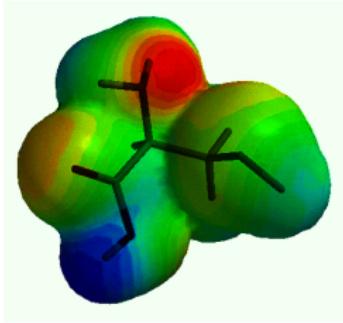


Finite-range kernel decompositions and asymptotic Optimal Transport between configurations

Mircea Petrache, PUC Chile

February 27, 2018

Density Functional Theory



Cystein molecule simulation,
(from [Walter Kohn's Nobel prize laudation page](#))

DENSITY FUNCTIONAL THEORY

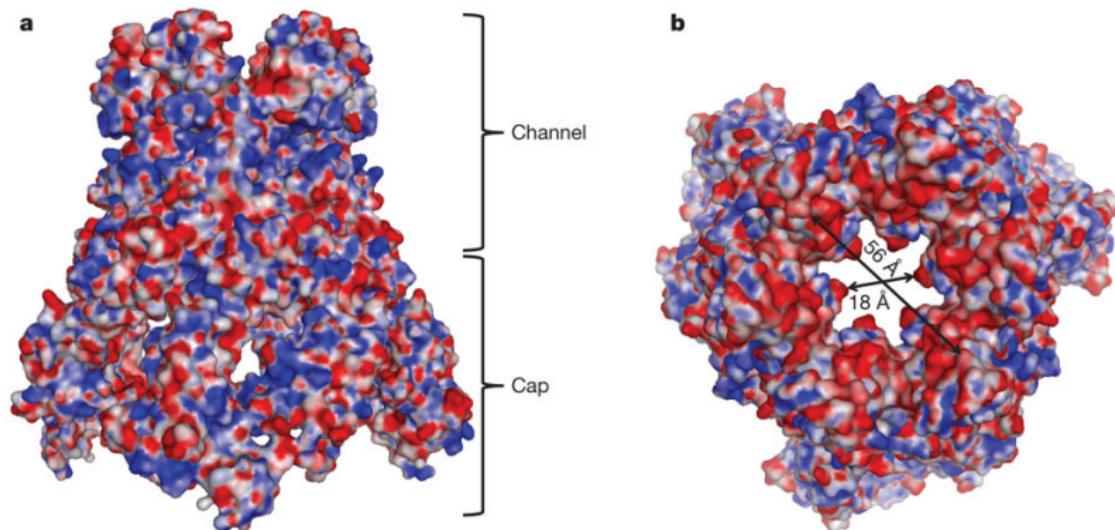
- ▶ The chemical behavior of atoms and molecules is captured by quantum mechanics via Schrödinger's eq. (Dirac '29)
- ▶ **Curse of dimensionality:**
 - ▶ The Schrödinger equation is of the form $H\Psi = E\Psi$, a second order PDE on \mathbb{R}^{3N} , Ψ represents the state of the N -particle system.
 - ▶ Chemical behavior \sim energy differences \ll total energy
- ▶ **Example:** carbon atom: $N = 6$, spectral gap = $10^{-4} \times$ (total energy). Discretize \mathbb{R} by 10 points $\Rightarrow 10^{18}$ total grid points.
- ▶ A scalable simplified reformulation of the precise equations is the **Hohenberg-Kohn-Sham** (HK) model (Levy '79 - Lieb '83). It is formulated in terms of the normalized one-particle density ρ .

DENSITY FUNCTIONAL THEORY

- ▶ The HK model boomed in computational chemistry since the 1990's.
- ▶ More than 15000 papers a year contain the keywords 'density functional theory'.
- ▶ There exist '**cheap**' versions which allow computations of large molecules (e.g. DNA, enzymes), routinely used in comp. chemistry, biochemistry, material science, etc.
- ▶ Lack of systematic improvability of the computations.

DENSITY FUNCTIONAL THEORY

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

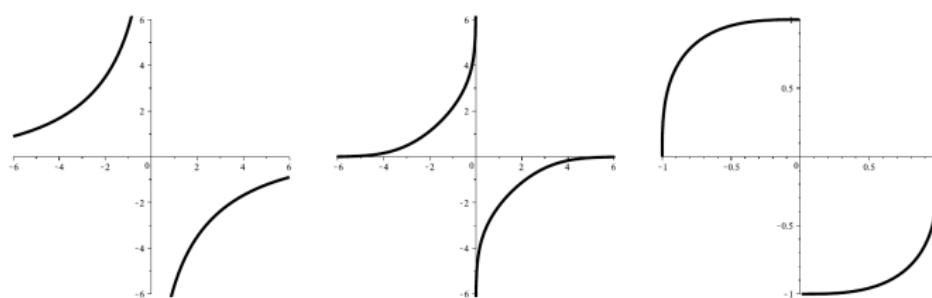


Simulation of heavy-metal pump in *E. Coli*
(Su & al., *Nature* '11)

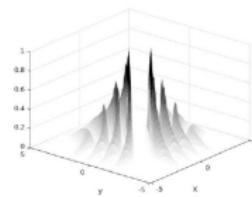
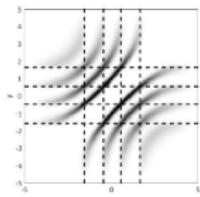
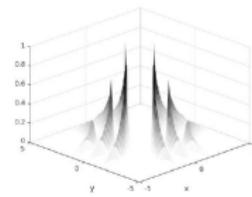
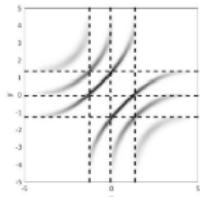
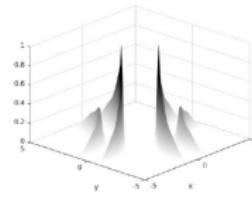
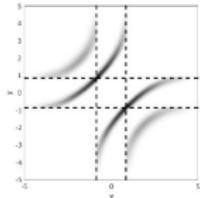
N-marginal Optimal Transport

AN N -MARGINAL OPTIMAL TRANSPORT PROBLEM:

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



Optimal γ_N (radial part) for $N = 2$, $s = 1$ and $d = 3$ and different ρ
from Cotar-Friesencke-Klüppenberg '13



Optimal γ_N for $N = 3, 4, 5$ points, and $s = 1, d = 1$
 (projected from \mathbb{R}^N to \mathbb{R}^2),
 from Di Marino-Gerolin-Nenna '15

ABOUT N -MARGINAL OPTIMAL TRANSPORT PROBLEMS:

$$F_{N,c}^{OT}(\rho) := \min \left\{ \int_{(\mathbb{R}^d)^N} \sum_{i \neq j}^N c(x_i - x_j) d\gamma_N(x_1, \dots, x_N) \mid \begin{array}{l} \gamma_N \in \mathcal{P}_{sym}((\mathbb{R}^d)^N), \\ \gamma_N \mapsto \rho \end{array} \right\}.$$

- ▶ Problem appeared naturally in OT theory (for tame $c(x - y)$)
Gangbo-Swiech '98, Carlier '03, Carlier-Nazaret '08
- ▶ Optimal transport community Colombo-De Pascale-Di Marino '13, Colombo-Di Marino '15, Di Marino-Gerolin-Nenna '15, De Pascale '15, Buttazzo-Champion-De Pascale '17, ..
- ▶ Link between OT and DFT/math physics
Cotar-Friesecke-Klüppelberg '13, '17, Cotar-Friesecke-Pass '15,..
- ▶ Regularity-type results Pass '13, Moameni '14, Moameni-Pass '17, Kim-Pass '17..

DFT AND MULTIMARGINAL OT

- **Hohenberg-Kohn functional:** energy of N electrons of density ρ
 (Hohenberg-Kohn '64, Levy '79, Lieb '83)

$$F_N^{HK}[\rho] := \min_{\Psi_N \in \mathcal{A}_N, \Psi_N \mapsto \rho} \langle \Psi_N, (\hbar^2 \hat{T} + \hat{V}_{ee}) \Psi_N \rangle.$$

- $\hat{T} = -\frac{1}{2} \Delta_{\mathbb{R}^{Nd}}$ quantum mechanical kinetic energy
- $V_{ee}(x_1, \dots, x_N) = \sum_{1 \leq i < j \leq N} 1/|x_i - x_j|^{d-2}$,
- $\mathcal{A}_N = \left\{ \Psi_N : (\mathbb{R}^d \times \mathbb{Z}_2)^N \rightarrow \mathbb{C}, \|\Psi_N\|_{L^2} = 1, \nabla \sqrt{|\Psi_N|} \in L^2, \text{ Antisymm. } \right\}$

- $\Psi_N \mapsto \rho$ means

$$\sum_{s_1, \dots, s_N \in \mathbb{Z}_2} \int |\Psi(x_1, s_1, \dots, s_N, x_N)|^2 dx_2 \dots dx_N = \rho(x_1).$$

- $\lim_{\hbar \rightarrow 0} F_N^{HK}[\rho] = F_N^{OT}(\rho)$ (Cotar-Friescke-Klüppelberg '13,'17,
 Lewin '17, De Pascale-Bindini '17)

MINIMUM ENERGY AND MULTIMARGINAL OT

- If $\omega_N = \{x_1, \dots, x_N\} \subset \mathbb{N}$ and $V : \mathbb{R}^d \rightarrow \mathbb{R}$ “confining” potential,

$$E_V(\omega_N) := \sum_{i \neq j} \frac{1}{|x_i - x_j|^s} + N \sum_{i=1}^N V(x_i).$$

- Let ω_N^* be minimum E_V -energy configurations. Then

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{p \in \omega_N^*} \delta_p = \mu_V \in \operatorname{argmin} \left[\int \int \frac{d\mu(x)d\mu(y)}{|x - y|^s} + \int V(x)d\mu(x) \right]$$

- $\gamma_N^* :=$ uniform on {permutations of ω_N^* }.
- Then $\gamma_N^* \in \mathcal{P}_{sym}((\mathbb{R}^d)^N)$ and we find

$$F_N^{OT}(\mu_V) \geq F_N^{OT} \left(\frac{1}{N} \sum_{p \in \omega_N^*} \delta_p \right) = E_V(\omega_N^*) - \int V d\mu_V.$$

Results and Open Problems

LEADING-ORDER ASYMPTOTICS, $0 \leq s < d$

- ▶ First-order “mean field” functional: Cotar-Friesecke-Pass ’15.
- ▶ Petrache ’15: generalization by convexity + De Finetti

Theorem

$$\lim_{N \rightarrow \infty} \binom{N}{2}^{-1} F_{N,c}(\rho) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} c(x-y) \rho(x) \rho(y) dx dy$$

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

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

NEXT-ORDER TERM, $0 < s < d$

- ▶ $d = 1$, general kernels: unpublished note by Di Marino
- ▶ $s = 1, d = 3$: Lewin-Lieb-Seiringer '17, using Graf-Schenker '95
- ▶ Improving upon the different strategy Fefferman '85, we get:

Theorem (Cotar-Petrache '17)

If $d \geq 1$, $0 < s < d$ and ρ s.t. the following integrals are finite, then

$$\begin{aligned} F_{N,s}^{OT}(\rho) &= N^2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\rho(x)\rho(y)}{|x-y|^s} dx dy \\ &\quad + N^{1+\frac{s}{d}} \left(C_{UG}(d,s) \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx + o(1) \right) \text{ as } N \rightarrow \infty. \end{aligned}$$

We can interpret $C_{UG}(d,s) = \min$ energy of an “Uniform Riesz Gas”
(special case: “Uniform Electron Gas” from DFT, for $s = d - 2$).

NEXT-ORDER TERMS: OT VS. ENERGY

Theorem (Cotar-Petrache '17)

If $0 < s < d$ and $d\mu(x) = \rho(x)dx$ then as $N \rightarrow \infty$

$$F_{N,s}^{OT}(\mu) = N^2 \mathcal{E}(\mu) + N^{1+\frac{s}{d}} \left(C_{UG}(d,s) \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx + o(1) \right).$$

We can interpret $C_{UG}(d,s) = \min \mathcal{E}_{UG}(\nu)$ “uniform gas” energy on microscale configurations. Recall:

Theorem (Petrache-Serfaty '15)

If $\max\{0, d-2\} \leq s < d$ under suitable assumptions on V , as $N \rightarrow \infty$

$$\min H_N \stackrel{(s \neq 0)}{=} N^2 \mathcal{E}(\mu_V) + N^{1+\frac{s}{d}} \left(C_{Jel}(d,s) \int \mu_V^{1+\frac{s}{d}}(x) dx + o(1) \right).$$

We can interpret $C_{Jel}(d,s) = \min \mathcal{E}_{Jel}(\nu)$, “Riesz Jellium” energy on microscale configurations.

NEXT-ORDER TERMS: OPEN PROBLEMS

Theorem (Cotar-Petrache '17)

For $d \geq 2$ and $d - 2 < s < d$ there holds $C_{Jel}(d, s) = C_{UG}(d, s)$.

- ▶ The above asymptotic microscale problems are then *equivalent* for $d \geq 2$ and $d - 2 < s < d$.
- ▶ Heuristics for $s = 1, d = 3$ in Lewin-Lieb '15:
 $C_{Jel}(d, d - 2) \neq C_{UG}(d, d - 2)$, questioning the physicists' conjecture that $C_{Jel}(d, d - 2) = C_{UG}(d, d - 2)$.
- ▶ **Open problem:** prove or disprove $C_{Jel}(d, d - 2) \neq C_{UG}(d, d - 2)$.
- ▶ **Open problem:** Sharp asymptotics of $\min H_N$ for $0 < s < d - 2$.
- ▶ *Possible ideas:*
 - ▶ $s \mapsto C_{Jel}(d, s)$ might have a jump at $s = d - 2$.
 - ▶ The (analytic continuation in α of the) fractional laplacian $(-\Delta)^\alpha$ from Petrache-Serfaty has a residue at $s = d - 2, d - 4, \dots$

NEXT-ORDER TERMS: OPEN PROBLEMS

“Exchange-correlation” energy = Part of the energy not encoded in 1-particle density

$$E_N^{xc}(\rho) := F_N^{OT}(\rho) - \frac{N^2}{\int_{\mathbb{R}^d} \rho} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\rho(x)\rho(y)}{|x-y|^s} dx dy.$$

In Cotar-Petrache '17 we prove

$$\lim_{N \rightarrow \infty} N^{-1-\frac{s}{d}} E_N^{xc}(\rho) = C_{UG}(d, s) \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx.$$

$C_{UG}(3, 1)$ = asymptotic Lieb-Oxford constant
 (cf. Dirac '30, Lieb-Oxford '81, Lewin-Lieb '15).

- **Open questions:** Let $d \geq 2$, let $0 < s < d$.
 What are the precise values of (any of)

$$\inf_{N \in \mathbb{N}} N^{-1-\frac{s}{d}} E_N^{xc}(1_{[0,1]^d}) \quad \text{or} \quad C_{UG}(d, s) ?$$

(most physically relevant for $s = 1, d = 3$)

Proof strategy

SHARP NEXT-ORDER TERM: PROOF FOR UNIFORM ρ

1. $E_{M_1+M_2}^{xc}\left(\frac{M_1\rho_1+M_2\rho_2}{M_1+M_2}\right) \leq E_{M_1}^{xc}(\rho_1) + E_{M_2}^{xc}(\rho_2).$
2. $E_N^{xc}(\alpha^d \rho_\alpha) = \alpha^{-s} E_N^{xc}(\rho)$ if $\rho_\alpha(x) = \rho(\alpha x).$
3. This and a subadditivity argument (**Robinson-Ruelle**) proves that for $\rho = 1_A$, $|A| = 1$, there holds:

$$\lim_{N \rightarrow \infty} N^{-1-\frac{s}{d}} E_N^{xc}(1_A) = C_{UG}(d, s)$$

This will give also the interpretation of $C_{UG}(d, s)$ as an energy on microscopic blow-up configurations. (Note that $C_{UG}(d, s) < 0.$)

SHARP NEXT-ORDER TERM: PIECEWISE CONSTANT ρ

$$\rho(x) = \sum_{i=1}^k \alpha_i \mu_i, \quad \mu_i \text{ uniform prob. on a hyperrectangle}$$

► **Upper bound:** subadditivity*

► **Lower bound:**

1. An ensemble (Ω, \mathbb{P}) of packings $\{F_\omega\}_{\omega \in \Omega}$
2. each F_ω consisting of balls of sizes $0 < R_1 < \dots < R_M$ in a geometric series,
3. if $\Sigma = spt(\mu)$ then $|\Sigma \setminus \cup_{A \in F_\omega} A| \rightarrow 0$ as $R_M \rightarrow 0$
4. at fixed F_ω , decompose the kernel + average:

$$5. \quad \sum_{\substack{i \neq j \\ i,j=1}}^N |x_i - x_j|^{-s} = \sum_{A \in F_\omega} \sum_{\substack{1 \leq i \neq j \leq N \\ x_i, x_j \in A}} |x_i - x_j|^{-s} + err_\omega(x_1, \dots, x_d),$$

$$\int_{\Omega} \left(\sum_{A \in F_\omega} E_{N_A}^{xc} \left(\frac{\rho|_A}{\int_A \rho} \right) \right) d\mathbb{P}(\omega) \leq E_N^{xc}(\rho) + err,$$

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 4. at fixed F_ω , decompose the kernel + average:

$$c(x-y) = \sum_{A \in F_\omega} 1_A(x) 1_A(y) c(x-y) + err_\omega(x-y),$$

5.

$$\int_{\Omega} \left(\sum_{A \in F_\omega} E_{N_A}^{xc} \left(\frac{\rho|_A}{\int_A \rho} \right) \right) d\mathbb{P}(\omega) \leq E_N^{xc}(\rho) + err,$$

5.

$$\int_{\Omega_l} \left(\sum_{A \in F_\omega} E_{N_A}^{xc} \left(\frac{\rho|_A}{\int_A \rho} \right) \right) d\mathbb{P}(\omega) \leq E_N^{xc}(\rho) + err,$$

6. If $\rho|_A$ constant $\equiv \frac{1}{|A|} \int_A \rho$ then (unif. marginal case), using the fact that $N_A = N \int_A \rho = |A|\rho|_A$:

$$\begin{aligned} E_{N_A}^{xc} \left(\frac{\rho|_A}{\int_A \rho} \right) &\simeq (N_A)^{1+\frac{s}{d}} |A|^{-\frac{s}{d}} C_{UG}(d, s) \\ &= N^{1+\frac{s}{d}} C_{UG}(d, s) \int_A (\rho|_A)^{1+\frac{s}{d}} dx, \end{aligned}$$

7. and we get as $R_M \rightarrow 0, N \rightarrow \infty$:

$$\int_{\Omega} \left(\sum_{A \in F_\omega} E_{N_A}^{xc} \left(\frac{\rho|_A}{N_A} \right) \right) d\mathbb{P}(\omega) = N^{1+\frac{s}{d}} C_{UG}(d, s) \left(\int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx + o(1) \right).$$

The new kernel truncation

The new kernel truncation

- ▶ Kernel decomposition like Fefferman '85, Gregg '89 ($s \sim 1, d = 3$).
- ▶ Three ingredients to tune:
 1. Packing strategy
 2. Positive definiteness criteria
 3. Scale separation

1. PACKING STRATEGY

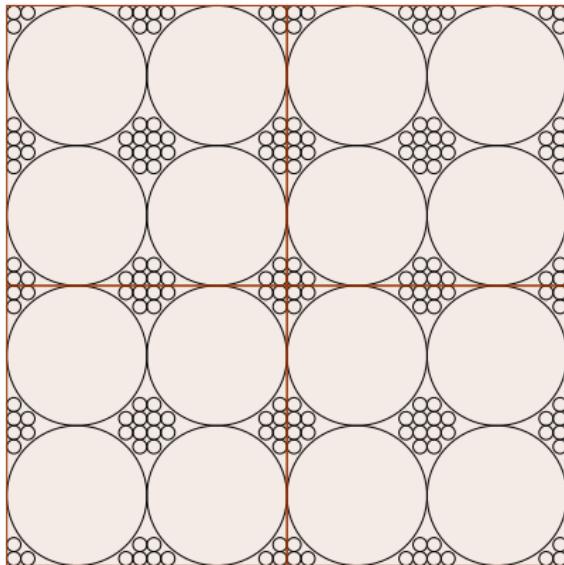
- ▶ “Swiss cheese” lemma Lebowitz-Lieb ’72: Cover $[0, l]^d$ by balls $\mathcal{F} = \{B\}_B$ of radii $0 < R_1 < \dots < R_M$ with
 - ▶ geometric growth: $R_{i+1} > C_d R_i$,
 - ▶ $c_i := (\text{volume fraction covered by } B_i\text{-balls}) = 1/M + O(M^{-2})$.

Extend by $(l\mathbb{Z})^d$ -periodicity.

- ▶ For $\langle f \rangle(x, y) := \int_{\mathbb{R}^d} f(x + p, y + p) dp$, write

$$\sum_{B \in \mathcal{F}} \langle 1_B(x) 1_B(y) c(x - y) \rangle = c(x - y) \sum_{i=1}^M c_i \frac{1_{B_{R_i}} * 1_{B_{R_i}}(x - y)}{|B_{R_i}|}.$$

OUR PACKING, $M = 2$



2. POSITIVE DEFINITENESS CRITERION

Lemma (perturbative positive-definiteness criterion)

$$|\partial_x^\beta g(x)| \lesssim |x|^{-s-|\beta|} \text{ for all multiindices } |\beta| \leq d.$$

\Rightarrow

$$|\hat{g}(\xi)| \lesssim |\xi|^{s-d}.$$

To use it we further mollify

$$Q_i(x) = \frac{1_{B_R} * 1_{B_R}(x)}{|B_R|} \quad \mapsto \quad Q_{i,\eta}(x) = \int_{1-\eta}^{1+\eta} \frac{1_{B_{tR}} * 1_{B_{tR}}(x)}{|B_{tR}|} \rho_\eta(t) dt.$$

(can still re-express as averaging over dilated packings)

THE ERROR ESTIMATE

Proposition (kernel localization + small error)

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

Moreover

1. w is positive definite.
2. we have

$$E_{N,w}^{xc}(\rho) \geq -\frac{C(w,s,d)}{M} N^{1+s/d} \int_{\mathbb{R}^d} \rho^{1+s/d}(x) dx - \frac{C}{M} R_1^{-s} N.$$

ERROR DECOMPOSITION

$$\begin{aligned}
err(x_1, x_2) &:= \frac{1}{|x_1 - x_2|^s} - \int_{\Omega_l} \left[\sum_{A \in F_\omega} \frac{1_A(x_1)1_A(x_2)}{|x_1 - x_2|^s} \right] d\mathbb{P}(\omega) \\
&= \frac{1}{|x_1 - x_2|^s} - \sum_{i=1}^M c_i \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}, \\
&= \frac{1}{M} \sum_{i=1}^M \frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} \\
&= \frac{1}{M} \sum_{i=1}^M \left(\frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} - \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \right) \\
&\quad + \frac{1}{M} \sum_{i=1}^M \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \\
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&= \frac{1}{|x_1 - x_2|^s} - \sum_{i=1}^M c_i \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}, \\
&= \frac{1}{M} \sum_{i=1}^M \frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} \\
&= \frac{1}{M} \sum_{i=1}^M \left(\frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} - \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \right) \\
&\quad + \frac{1}{M} \sum_{i=1}^M \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \\
&\quad + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}.
\end{aligned}$$

ERROR DECOMPOSITION

$$\begin{aligned}
w(x_1, x_2) &:= \left(1 + \frac{2C}{M}\right) \frac{1}{|x_1 - x_2|^s} - \int_{\Omega_l} \left[\sum_{A \in F_\omega^l} \frac{1_A(x_1)1_A(x_2)}{|x_1 - x_2|^s} \right] d\mathbb{P}_l(\omega) \\
&= \frac{1}{|x_1 - x_2|^s} + \frac{2C}{M} \frac{1}{|x_1 - x_2|^s} - \sum_{i=1}^M c_i \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}, \\
&= \frac{2C}{M} \frac{1}{|x_1 - x_2|^s} + \frac{1}{M} \sum_{i=1}^M \frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}. \\
&= \frac{C}{M} \frac{1}{|x_1 - x_2|^s} + \frac{1}{M} \sum_{i=1}^M \left(\frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} - \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \right) \\
&\quad + \frac{1}{M} \sum_{i=1}^M \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \\
&= \frac{C}{M} \frac{1}{|x_1 - x_2|^s} + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}.
\end{aligned}$$

3. SCALE SEPARATION

$$\begin{aligned}
w(x_1, x_2) &:= \left(1 + \frac{2C}{M}\right) \frac{1}{|x_1 - x_2|^s} - \int_{\Omega_l} \left[\sum_{A \in F_\omega^l} \frac{1_A(x_1)1_A(x_2)}{|x_1 - x_2|^s} \right] d\mathbb{P}_l(\omega) \\
&= \frac{1}{|x_1 - x_2|^s} + \frac{2C}{M} \frac{1}{|x_1 - x_2|^s} - \sum_{i=1}^M c_i \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}, \\
&= \frac{2C}{M} \frac{1}{|x_1 - x_2|^s} + \frac{1}{M} \sum_{i=1}^M \frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}. \\
(w_{\text{multiscale}}) &= \frac{C}{M} \frac{1}{|x_1 - x_2|^s} + \frac{1}{M} \sum_{i=1}^M \left(\frac{1 - Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s} - \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \right) \\
(w_{\text{tail}}) &+ \frac{1}{M} \sum_{i=1}^M \left(\int_{\mathbb{R}^d} Q_{i,\eta} \right)^{-1} \int_{\mathbb{R}^d} \frac{Q_{i,\eta}(y)}{|x_1 - x_2 - y|^s} dy \\
(w_{\text{cover-error}}) &+ \frac{C}{M} \frac{1}{|x_1 - x_2|^s} + \sum_{i=1}^M \left(\frac{1}{M} - c_i \right) \frac{Q_{i,\eta}(x_1 - x_2)}{|x_1 - x_2|^s}.
\end{aligned}$$

BOUNDS FOR THE PIECES

Lemma

If $w_{\text{multiscale}}$, w_{tail} , $w_{\text{cover-error}}$ are the last 3 lines of the previous slide, then

1. $w_{\text{multiscale}}$ is positive definite.
2. w_{tail} is positive definite and $w_{\text{tail}}(x) \leq \frac{C}{M} R_1^{-s}$.
3. $w_{\text{cover-error}}$ is positive definite.

Moreover, for all $\mu \in \mathcal{P}(\mathbb{R}^d)$ with density $\rho \in L^{1+\frac{s}{d}}(\mathbb{R}^d)$ we have

$$E_{N,w_{\text{multiscale}}}^{xc}(\rho) \geq -\frac{C(w_{\text{multiscale}}, s, d)}{M} N^{1+\frac{s}{d}} \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx$$

$$E_{N,w_{\text{cover-error}}}^{xc}(\rho) \geq -\frac{C(w_{\text{cover-error}}, s, d)}{M} N^{1+\frac{s}{d}} \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x) dx.$$

SUMMARY

- ▶ Pack by geometric-decreasing balls (cheese lemma)
- ▶ Averaging + transl. invariance: reduce to truncated kernel
- ▶ Divide the error into positive-definite contributions.

PARALLEL TO WAVELET ANALYSIS

- ▶ *Littlewood-Paley / multiplier methods:*
 - ▶ truncate in Fourier
 - ▶ bookkeeping on function norm bounds (real side)
 - ▶ regularity theory / control on oscillations
 - ▶ model case: PDEs with the Laplacian
- ▶ *Finite range decomposition / truncation methods:*
 - ▶ truncate in real space
 - ▶ bookkeeping on ellipticity/pos.-def. bounds (Fourier side)
 - ▶ sharp asymptotics / control on asymptotic terms
 - ▶ model case: pairwise interaction = kernel of the Laplacian
- ▶ *Very robust method:*
vector potentials, nonlinear/curved models, oscillating kernels..
- ▶ other finite-range decompositions Adams, Bauerschmidt, Brydges, Kotecky, Mitter, Müller, Slade, Talarczyk, .. especially worked out in lattice-models so far.

THANK YOU!