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

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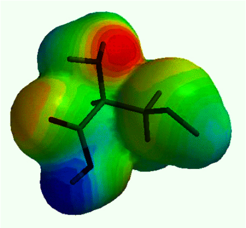


Cysteine molecule simulation,
(from Walter Kohn's Nobel prize laudation page)

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 $\longrightarrow$ 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 Schrodinger 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 Schroedinger equation) for a function Ψ 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
- $$|\Psi(x_1, \ldots, x_N)|^2 = \text{probability density that the electrons are at positions } x_i \,.$$

  Ψ 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 determined accurately.
- Unfortunately, there is neither an accurate nor an efficient method to solve these problems.

Density Functional Theory (DFT)

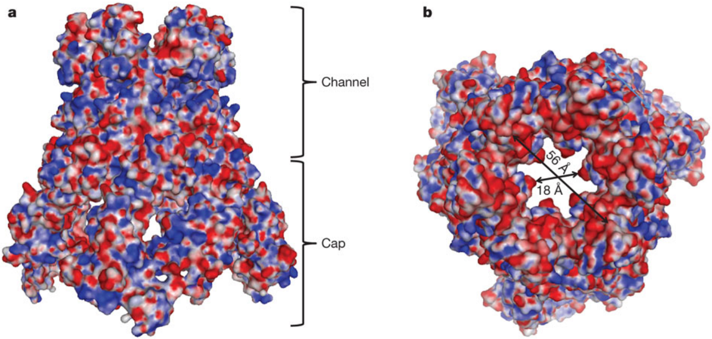
- To simulate chemical behaviour, approximations are needed.
- Curse of dimensionality: carbon atom: $N = 6$. Discretise $\mathbb{R}$ by 10 points→10^{18} total grid points.
- DFT is a simplified version of quantum mechanics (QM), widely used in molecular simulations in chemistry, physics, materials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

  $$\mathcal{A}_N = \{\Psi \in L^2((\mathbb{R}^{3N}) \,|\, \nabla\Psi \in L^2,\ \Psi \text{ antisymmetric}, \ ||\Psi||_{L^2} = 1\}$$

- $V_{ee}[\Psi]$, $V_{ne}[\Psi]$ 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 ρ

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

- Pair electrons density

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

- $\mathcal{R}_N := \{\rho \,:\, \mathbb{R}^3 \to \mathbb{R} \,|\, \rho \text{ is the density of some } \Psi\}$

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

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

  with

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

  $\mathrm{HK}_{h[\rho]}$ 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 ρ_2 in terms of ρ.
- 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

$$\text{Mean field } + \text{ additive corrections.}$$

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:

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

Many-marginals Optimal Transportation

- γ measure in $\mathbb{R}^{Nd}$, $\mu_1, \mu_2, \ldots, \mu_N$ measures in $\mathbb{R}^d$
- The Cost Function $c : \mathbb{R}^d \times \mathbb{R}^d \ldots \times \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$
- We want to transport mass from a given pile ρ_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

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

$$\int_{\mathbb{R}^{(N-1)d}} \gamma(x_1, x_2, \ldots, x_N) dx_1 \ldots dx_{N-1} = \mu_N(x_N),$$

$$F^{\mathrm{OT}}_{N,\mathrm{c}}(\mu) := \min\left\{ \int_{(\mathbb{R}^d)^N} \sum_{\substack{i,j=1\\ i\neq j}}^{N} c(x_i - x_j)\, d\gamma_N(x_1,\dots,x_N) \;\middle|\; \begin{array}{l} \gamma_N \in \mathcal{P}_{sym}((\mathbb{R}^d)^N) \\ \gamma_N \mapsto \mu \end{array} \right.$$

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

$$F^{\mathrm{OT}}_{N,s}(\mu) := \min\left\{ \int_{(\mathbb{R}^d)^N} \sum_{\substack{i,j=1\\ i\neq j}}^{N} \frac{1}{|x_i - x_j|^s}\, d\gamma_N(x_1,\dots,x_N) \;\middle|\; \begin{array}{l} \gamma_N \in \mathcal{P}_{sym}((\mathbb{R}^d)^N) \\ \gamma_N \mapsto \mu \end{array} \right.$$

The case $s = d - 2$ is the Coulomb cost.

Semiclassical limit

Theorem

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

$$\lim_{h \to 0} \mathrm{HK}_h[\rho] = F^{\mathrm{OT}}_{N,1}(\rho)$$

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

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

- Cotar, Friesecke, Klueppelberg: $N = 2$ (2011)
- Bindini - De Pascale (2017): extension to $N = 3$.
- Cotar, Friesecke, Klueppelberg (2017 - extension for $N \geq 3$ to the full model); Lewin (2017 - extension for $N \geq 3$ to a relaxed model)
- In physics literature: Seidl'99, Seidl/Perdew/Levy 1999, Seidl/Gori-Giorgi/Savin 2007

Optimal transport DFT community

- C-Friesecke-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), ..
- Regularity-type results: Pass (2013), Moameni (2014), Moameni-Pass (2017), Kim-Pass (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)

$$\lim_{N\to\infty}\binom{N}{2}^{-1}F^{\mathrm{OT}}_{N,\mathrm{c}}(\mu)=F^{\mathrm{OT}}_{\infty,\mathrm{c}}[\mu]=\frac{1}{2}\int_{\mathbb{R}^{2d}}l(x-y)d\mu(x)d\mu(y).$$

$(c(x,y)=l(x-y)$ 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 $E^{\mathrm{xc}}_{N,s}$

- Lieb-Oxford bound

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

- Trivially, we also have

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

- Question: Does the limit below exist

$$\lim_{N\to\infty} N^{-1-s/d}\left(F^{\mathrm{OT}}_{N,s}[\mu] - N^2\int_{\mathbb{R}^{2d}}\frac{1}{|x-y|^s}\rho(x)\rho(y)dxdy\right) =?$$

Second-order term $0 < s < d$

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

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

  (Lewin-Lieb-Seiringer 2017, via Graf-Schenker (1995) decomposition)
- $0 < s < d$, 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.)

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*

$$\lim_{N\to\infty} N^{-1-s/d}\underbrace{\left(F^{\text{OT}}_{N,s}(\mu) - N^2\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\frac{\rho(x)\rho(y)}{|x-y|^s}dx\,dy\right)}_{=:E^{\text{xc}}_{N,s}(\mu)} = -C_{\text{UEG}}(s,d)\int_{\mathbb{R}^d}\rho^{1+\frac{s}{d}}(x)dx.$$

- 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, ϵ, a family Ω of ball packings F_ω of $\mathbb{R}^d, \omega \in \Omega$, a radius $R_1 > 0$ and a probability measure $\mathbb{P}$ on Ω 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.

Grand canonical optimal transport

Let $N \in \mathbb{R}_{>0}, N \geq 2$, $\mu \in \mathcal{P}(\mathbb{R}^d)$

- The grand-canonical optimal transport

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

where infimum is taken over

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

with $\mu_n \in \mathcal{P}(\mathbb{R}^d), \; \alpha_n \geq 0, \quad n \in \mathbb{N}.$

- The grand-canonical exchange correlation energy

$$E^{\mathrm{xc}}_{\mathrm{GC},N,\mathsf{c}}(\mu) := F^{\mathrm{OT}}_{\mathrm{GC},N,\mathsf{c}}(\mu) - N^2 \int_{\mathbb{R}^d \times \mathbb{R}^d} \mathsf{c}(x,y)d\mu(x)d\mu(y).$$

- We have

$$F^{\mathrm{OT}}_{\mathrm{GC},N,\mathsf{c}}(\mu) \leq F^{\mathrm{OT}}_{N,\mathsf{c}}(\mu) \quad \text{and} \quad E^{\mathrm{xc}}_{\mathrm{GC},N,s}(\mu) \leq E^{\mathrm{xc}}_{N,s}(\mu).$$

Speed of convergence (small oscillations) result

Theorem (**Cotar-Petrache - Adv. Math. 2019**)

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*

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

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

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

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

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

(Lieb & Narnhofer 1975 for $s = d - 2$; Cotar-Petrache March 2019 for $d - 2 \le s < d$)

Connection to the Jellium model

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

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

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

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

(Cotar-Petrache 2019 for $d-2 \le s < d$)

- $$\mathrm{Jel}_{N,s}(\mu) \leq E^{\mathrm{xc}}_{N,s}(\mu)$$
- Lewin-Lieb (2015): comparison with uniform electron gas constant in $s = 1, d = 3$
- Heuristics for $s = 1, d = 3$ in Lewin-Lieb (2015): $C_{\mathrm{Jel}}(d, d-2) \neq C_{\mathrm{UEG}}(d, d-2)$, questioning the physicists' conjecture that $C_{\mathrm{Jel}}(d, d-2) = C_{\mathrm{UEG}}(d, d-2)$.

Minimum-energy point configurations (Coulomb and Riesz gases)

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

$V:\mathbb{R}^d\to]-\infty,+\infty]$ confining potential growing at infinity ($s=0$: 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 μ_V be the minimizer (among probability measures) of

$$\mathcal{E}_V^s(\mu) = \int\int \frac{1}{|x-y|^s} d\mu(x) d\mu(y) + \int V(x) d\mu(x)$$

Theorem

Under suitable assumptions on V, and if the density ρ_V is smooth enough, we have

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

and $-C_{\text{Gas}}(s,d)$ is the minimim value of a ***functional*** $\mathcal{W}$ ***on microscopic configurations*** ν.

- $C_{\text{Gas}}(s,d)$ 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

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

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

$$C_{\mathrm{UEG}}(s,d) = C_{\mathrm{Jel}}(s,d) = C_{\mathrm{Gas}}(s,d).$$

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

$$C_{\mathrm{UEG}}(s,d) = C_{\mathrm{Jel}}(s,d) = C_{\mathrm{Gas}}(s,d).$$

Continuity of $C_{\mathrm{UEG}}(s,d)$

- For $0 < s < d$, the function

  $$s \to C_{\mathrm{UEG}}(s,d)$$

  is continuous
- The proof works by interchanging the limits of $s \to s_0$ and $N \to \infty$ in

  $$N^{-1-s/d}\left(F_{\mathrm{GC},N,s}^{\mathrm{OT}}(\mu) - N^2 \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \frac{\rho(x)\rho(y)}{|x-y|^s} dxdy\right)$$

Key steps of the proof for Riesz costs (Cotar-Petrache July 2017)

- **Step 1**: Our crucial idea was to reduce the Jellium minimization problem to a Jellium problem with minimization over peridioc configurations
- In particular, this reduction allows to prove for $d-2 \leq s < d$

$$C_{\mathrm{Gas}}(s,d) = C_{\mathrm{Jel}}(s,d) = C_{\mathrm{Per}}(s,d).$$

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

$$C_{\mathrm{Gas}}(s,d) = C_{\mathrm{Per}}(s,d).$$

- **Step 2:** Our crucial idea was to use the periodic minimizing configurations to construct a competitor for the $E^{\mathrm{xc}}_{N,s}$ problem, albeit with the *wrong marginal*, depending on N
- Use the subadditivity of the $E^{\mathrm{xc}}_{N,s}$ 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 suabdditivity 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 $0 < \epsilon \leq \min(2, d/2)$. Then for $0 < d-2 \leq s \leq d-\epsilon$

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

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

Next-order terms: open problems

- **Open problem**: Find $C_{\mathrm{UEG}}(s,d)$ (connected to the crystallization conjecture)
- **Open problem**: Prove or disprove $E^{\mathrm{xc}}_{N,s}/N^{1+s/d}$ is decreasing in N (recall that E^{xc}_{N} is negative here)