_s(x) - \rho \int_{\mathbb{R}^d \setminus B_1} \frac{\mathrm{d}y}{|y|^s} = \Phi_s(x) - \frac{\rho |\mathbb{S}^{d-1}|}{s - d}$$

- For $d - 2 < \Re(s) < d$

$$f(s) = \lim(\cdots) + \rho \int_{B_1} \frac{\mathrm{d}y}{|y|^s} = \lim(\cdots) + \frac{\rho |\mathbb{S}^{d-1}|}{d - s}$$

Rmk. Quadrupole depends on s, given in terms of $d \times d$ matrix $(s+2)xx^T - |x|^2$

Conendrum in periodic case

Lemma (Borwein *et al* '88)

Let $X = v_1\mathbb{Z} + \cdots + v_d\mathbb{Z}$ be a lattice and $Q = \{|y| < |y - z|,\ z \in X \setminus \{0\}\}$ be its unit cell. Then $\Phi_s(x) := \sum_{z\in X} |x - z|^{-s}$, initially defined for $\{\Re(s) > d\}$, admits a meromorphic extension to $\mathbb{C} \setminus \{d\}$ with a simple pole at $s = d$ of residue $\rho|\mathbb{S}^{d-1}|$. If there is no quadrupole, $d \int_Q y_j y_k\, dy = \int_Q |y|^2\, dy$, then at $s = d - 2$ $(d \geq 3)$ we have

$$\lim_{R\to\infty}\left(\sum_{x_j\in B_R}\frac{1}{|x-x_j|^{d-2}} - \rho\int_{\bigcup_{x_j\in B_R}(x_j+Q)}\frac{dy}{|x-y|^{d-2}}\right) = \Phi_{d-2}(x) + \frac{|\mathbb{S}^{d-1}|}{2d}\int_Q |y|^2\, dy$$

- Fuchs (1935): energy per particle e of BCC lattice in background. Used $e = \frac{\Phi^{(0)}}{2}$,
$$\Phi^{(0)} := \lim_{x\to 0}\left(\Phi_{d-2}(x) - \frac{1}{|x|^{d-2}}\right)$$
is the interaction of any point with rest of the system (Madelung cnst). Important here to use analytic continuation and not the background.
- Nijboer–Ruijgrok (1988): different shifts depending on how background grows
- Additional log in $d = 2$ (Lauritsen, 2021)

Proof

$[|Q| = \rho^{-1} = 1]$

- no-quadrupole $\Rightarrow f_s = |x|^{-s} - \mathbb{1}_Q * |x|^{-s}$ also integrable for $s = d-2$, hence

$$\lim_{R\to\infty}\left(\sum_{x_j\in B_R}\frac{1}{|x-x_j|^s} - \int_{\bigcup_{x_j\in B_R}\Omega_j}\frac{dy}{|x-y|^s}\right) = \sum_j f_s(x-x_j) =: F_s(x)$$

for all $d-2 \leq s < d$. Already known that $F_s = \Phi_s$ for $d-2 < s < d$

- F_s is periodic function with Fourier coefficients $\{\widehat{f_s}(k)\}_{k\in X^*}$

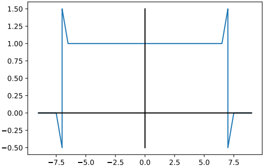
$$\widehat{f_s}(k) \propto \frac{1-\widehat{\mathbb{1}_Q}(k)}{|k|^{d-s}} = \begin{cases} \frac{1}{|k|^{d-s}} & \text{for } k \in X^*\setminus\{0\} \\ 0 & \text{for } k = 0 \text{ and } s > d-2 \\ \frac{1}{d}\int_Q |x|^2\,dx & \text{for } k = 0 \text{ and } s = d-2 \end{cases}$$

since

$$\widehat{\mathbb{1}_Q}(k) = \int_Q e^{-ik\cdot x}\,dx = 1 + \frac{|k|^2}{d}\int_Q |x|^2\,dx + o(|k|^2))$$

Remark: would work for $\Re(s) > d-4$ with $|1-\widehat{\mathbb{1}_Q}(k)|^2$ $\Longleftrightarrow$ big background $2\mathbb{1}_\Omega - \mathbb{1}_\Omega * \mathbb{1}_Q$ instead of $\mathbb{1}_\Omega$

Energy involves $|x|^{-s} - 2\mathbb{1}_Q * |x|^{-s} + \mathbb{1}_Q * \mathbb{1}_Q * |x|^{-s}$ hence analytic extension



Jellium ground state

Jellium energy of N points in background $\rho\mathbb{1}_\Omega$

$$\mathcal{E}_s(x_1,\dots,x_N,\Omega,\rho) := \sum_{1\le j<k\le N}\frac{1}{|x_j-x_k|^s} - \rho\sum_{j=1}^N\int_\Omega\frac{dy}{|x_j-y|^s} + \frac{\rho^2}{2}\iint_{\Omega\times\Omega}\frac{dx\,dy}{|x-y|^s}$$

$$E_s(N,\Omega,\rho) := \min_{x_1,\dots,x_N\in\overline{\Omega}}\mathcal{E}_s(x_1,\dots,x_N,\Omega,\rho)$$

Theorem (Thermodynamic limit)

Let $0<s<d$ and $\Omega=\ell\omega$ with ω smooth and convex, with $|\omega|=1$.

The following limits exist and are independent of ω:

- *Grand-canonical:* $\lim_{\ell\to\infty}\ell^{-d}\min_n\left\{E_s(n,\ell\omega,\rho)-\mu\,n\right\} = e(s)\rho^{1+\frac{s}{d}}-\mu\rho$
- *Canonical for $d-2\le s<d$:* $\lim_{\substack{N,\ell\to\infty\\ \ell^{-\frac{d+s}{2}}(N-\rho\ell^d)\to0}}\ell^{-d}E_s(N,\ell\omega,\rho) = e(s)\rho^{1+\frac{s}{d}}$

Lieb–Narnhofer '75, Sari–Merlini '76, Fefferman–Gregg '80s, Serfaty *et al* '10s, ML '22

Same result at $T>0$

Infinite equilibrium configurations

Theorem (ML '22)

Let $0 < s < d$ in $d \in \{1,2\}$ and $d-2 \leq s < d$ in $d \geq 3$. Let $\rho > 0$, $\mu \in \mathbb{R}$. Consider any minimizer $X_\ell = \{x_{1,\ell}, ..., x_{N_\ell,\ell}\} \subset \ell\omega$ for the grand-canonical problem. Up to a subsequence and space translation, we have $X_\ell \to X$ locally. The potential

$$\Phi_\ell(x) := \sum_{j=1}^{N_\ell} \frac{1}{|x - x_{j,\ell}|^s} - \rho \int_{\ell\omega} \frac{\mathrm{d}y}{|x-y|^s} \xrightarrow[\ell\to\infty]{} \Phi(x)$$

in $L^1_{\rm loc}(\mathbb{R}^d)$ and locally uniformly away from the x_j's. For $s > d-2$ we have

$$\Phi(x) = C_{j_0} + \frac{1}{|x-x_{j_0}|^s} + \sum_{j\neq j_0} \left(\frac{1}{|x-x_j|^s} - \frac{1}{|x_{j_0}-x_j|^s} + s\frac{(x-x_{j_0})\cdot(x_{j_0}-x_j)}{|x_{j_0}-x_j|^{s+2}} \right).$$

If $s = d-2$, Φ solves the equation $-\Delta\Phi = (d-2)|\mathbb{S}^{d-1}|(\sum_j \delta_{x_j} - \rho)$ and is uniquely determined up to a constant. For any $D \subset \mathbb{R}^d$, any $Y = \{y_1, ..., y_n\} \subset \overline{D}$ we have the **D***obrušin–***L***anford–***R***uelle equation*

$$\sum_{j=1}^n \Phi_{D^c}(y_j) + \mathcal{E}_s(Y, D, \rho) - \mu n \geq \sum_{x_j\in\overline{D}} \Phi_{D^c}(x_j) + \mathcal{E}_s(X_D, D, \rho) - \mu N,$$

where $X_D := X \cap \overline{D}$, $N = \# X_D$ and $\Phi_{D^c}(x) := \Phi(x) - \sum_{x_j\in\overline{D}} \frac{1}{|x-x_j|^s} + \rho\int_D \frac{\mathrm{d}y}{|x-y|^s}$.

- Positive distance between the points in the bulk (Lieb, Petrache–Serfaty '17)
- Φ_ℓ locally bounded, up to the obvious singularities at the $x_{j,\ell}$
- Limiting Φ only known up to a constant. Corresponds to **renormalizing the chemical potential** μ (Imbrie '82, Brydges–Martin '99)
- Existence for only one $\mu_{\rm ren}$?
- How is $\Phi(x)$ renormalized?

Crystallization conjecture

The equilibrium infinite configurations X are periodic, of minimal energy per unit volume

$$e(s) = \min_{\mathcal{L},\ |Q|=1} \zeta_{\mathcal{L}}(s)$$

where $\zeta_{\mathcal{L}}(s) = \frac{1}{2}\sum_{z\in\mathcal{L}\setminus\{0\}} |z|^{-s}$ for $\{\Re(s) > d\}$ meromorphically continued to $\mathbb{C}\setminus\{d\}$ (Epstein Zeta function).

- Formula for $e(s)$ known for all $s \geq \max(0, d-2)$ in $d \in \{1, 8, 24\}$ (Cohn–Kumar–Miller–Radchenko–Viazovska '22, Petrache–Serfaty '20)
- Expect triangular $\forall s > 0$ in $d = 2$
- Expect BCC for $0 < s \leq 3/2$ and FCC for $s \geq 3/2$ in $d = 3$ (Wigner '34, Nijboer '75, Sarnak-Strömbergsson '04)
- no result for X to our knowledge, except for $s = -1$ in 1D (Kunz '74)

Positive temperature case

Dereudre–Vasseur (arXiv): $d-1<s<d$

- use of move function $\widetilde{\Phi}_s(x):=\sum_j\left(\frac{1}{|x-x_j|^s}-\frac{1}{|x_j|^s}\right)$ to define infinite canonical stationary Gibbs measure
- Study cost of adding or removing one point to the infinite system, through Campbell measures. Show they are absolutely continuous w.r.t. Gibbs point process
- Solution to grand-canonical DLR, with unknown potential $\Phi_s=\widetilde{\Phi}_s+C$, for an unknown constant