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

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Many-marginals optimal transport problem

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

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

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

The infinite-dimensional Optimal Transportation problem

- Let γ be an infinite dimensional measure, γ symmetric (exchangeable), μ probability measure in $\mathbb{R}^d$ and $c(x,y) = l(x-y)$.

$$F^{\mathrm{OT}}_{\infty,\mathrm{c}}(\mu) = \inf_{\substack{\gamma\in\mathcal{P}^{\infty}_{\mathrm{sym}}(\mathbb{R}^d)\\ \gamma\mapsto\mu}} \lim_{N\to\infty} \frac{1}{\binom{N}{2}} \int_{\mathbb{R}^{dN}} \sum_{1\leq i<j\leq N} l(x_i-x_j)d\gamma(x_1,..,x_N),$$

subject to the constraint

$$\int_{\mathbb{R}\times\mathbb{R}\times\ldots} \gamma(x_1,x_2,\ldots,x_N,\ldots)dx_2dx_3\ldots dx_N\ldots = \mu(x_1).$$

Theorem

(Cotar, Friesecke, Pass - Calc Var PDEs 2015)

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

(l with positive Fourier transform)

Proof by Fourier analysis and de Finetti arguments

Theorem

(Petrache-2015: generalization by convexity)

$$\lim_{N\to\infty} \binom{N}{2}^{-1} F^{\mathrm{OT}}_{N,\mathrm{c}}(\mu) = \int_{d} \int_{d} c(x-y)d\mu(x)d\mu(y)$$

if and only if $c(x-y)$ *is balanced positive definite, i.e.*

$$\int \int \rho(x)\rho(y)c(x-y)dxdy \geq 0 \quad \textit{whenever} \quad \int \rho = 0 \, .$$

Second-order term, $0 < s < d$

- $d = 1$, very general kernels: 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)

Theorem

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

Connection to Jellium

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

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

- Let minimization be $\xi(N, \Omega)$, then the limit (Lieb & Narnhofer 1975)

$$\lim_{N\to\infty} \frac{\xi(N,\Omega)}{N} = -C_{jel}(s,d).$$

Connection to Jellium

- Alternatively, take Ω with $|\Omega| = 1$.
- Minimize over x_i

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

- Let minimization be $\xi(\Omega)$, then the limit

$$\lim_{N \to \infty} \frac{\xi(N, \Omega)}{N^{1+s/d}} = -C_{jel}(s, d).$$

- Lewin-Lieb (2015): comparison with uniform electron gas constant in $d = 3$

Minimum-energy point configurations

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

$\mathsf{c}(x) = |x|^{-s}$ interaction potential, $V : \mathbb{R}^d \to]-\infty, +\infty]$ 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
- **Possible Modifications**:
  - (a) replace the V-term by imposing $x_i \in A$ for $A \subset X$ fixed compact set.
  - (b) change c (e.g. Gaussian, or add perturbations).
  - (c) replace $\mathbb{R}^d$ by another space X

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

$$\min H_{N,V} = \begin{cases} N^2\mathcal{E}^s(\mu_V) - N^{1+\frac{s}{d}} C_{\mathrm{Jel}}(s,d) \int \mu_V^{1+\frac{s}{d}}(x)dx + o(N^{1+\frac{s}{d}}) \\ N^2\mathcal{E}^{\log}(\mu_V) - \frac{N}{d}\log N - N\left(C_{\mathrm{Jel}}(\log) - \frac{1}{d}\int \mu_V(x)\log \mu_V(x)\, dx\right) \\ +o(N), \end{cases}$$

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

- $C_{\text{Jel}}(s,d)$ 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 Jellium minimizers are not lattices, although this is very much speculative at the moment.
- Open for all $d \geq 2$ dimensions.
- For $s = 1, d = 3$, the value of $C_{\text{Jel}}(1,3)$ is thought to be approx. 1.4442

Comparison between Jellium and UEG ($d-2<s<d$)

- Lewin-Lieb (2015): comparison between minimum when $|\Omega| = N$ (and the minimum is taken only of configurations forming lattices) of the Jellium problem

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

and the following quantity

- $$E_{\text{UEG}}(\Omega, \vec{x}) := \sum_{\substack{1\leq i,j\leq N\\ i\neq j}} \frac{1}{|x_i - x_j|} - \int_\Omega \int_\Omega \frac{1}{|x-y|} dxdy.$$

- The quantity

$$\min\left\{\int E_{\mathrm{UEG}}(\Omega,\vec{x})d\gamma_N(\vec{x})\,:\,\gamma_N\mapsto\frac{1_{|\Omega|}}{N}\right\}$$

  is equal to

$$E^{\mathrm{xc}}_{N,1}\left(\frac{1_{|\Omega|}}{N}\right)$$

- $$\lim_{N\to\infty}\frac{1}{N}\min\left\{\int E_{\mathrm{UEG}}(\Omega,\vec{x})d\gamma_N(\vec{x})\,:\,\gamma_N\mapsto\frac{1_{|\Omega|}}{N}\right\}=-C_{\mathrm{UEG}}(1,3).$$

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

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

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

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

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

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

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

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

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

Next-order terms: open problems

- Heuristics for $s = 1, d = 3$ in **Lewin-Lieb '15**: $C_{Jel}(d, d-2) \neq C_{UEG}(d, d-2)$, questioning the physicists' conjecture that $C_{Jel}(d, d-2) = C_{UEG}(d, d-2)$.
- **Open problem**: prove or disprove $C_{Jel}(d, d-2) \neq C_{UEG}(d, d-2)$.
- **Open problem**: Sharp asymptotics of $\min H_N$ for $0 < s < d-2$.
- **Open problem**: Find $C_{UEG}(s, d)$ (connected to the crystallization conjecture)
- **Open problem**: Prove or disprove $E^{xc}_{N,s}/N^{1+s/d}$ is decreasing in N (recall that E^{xc}_N is negative here)