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

Codina Cotar
(joint works with M. Petrache)

Mary 11, 2022

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)

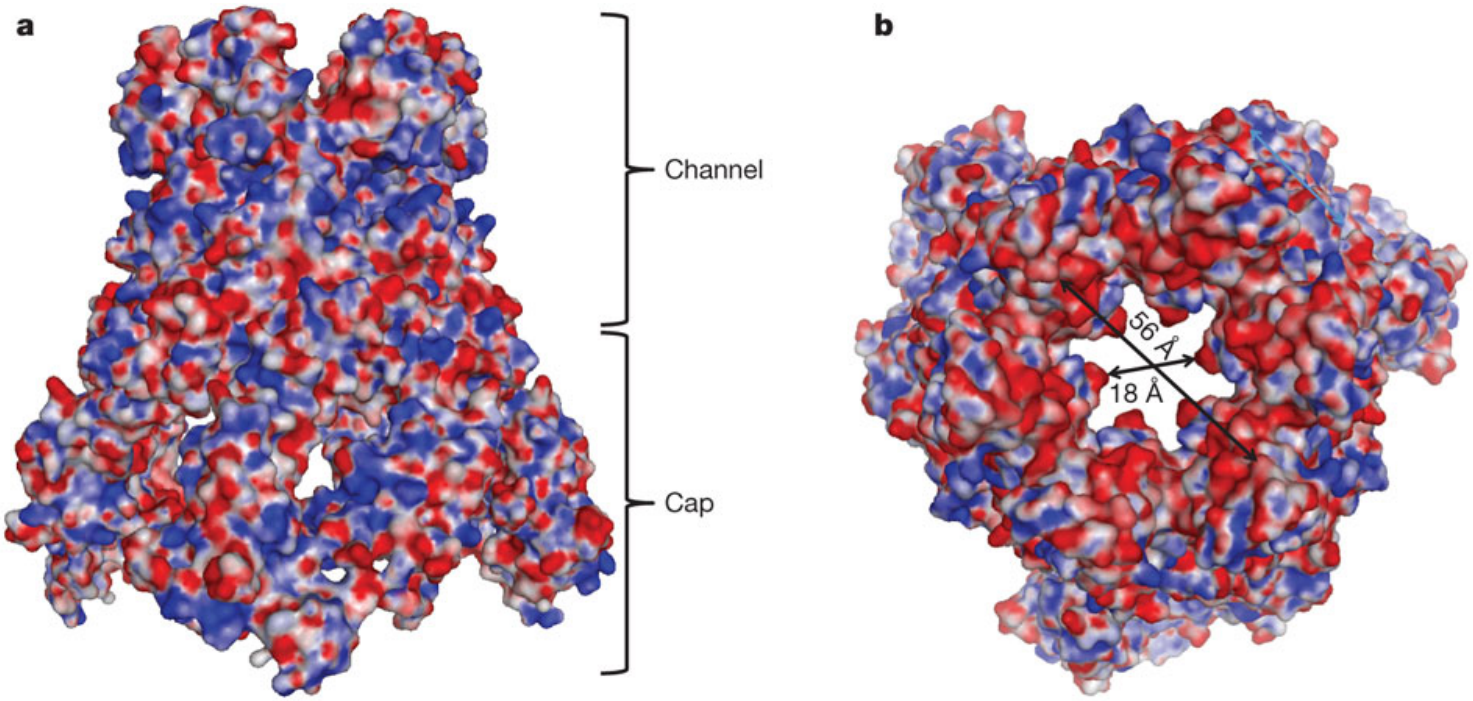
- To simulate chemical behaviour, approximations are needed.
- Curse of dimensionality: carbon atom: $N = 6$. Discretise $\mathbb{R}$ by 10 points$\rightarrow 10^{18}$ total grid points.
- DFT is a simplified version of quantum mechanics (QM), widely used in molecular simulations in chemistry, physics, 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 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 (345,580 Google Scholar paper citations as of this morning, compared to 152,344 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

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

- $V_{ee}[\Psi]$ and $V_{ne}[\Psi]$ are expectations 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:

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

New mathematical approach

Fresh look at the DFT correlation problem from the point of view of: (i) optimal transport (analysis+probability theory); (ii) exchangeable processes and other probabilistic tools; (iii) finite decomposition methods (applied math/mathematical physics)

- Cotar, Friesecke, Klueppelberg (CPAM-2013, ARMA-2018): in a natural scaling limit (i.e. taking the small Planck's constant h to 0), the celebrated Hohenberg-Kohn functional from DFT reduces for any $N \geq 2$ to an optimal transport problem F_N with marginal density ρ.
  - Novel functional form, complete anticorrelation
  - Opposite starting point for designing approximations than usual

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

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

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

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

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),..

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

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.

Asymptotics for F_N for large N

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

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

  $(c(x,y) = l(x-y)$ 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* $C_{\mathrm{UEG}}(d,s) > 0$ *such that*

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

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

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

Main tool: 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 $0 < s < d$.

Main tool: 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.

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

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

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

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

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

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

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

Jellium model

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

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

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

Jellium model

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

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

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

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

(Cotar-Petrache 2020 for $0 < s < d$)

Comparison between Jellium and UEG

- $$\mathrm{Jel}_{N,s}(\mu) \leq E^{\mathrm{xc}}_{N,s}(\mu)$$
- 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)

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

$V:\mathbb{R}^d\to]-\infty,+\infty]$ 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 $\max(0, d-2) \leq s < d$
- Their methods break down for $0 < s < d-2$
- Cotar-Petrache, 2020 - all previous cases + $0 < s < d-2$ by using a new screening procedure based on the Fefferman-Gregg decomposition

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

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

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

- $C_{\mathrm{Gas}}(s,d)$ 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 $C_{\mathrm{Gas}}(1,3)$ is thought to be approx. 1.4442

Comparison between Jellium, UEG and Riesz Gases

- 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)

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

- For $s = d-2$, Lewin, Lieb and Seiringer (May 2019) - same strategy as Cotar-Petrache 2017, with a better competitor
- Extension of the equality to $0 < s < d-2$ (Cotar-Petrache 2020)

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

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

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

  is continuous and $\lim_{s\to 0} C_{\mathrm{UEG}}(s,d) = -1$.
- The proof works by interchanging the limits of $s \to s_0$ and $N \to \infty$ in

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

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

- **Step 1**: The main 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 $d-2 \leq s < d$

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

- Cotar-Petrache 2017 was the first time where the first equality was proved. Previously, it was only proved for Coulomb and Riesz gases that

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

- **Step 2:** The key 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.

Main 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 $0 < d - 2 \leq s \leq d - \epsilon$

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

- 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 $C_{\mathrm{UEG}}(s, d)$ for $0 < s < d$.

Extension past Coulomb costs

- $c(x) = f(|x|)/|x|^s$, with $0 < c \leq f(|x|) \leq C$, where f is radial and decreasing.
- Potentials which are not rotation-invariant,such as

$$\mathsf{c}(x,y) := g(x-y), \text{ with } g(x) = |x|^{-s} f(x/|x|),$$

where $f \in C^0(\mathbb{S}^{d-1})$ and $0 < s < d$.

- For $0 < \alpha < 1$

$$\mathsf{c}(x,y) := \prod_{i=1}^{d} |x_i - y_i|^{-\alpha}, x = (x_1, \ldots, x_d), y = (y_1, \ldots, y_d) \in \mathbb{R}^d.$$

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)

Research summer school coming up!

https://sites.google.com/view/pointconfig2020

LONDON MATHEMATICAL SOCIETY EST. 1865 · CMI · Heilbronn Institute for Mathematical Research · UCL

Point Configurations: Deformations and Rigidity

LMS Research School at the University College London

27th JUNE - 1st JULY 2022

(The conference will be in hybrid format)

Organisers: Codina Cotar (UCL, London) and Mircea Petrache (PUC, Santiago)

Location: Department of Statistical Science, University College London, UK

The aim of the research summer school is to present several different modern perspectives on the rigidity and deformability of optimum point configurations. Three main points of view are presented in the lecture courses: the point of view of material science and elasticity; the point of view of approximation theory; and the point of view of the methods of Viazovska, based on linear programming bounds.

The research school is funded by the London Mathematical Society, Clay Mathematics Institute, Heilbronn Institute for Mathematical Research and UCL.

Lecturers and Plenary Speakers

There will be three main lecture courses (of six hours each), accompanied by tutorial classes (of four hours each), on the following topics (click on the title to see the abstract):

- Crystallization in classical particle systems by Gero Friesecke, from Technical University of Munich (tutorial classes by Gero Friesecke)
- Optimal and Near Optimal Energy Minimizing Point Configurations by Douglas Hardin and Edward Saff, from Vanderbilt University (tutorial classes by Alex Vlasiuk from Vanderbilt University)
- Modular forms, universal optimality and Fourier interpolation by Danylo Radchenko, from ETH Zurich (tutorial classes by Steven Charlton, from University of Hamburg)

Additionally, there will be distinguished plenary lectures by:

- Keith Ball (Warwick University)
- Werner Krauth (Ecole Normale Superieure)
- Franz Merkl (Ludwig Maximilian University of Munich)
- Sylvia Serfaty (New York University)

There will also be an opportunity for the participants to present posters or give short talks on their own research. Further information will be added closer to the summer school.

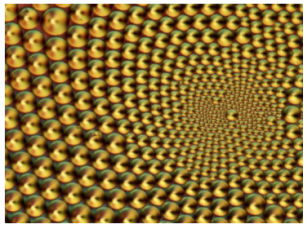


Photo by Vance Williams

THANK YOU!