Equality of the Jellium and Uniform Electron Gas next-order asymptotic terms for Coulomb and Riesz potentials

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May 06, 2020
Cysteine molecule simulation,
(from Walter Kohn’s Nobel prize laudation page)
Quantum mechanics

- **Quantum mechanics** describes nature at the smallest scales of energy levels of atoms and subatomic particles.

- Important applications of quantum mechanics: quantum chemistry, quantum optics, quantum computing, superconducting magnets, light-emitting diodes, the laser, the transistor and semiconductors such as the microprocessor, medical and research imaging such as magnetic resonance imaging and electron microscopy.

- Explanations for many biological and physical phenomena are rooted in the nature of the chemical bond, most notably the macro-molecule DNA — quantum biology.
Informal introduction to Quantum mechanics/DFT

- All materials systems we study essentially consist of electrons and nuclear charge.
- Mechanical, electronic, magnetic etc. properties are due to electrons and their interaction with other electrons.
- In order to define electrons and their interaction we use Schrödinger equation (Dirac 1929).
- It allows to predict, e.g., binding energies, equilibrium geometries, intermolecular forces
- Quantum mechanics for a molecule with $N$ electrons reduces to a PDE of form $H \Psi = E \Psi$ (called Schrödinger equation) for a function $\Psi$ on $\mathbb{R}^{3N}$. 
The solution $\Psi(x_1, \ldots, x_N)$ is called wave function and represents the state of the $N$-particles system.

- $N$ - number of electrons, $x_i$ position of electron $i$

$$|\Psi(x_1, \ldots, x_N)|^2 = \text{probability density that the electrons are at positions } x_i.$$

$\Psi$ is an anti-symmetric function, which makes $|\Psi|^2$ a symmetric ($N$-exchangeable) probability measure.

- If Schrodinger equation for the many electrons problem could be solved accurately and efficiently then almost any property of the materials could be determined accurately.

- Unfortunately, there is neither an accurate nor an efficient method to solve these problems.
Density Functional Theory (DFT)

- To simulate chemical behaviour, approximations are needed.
- Curse of dimensionality: carbon atom: $N = 6$. Discretise $\mathbb{R}$ by 10 points $\rightarrow 10^{18}$ total grid points.
- DFT is a simplified version of quantum mechanics (QM), widely used in molecular simulations in chemistry, physics, materials science.

**Main idea**: describe complicated N-particle system (a probability on $\mathbb{R}^{3N}$) using only its single-electron marginal density

$$\rho(x_1) = \int_{\mathbb{R}^{3(N-1)}} |\Psi(x_1, \ldots, x_N)|^2 \, dx_2 \ldots dx_N$$

- Feasible system size: systems with more than a dozen or so electrons.
Density Functional Theory

How to devise faster methods for the full model at large $N$?

“cheap” simulation of heavy-metal pump in *E. Coli* (Su & al., *Nature ’11*)
Some history of DFT

- Thomas-Fermi: 1920s simple model
- Hohenberg-Kohn-Sham (1963-1964): practical method based on semi-empirical functions of $\rho$
- Levy (1979), Lieb (1983): mathematical justification and simplified reformulation of the equation
- 1970s: popular in solid state physics, but not so accurate
- 1990s: explosion in quantum chemistry, due to increase of computational resources + discovery of efficient semi-empirical functionals of $\rho$
- 1998 Nobel Prize for ‘founding father’ Walter Kohn
Fun facts

- More than 15,000 papers per year with the keyword ‘density functional theory’
- Most cited physicist of all time is a designer of DFT models, J. Perdew (275,877 Google Scholar paper citations as of this morning, compared to 130,029 citations for Einstein).
Turning this into math

- **Key** quantum mechanics quantity is the **ground state energy** $E_0$ (state of lowest energy)

\[
E_0 = \inf \Psi E[\Psi]
\]

where

\[
E[\Psi] = T_h[\Psi] + V_{ee}[\Psi] + V_{ne}[\Psi]
\]

and

\[
A_N = \left\{ \Psi \in L^2(\mathbb{R}^{3N}) \mid \nabla \Psi \in L^2, \Psi \text{ antisymmetric}, ||\Psi||_{L^2} = 1 \right\}
\]

- $V_{ee}[\Psi], V_{ne}[\Psi]$ involve expectations for the Coulomb potential $(1/|x|)$ with respect to symmetric probability measures on $\mathbb{R}^{3N}$
A simplified reformulation of the above equation is the Hohenberg-Kohn-Sham (HK) model (Levy 1979 - Lieb 1983).

It is formulated in terms of the single-electron density $\rho$

$$\rho(x_1) = \int_{\mathbb{R}^{3(N-1)}} |\Psi(x_1, \ldots, x_N)|^2 dx_2 \ldots dx_N.$$ 

**Pair electrons density**

$$\rho_2(x_1, x_2) = \int_{\mathbb{R}^{3(N-2)}} |\Psi(x_1, \ldots, x_N)|^2 dx_3 \ldots dx_N$$

$${\mathcal{R}}_N := \{ \rho : \mathbb{R}^3 \to \mathbb{R} \mid \rho \text{ is the density of some } \Psi \}$$
Variational formulation of density functional theory

(Hohenberg/Kohn 1964, M. Levy 1979, E. Lieb 1983)
For any external potential $v$, the exact Schroedinger eqn. satisfies

$$E_0 = \inf_{\rho \in \mathcal{R}_N} \left\{ \text{HK}_h[\rho] + N \int_{\mathbb{R}^3} \frac{1}{|x|} \rho(x) dx \right\}$$

with

$$\text{HK}_h[\rho] = \inf_{\Psi \in \mathcal{A}_N, \Psi \mapsto \rho} \left\{ T_h[\Psi] + V_{ee}[\Psi] \right\},$$

$\text{HK}_h[\rho]$ is the famous Hohenberg-Kohn functional.

Not useful for computations (definitely still contains the big space of $\Psi(x_1, \ldots, x_N)$). But useful starting point for model reduction in asymptotic limits.
Correlations in DFT

- Mathematical structure: Minimize an approximate energy functional $E[\rho]$ which depends on the electron density $\rho(x)$, a function on $\mathbb{R}^3$.
- Catch: exact QM energy requires knowledge of electron-pair density

$$\rho_2(x_1, x_2) = \int_{\mathbb{R}^{3(N-2)}} |\Psi(x_1, \ldots, x_N)|^2 \, dx_3 \ldots dx_N,$$

a function on $\mathbb{R}^6$, which entails correlations.
- Roughly, DFT models $\approx$ semi-empirical models of the pair density $\rho_2$ in terms of $\rho$.
- Standard way out: start by assuming independence (called mean field in physics), add semi-empirical corrections to $E[\rho]$ accounting for correlations. Often but not always accurate/reliable.
Popular functionals

All functionals used in practice are of form

Mean field  +  additive corrections.

Why mean field? Interactions not weaker than single-particle terms.

- The mean field approximation:

\[ V_{ee}(\psi) \approx \frac{N^2}{2} \int_{\mathbb{R}^6} \frac{1}{|x-y|} \rho(dx)\rho(dy) =: J[\rho]. \]

- Local Density Approximation:

\[ V_{ee}(\psi) \approx J[\rho] - \frac{4}{3} \left( \frac{3}{\pi} \right)^{1/3} N^{4/3} \int_{\mathbb{R}^3} \rho(x)^{4/3} dx. \]
Many-marginals Optimal Transportation

- $\gamma$ measure in $\mathbb{R}^{Nd}$, $\mu_1, \mu_2, \ldots, \mu_N$ measures in $\mathbb{R}^d$

- **The Cost Function** $c : \mathbb{R}^d \times \mathbb{R}^d \cdots \times \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$

- We want to transport **mass** from a given pile $\rho_1$ into a number of given holes $\mu_2, \mu_3, \ldots, \mu_N$, so as to minimize the transportation cost

$$\int c(x_1, x_2, \ldots, x_N) d\gamma(x_1, x_2, \ldots, x_N).$$

subject to the constraints

$$\int_{\mathbb{R}^{(N-1)d}} \gamma(x_1, x_2, \ldots, x_N) dx_2 \cdots dx_N = \mu_1(x_1), \ldots$$

$$\int_{\mathbb{R}^{(N-1)d}} \gamma(x_1, x_2, \ldots, x_N) dx_1 \cdots dx_{N-1} = \mu_N(x_N),$$
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\[ F_{N,c}^{\text{OT}}(\mu) := \min \left\{ \int_{(\mathbb{R}^d)^N} \sum_{i,j=1}^{N} c(x_i - x_j) d\gamma_N(x_1, \ldots, x_N) \mid \gamma_N \in \mathcal{P}_{\text{sym}}((\mathbb{R}^d)^N) \right\} \]

We are mostly interested in the case \( c(x, y) = \frac{1}{|x-y|^s} \), \( 0 < s < d \), i.e.

\[ F_{N,s}^{\text{OT}}(\mu) := \min \left\{ \int_{(\mathbb{R}^d)^N} \sum_{i,j=1}^{N} \frac{1}{|x_i - x_j|^s} d\gamma_N(x_1, \ldots, x_N) \mid \gamma_N \in \mathcal{P}_{\text{sym}}((\mathbb{R}^d)^N) \right\} \]

The case \( s = d - 2 \) is the Coulomb cost.
Semiclassical limit

**Theorem**

Fix $\rho \in \mathcal{R}_N$. Let $N \geq 2$. Then in $d = 3$

$$
\lim_{h \to 0} HK_h[\rho] = F_{N,1}^{OT}(\rho)
$$

for every $\rho \in \mathcal{R}_N$, where recall that

$$
HK_h[\rho] := \inf_{\Psi \in A_N, \Psi \mapsto \rho} \left\{ T_h[\Psi] + V_{ee}[\Psi] \right\}.
$$
- Cotar, Friesecke, Klueppelberg: $N = 2$ (2011)
- Cotar, Friesecke, Klueppelberg (2017 - extension for $N \geq 3$ to the full model); Lewin (2017 - extension for $N \geq 3$ to a relaxed model)
Optimal transport DFT community

- C-Frieseecke-Klüpperberg (CPAM 2013): characterization for a class of repulsive costs of the minimizing measure for $N = 2$
- Colombo-Di Marino (2017): Kantorovich problem coincides with infimum over Monge states for $N \geq 2$ and $d \geq 1$
- Colombo-De Pascale-Di Marino (2013): Existence and uniqueness of Monge solution for $N \geq 2$ and $d = 1$
- Duality and bounds on the support of the optimal transport measure: De Pascale (2015), Buttazzo-Champion-De Pascale (2017), ..
- Numerics: Benamou-Carlier-Nenna (2015); Di Marino-Gerolin-Nenna (2017),..
Asymptotics for $F_N$ for large $N$

- First-order "mean field" functional (Cotar-Friesecke-Pass, Calc. Var. PDE-2013; Petrache 2015)

$$
\lim_{N \to \infty} \left( \begin{array}{c} N \\ 2 \end{array} \right)^{-1} F_{N,c}^{\text{OT}}(\mu) = F_{\infty,c}^{\text{OT}}[\mu] = \frac{1}{2} \int_{\mathbb{R}^{2d}} l(x - y) d\mu(x) d\mu(y).
$$

$(c(x, y) = l(x - y)$ with positive Fourier transform)$

- Proof by use of de Finetti theorem: exchangeable observations are conditionally independent relative to some latent variable
Next-order term

Study of the energy not encoded in the mean field functional, called in physics Exchange-correlation energy $E_{N,s}^{xc}$

- Lieb-Oxford bound

$$N^{-1-s/d} \left( F_{N,s}^{\text{OT}}(\mu) - N^2 \int_{\mathbb{R}^{2d}} \frac{1}{|x-y|^s} \rho(x) \rho(y) dxdy \right) \geq -C_{LO} \int_{\mathbb{R}^d} \rho(x)^{1+s/d} dx.$$ 

- Trivially, we also have

$$F_{N,s}^{\text{OT}}(\mu) - N^2 \int_{\mathbb{R}^{2d}} \frac{1}{|x-y|^s} \rho(x) \rho(y) dxdy \leq 0.$$ 

- Question: Does the limit below exist

$$\lim_{N \to \infty} N^{-1-s/d} \left( F_{N,s}^{\text{OT}}[\mu] - N^2 \int_{\mathbb{R}^{2d}} \frac{1}{|x-y|^s} \rho(x) \rho(y) dxdy \right) = ?$$
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Optimal Transport Connection to DFT

Second-order term $0 < s < d$

- $d = 1$, Coulomb and Riesz costs: Di Marino (2017)
- $s = 1, d = 3$ for $\mu$ with continuous, slow-varying density $\rho$, i.e., densities satisfying

$$\sum_{k \in \mathbb{Z}^d, x \in [0,1)^d + k} \max_{\rho(x)} \rho(x) < \infty$$


- $0 < s < d$, any $d$, any $\rho > 0$ such that $\int_{\mathbb{R}^d} \rho^{1 + \frac{s}{d}} < \infty$, via new type of Fefferman-Gregg decomposition (1985, 1989) + optimal transport tools (Cotar-Petrache 2017-Adv. Math.)
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Optimal Transport Connection to DFT

Theorem

(Cotar-Petrache- Adv. Math 2019) If $0 < s < d$ and $d\mu(x) = \rho(x)dx$ then then exists $C_{\text{UEG}}(d, s) > 0$ such that

$$\lim_{N \to \infty} N^{-1-s/d} \left( F_{N,s}^\text{OT}(\mu) - N^2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\rho(x)\rho(y)}{|x-y|^s} dx \, dy \right)$$

$$=: E_{N,s}^{\text{xc}}(\mu)$$

$$= -C_{\text{UEG}}(s, d) \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx.$$

- Uniform marginal (uniform electron gas UEG): Dirac (1929)
- Exact value of $C_{\text{UEG}}(d, s)$ for $s = 1, d = 3$, is unknown, although the physics community thought for a long time that it is approx 1.4442
Some tools: Fefferman-Gregg decomposition

- Introduced by Fefferman (1985) for $s = 1, d = 3$
- Extended by Gregg (1989) to $0 < s < 2 + [(d − 1)/2]$
- Further extended by Cotar, Petrache (Adv. Math 2019) to all $0 < s < d$. 
Some tools: Fefferman-Gregg type decomposition

Let $M \in \mathbb{N}_+$, $0 < \epsilon < d/2$ and $\epsilon \leq s \leq d - \epsilon$. Then there exists a constant $C$ depending only on $d, \epsilon$, a family $\Omega$ of ball packings $F_\omega$ of $\mathbb{R}^d$, $\omega \in \Omega$, a radius $R_1 > 0$ and a probability measure $\mathbb{P}$ on $\Omega$ such that the cost $|x_1 - x_2|^{-s}$ can be decomposed as follows:

$$\frac{1}{|x_1 - x_2|^s} = \frac{M}{M + C} \left\{ \int_\Omega \left( \sum_{A \in F_\omega} \frac{1_A(x_1)1_A(x_2)}{|x_1 - x_2|^s} \right) d\mathbb{P}(\omega) + w(x_1 - x_2) \right\} ,$$

where $w$ is positive definite.
Let $N \in \mathbb{R}_{>0}$, $N \geq 2$, $\mu \in \mathcal{P}(\mathbb{R}^d)$

The **grand-canonical optimal transport**

$$F_{GC,N,c}^{\text{OT}}(\mu) := \inf \left\{ \sum_{n=2}^{\infty} \alpha_n F_{n,c}^{\text{OT}}(\mu_n) \right\},$$

where infimum is taken over

$$\sum_{n=0}^{\infty} \alpha_n = 1, \quad \sum_{n=1}^{\infty} n \alpha_n \mu_n = N \mu,$$

with $\mu_n \in \mathcal{P}(\mathbb{R}^d)$, $\alpha_n \geq 0$, $n \in \mathbb{N}$. 
The grand-canonical exchange correlation energy

\[ E_{\text{GC},N,c}^{\text{xc}}(\mu) := F_{\text{GC},N,c}^{\text{OT}}(\mu) - N^2 \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x,y) d\mu(x)d\mu(y). \]

We have

\[ F_{\text{GC},N,c}^{\text{OT}}(\mu) \leq F_{N,c}^{\text{OT}}(\mu) \quad \text{and} \quad E_{\text{GC},N,s}^{\text{xc}}(\mu) \leq E_{N,s}^{\text{xc}}(\mu). \]

Fix $0 < \epsilon < d/2$ and let $\epsilon < s < d - \epsilon$. Let $\mu \in \mathcal{P}(\mathbb{R}^d)$ be a probability measure with compactly-supported density. Then there exists $C(d, \epsilon, \mu) > 0$ such that for all $N, \tilde{N} \in \mathbb{R}_+$, $N \geq \tilde{N} \geq 2$, we have

$$\left| \frac{E^{xc}_{GC,N,s}(\mu)}{N^{1+s/d}} - \frac{E^{xc}_{GC,\tilde{N},s}(\mu)}{\tilde{N}^{1+s/d}} \right| \leq \frac{C(d, \epsilon, \mu)}{\log \tilde{N}}.$$
Some consequences of Small Oscillations

Let $\mu \in \mathcal{P}(\mathbb{R}^d)$ be a probability measure with compactly-supported density.

- Fix $0 < \epsilon < d/2$ and let $\epsilon \leq s \leq d - \epsilon$. Then the sequence of functions

$$f_s(N) := \frac{E_{GC,N,s}^{xc}(\mu)}{N^{1+s/d}}$$

converges as $N \to \infty$ uniformly with respect to the parameter $s \in [\epsilon, d - \epsilon]$. 
Connection to the Jellium model

- **N** electrons and a neutralizing background in a domain Ω with \(|\Omega| = N\).
- Minimize over \(x_i\) in Ω

\[
\sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|^s} - \sum_{j=1}^{N} \int_{\Omega} \frac{1}{|x_j - y|^s} dy + \frac{1}{2} \int_{\Omega} \int_{\Omega} \frac{1}{|x - y|^s} dxdy
\]

- Let minimization be \(\text{Jel}_{N,s}(\Omega)\), then the limit

\[
\lim_{N \to \infty} \frac{\text{Jel}_{N,s}(\Omega)}{N} = -C_{\text{Jel}}(s,d).
\]

(Lieb & Narnhofer 1975 for \(s = d - 2\); Cotar-Petrache March 2019 for \(d - 2 \leq s < d\))
Connection to the Jellium model

- More generally, take $\mu \in \mathcal{P}(\mathbb{R}^d)$ and density $\rho$.
- Minimize over $x_i \in \mathbb{R}^d$

$$
\sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|^s} - N \sum_{j=1}^{N} \int \frac{d\mu(y)}{|x_j - y|^s} + \frac{N^2}{2} \int \int \frac{d\mu(x)d\mu(y)}{|x - y|^s}
$$

- Again the minimization is $\text{Jel}_{N,s}(\mu)$, then the limit

$$
\lim_{N \to \infty} \frac{\text{Jel}_{N,s}(\Omega)}{N^{1+s/d}} = -C_{\text{Jel}}(s, d) \int \rho^{1+s/d}(x)dx.
$$

(Cotar-Petrache 2019 for $d - 2 \leq s < d$)
Equality of the Jellium and Uniform Electron Gas next-order asymptotic terms for Coulomb and Riesz potentials

Equality of second-order constants

\[ \text{Jel}_{N,s}(\mu) \leq E_{N,s}^{xc}(\mu) \]

- Lewin-Lieb (2015): comparison with uniform electron gas constant in \( s = 1, d = 3 \)

- Heuristics for \( s = 1, d = 3 \) in Lewin-Lieb (2015):
  \[ C_{\text{Jel}}(d, d - 2) \neq C_{\text{UEG}}(d, d - 2) \]
  questioning the physicists’ conjecture that \( C_{\text{Jel}}(d, d - 2) = C_{\text{UEG}}(d, d - 2) \).
Minimum-energy point configurations (Coulomb and Riesz gases)

\[ H_{N,V}(x_1, \ldots, x_N) = \sum_{i \neq j} \frac{1}{|x_i - x_j|^s} + N \sum_{i=1}^{N} V(x_i), \quad x_1, \ldots, x_N \in \mathbb{R}^d, \]

\( V : \mathbb{R}^d \rightarrow ] - \infty, +\infty] \) confining potential growing at infinity \((s = 0: \text{let then } c(x) = -\log |x|)\)

- \( 0 \leq s < d \): Riesz gas, integrable kernel.
- \( s = d - 2 \): Coulomb gas.
- \( s > d \): short-ranged, Hypersingular kernel.
- \( s \to \infty \): Best packing problem
Second-order asymptotics $d - 2 \leq s < d$

- Sandier-Serfaty, 2010-2012: $d = 1, 2$, $c(x) = -\log |x|$
- Rougerie-Serfaty, 2016: $c(x) = 1/|x|^{d-2}$
- Petrache-Serfaty, 2017: all previous cases plus Riesz cases
  $\max(0, d - 2) \leq s < d$

Let $\mu_V$ be the minimizer (among probability measures) of

$$\mathcal{E}_V^s(\mu) = \int \int \frac{1}{|x-y|^s} d\mu(x)d\mu(y) + \int V(x)d\mu(x)$$
Equality of the Jellium and Uniform Electron Gas next-order asymptotic terms for Coulomb and Riesz potentials

Equality of second-order constants

Theorem

Under suitable assumptions on $V$, and if the density $\rho_V$ is smooth enough, we have

$$
\min H_{N,V} =
N^2 E_V^s(\mu_V) - N^{1+\frac{s}{d}} C_{\text{Gas}}(s,d) \int \mu_{\frac{1}{V}}^{1+\frac{s}{d}}(x)dx + o(N^{1+\frac{s}{d}}),
$$

and $-C_{\text{Gas}}(s,d)$ is the minimim value of a functional $\mathcal{W}$ on microscopic configurations $\nu$. 
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Equality of second-order constants

- $C_{\text{Gas}}(s, d)$ minimizer of a limiting energy $\mathcal{W}$
- Abrikosov crystallization conjecture: in $d = 2$, the regular triangular lattice is a minimizing configuration for $\mathcal{W}$.
- For $d = 3$, it is conjectured that for $0 < s < 3/2$ the minimizer should be a BCC lattice and for $3/2 < s < 3$ it should be an FCC lattice.
- In high dimensions, there is more and more evidence that Coulomb and Riesz gases minimizers are not lattices, although this is very much speculative at the moment.
- Open for all $d \geq 2$ dimensions, except $d = 8, 24$ (Viazovska).
- For $s = 1, d = 3$, the value of $C_{\text{Gas}}(1, 3)$ is thought to be approx. 1.4442
Comparison between Jellium, UEG and Riesz Gases

\((d - 2 \leq s < d)\)

- For \(0 < s < d\) we can show

\[
\text{Jel}_{N,s}(\mu_V) \leq H_{N,V} - N^2 \mathcal{E}_V^s(\mu_V) \leq E_{N,s}^{xc}(\mu_V)
\]

- For \(d - 2 < s < d\), we have (Cotar-Petrache - July 2017)

\[
C_{\text{UEG}}(s,d) = C_{\text{Jel}}(s,d) = C_{\text{Gas}}(s,d).
\]

- For \(s = d - 2\), we have (Cotar-Petrache - March 2019)

\[
C_{\text{UEG}}(s,d) = C_{\text{Jel}}(s,d) = C_{\text{Gas}}(s,d).
\]
Continuity of $C_{\text{UEG}}(s, d)$

- For $0 < s < d$, the function
  $$s \to C_{\text{UEG}}(s, d)$$

  is continuous.

- The proof works by interchanging the limits of $s \to s_0$ and $N \to \infty$ in
  $$N^{-1-s/d} \left( F_{\text{GC},N,s}^{\text{OT}}(\mu) - N^2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\rho(x)\rho(y)}{|x-y|^s} \, dx\, dy \right)$$
Key steps of the proof for Riesz costs (Cotar-Petrachê July 2017)

- **Step 1:** Our crucial idea was to reduce the Jellium minimization problem to a Jellium problem with minimization over periodic configurations.

- In particular, this reduction allows to prove for \( d - 2 \leq s < d \)

\[
C_{\text{Gas}}(s, d) = C_{\text{Jel}}(s, d) = C_{\text{Per}}(s, d).
\]

- Note that Cotar-Petrachê 2017 is the first time where these equalities were proved for Jellium. Previously, it was only proved for Coulomb and Riesz gases that

\[
C_{\text{Gas}}(s, d) = C_{\text{Per}}(s, d).
\]
Step 2: Our crucial idea was to use the periodic minimizing configurations to construct a competitor for the $E_{N,s}^{xc}$ problem, albeit with the wrong marginal, depending on $N$.

Use the subadditivity of the $E_{N,s}^{xc}$ problem to get back to the OT problem with the correct marginal.
Key steps in the proof for Coulomb costs (Cotar-Petrache March 2019)

■ Prove (for the first time) a subadditivity for Jellium: Let $N_1, N_2 \geq 2$, $N := N_1 + N_2$, and let $\Omega_N = \Omega_{N_1} \cup (\Omega_N \setminus \Omega_{N_1})$. Set $0 < \epsilon \leq \min(2, \frac{d}{2})$. Then for $0 < d - 2 \leq s \leq d - \epsilon$

$$
\text{Jel}_{N_1+N_2,s}(\Omega_N) \leq \text{Jel}_{N_1,s}(\Omega_{N_1}) + \text{Jel}_{N_2,s}(\Omega_N \setminus \Omega_{N_1}) + C_{\text{add}}(\epsilon, d) \frac{N_1 + N_2}{\log(\min(N_1, N_2))}.
$$

■ Use the equality of $C_{\text{Jel}}(s, d)$ and $C_{\text{UEG}}(s, d)$ from Riesz costs $d - 2 < s < d$ and the continuity of $C_{\text{UEG}}(s, d)$. 

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Equality of second-order constants
Next-order terms: open problems

- **Open problem**: Find $C_{\text{UEG}}(s, d)$ (connected to the crystallization conjecture)

- **Open problem**: Prove or disprove $E_{N,s}^{xc}/N^{1+s/d}$ is decreasing in $N$ (recall that $E_{N}^{xc}$ is negative here)