Density functional theory and optimal transport with Coulomb cost

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TU Munich

Workshop at MSRI, October 17, 2013

Organizers: Yann Brenier, Michael Cullen, Wilfrid Gangbo, Allen Tannenbaum

Ch. Mendl (TUM), C. Klüppelberg (TUM),
C. Cotar (University College London), Brendan Pass (Alberta)

Optimal transport with Coulomb cost

Minimize

$$\int_{\mathbb{R}^{3N}} \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \, d\gamma(x_1, .., x_N)$$

over symmetric N-body probability measures γ on $\mathbb{R}^{3N}$ with given one-body marginal ρ, i.e.

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- Qualitative theory
- Exactly soluble examples
- Large N

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C.Cotar, G.F., C.Klüppelberg, CPAM 66, 548-599, 2013 (arXiv 2011)
G.F., Ch.Mendl, B.Pass, C.C, C.K., arXiv 2013 (to appear in J.Chem.Phys.)
C.C., G.F., B.Pass, arXiv 1307.6540, 2013

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To simulate chemical behaviour, approximations are needed. (Full Schröd.eq.: $\mathbb{R} \to 10$ gridpoints means $\mathbb{R}^{3N} \to 10^{3N}$ gridpoints. E.g., H_2O has 10 electrons, so 10^{30} gridpts! Curse of dimension.)

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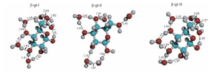

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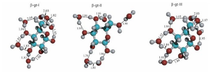

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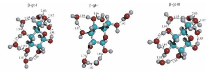

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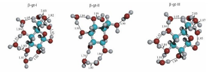

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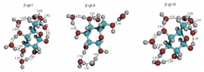

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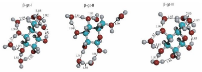

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– Accuracy not that high; lack of systematic derivability/improvability of functionals

Quantum mechanics of atoms and molecules – Details

- Goal: compute lowest eigenvalue ("ground state energy") E_0 of the following linear operator ("electronic Hamiltonian")

$$H_{e\ell} = \sum_{i=1}^{N}(-\frac{\hbar^2}{2}\Delta_{x_i}) + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} + \sum_{i=1}^{N} v_R(x_i)$$

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- Rayleigh-Ritz variational principle:

$$E_0 = \min_{||\Psi||=1}\left\langle \Psi, H_{e\ell}\Psi \right\rangle_{L^2}$$

Connection quantum mechanics $\leftrightarrow$ DFT

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Hohenberg-Kohn-Theorem (1964) There exists a universal (i.e., molecule-independent) functional F^{HK} of the single-particle density ρ such that for any potential v_R, the exact QM ground state en. satisfies

$$E_0 = \min_{\rho} \Big(F^{HK}[\rho] + N \int_{\mathbb{R}^3} v_R(x)\rho(x)\, dx \Big),$$

where the min is over $\rho : \mathbb{R}^3 \to \mathbb{R}$, $\rho \geq 0$, $\int \rho = 1$.

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Proof 1. The non-universal part of the energy only depends on ρ_Ψ:

$$\langle \Psi, \sum_i v(x_i)\Psi \rangle = \int \sum_i v(x_i)|\Psi(x_1, .., x_N)|^2 = N \int_{\mathbb{R}^3} v(x)\, \rho_\Psi(x)\, dx.$$

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2. Partition the min over Ψ into a double min, first over Ψ subject to fixed ρ, then over ρ: letting $H_{e\ell}^{univ} := -\frac{\hbar^2}{2}\Delta + \sum_{i<j} \frac{1}{|x_i - x_j|}$,

$$\begin{aligned} E_0 &= \inf_\Psi \Big(\langle \Psi, H_{e\ell}^{univ} \Psi \rangle + N \int v(r)\, \rho_\Psi(r)\, dr \Big) \\ &= \inf_\rho \underbrace{\inf_{\Psi \mapsto \rho} \Big(\langle \Psi, H_{e\ell}^{univ} \Psi \rangle \Big)}_{=: F^{HK}[\rho]} + N \int v(r)\, \rho(r)\, dr. \end{aligned}$$

Existence of a universal map $\rho \to \rho_2$

Corollary of the HK theorem There exists a universal (i.e., molecule-independent) map from single-particle densities $\rho(x_1)$ to pair densities $\rho_2(x_1, x_2)$ which gives the exact pair density of any N-electron molecular ground state $\Psi(x_1, .., x_N)$ in terms of its single-particle density.

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$\rho_2 :=$ pair density of minimizer, i.e.
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Analogously, $\rho_k(x_1, .., x_k) := \int |\Psi_*(x_1, .., x_k, .., x_N)|^2 dx_{k+1}..dx_N$
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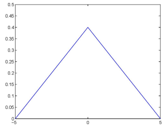
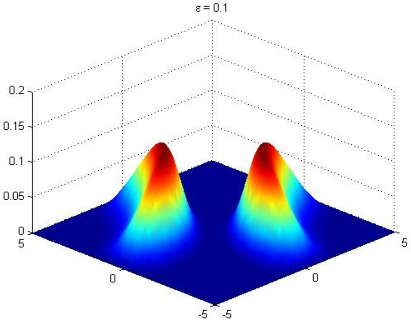
ρ_2 may be nonunique since GS may be degenerate

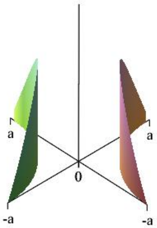
Map highly nontrivial and not comp'ly feasible – still uses high-dim. wavefunctions.

Design comp'ly feasible DFT's $\approx$ approximate the map

Connection DFT $\longleftrightarrow$ OT (simulation)







Left: simulation of the universal map $\rho \to \rho_2$. Right: optimal transport prediction.

Connection DFT $\longleftrightarrow$ OT (theory)

In the semiclassical limit, exact DFT reduces to an OT problem.

Theorem (Cotar/GF/Klüppelberg, CPAM 2013)

$$F^{HK}[\rho] = \min_{\Psi\in H^1,\,\Psi\mapsto\rho} \left(\langle \Psi, (-\frac{\hbar^2}{2}\Delta + \sum_{i<j} \frac{1}{|x_i - x_j|})\Psi\rangle_{L^2} \right)$$

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where $\mathcal{P}_N$ is the set of symmetric probability measures on $\mathbb{R}^{3N}$.

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- Difficulty (regularity issue): Any Ψ with $|\Psi|^2 = \gamma$=optimal plan of OT pb. has $\Psi \not\in H^1$, $\Psi \not\in L^2$, $T[\Psi] = +\infty$, and hence cannot be used as trial state in var. principle for F^{HK}. Smoothing the optimal OT plan doesn't work either, since this destroys the marginal constraint.

Way out: new smoothing technique which preserves marginals

Given: arbitrary (nonsmooth) transport plan γ with smooth marginals ρ_A

Goal: smooth transport plan $\tilde{\gamma}$ close to γ, with same marginals

- Smoothen γ. Note: this modifies the marginals.
- Make it "strongly positive" (i.e. bigger or equal a positive constant times the tensor product of its marginals), by mixing in a small amount of the tensor product plan.
- Re-instate the marginal constraint (see next slide)

Re-instating the marginal constraint

Given: two measures ρ_A and ρ_B in $L^1(\mathbb{R}^d)$, a transport plan $\gamma_{A\to A}$ with $\sqrt{\gamma} \in W^{1,2}(\mathbb{R}^{2d})$.

Goal: transport plan $\gamma_{B\to B}$ which is "close" to $\gamma_{A\to A}$ if ρ_B is close to ρ_A, and also has $\sqrt{\gamma} \in W^{1,2}$. Available regularity on opt. maps far too weak to achieve this. Use a hybrid map/plan.

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First, define a suitable plan $\gamma_{A\to B}$: Let $f(x) := \min\{\rho_A(x), \rho_B(x)\}$, $f_A := (\rho_A - f)_+$, $f_B = (\rho_B - f)_+$. Do nothing on f, and move f_A to f_B via the tensor product plan.

Let $\gamma_{B\to A}$ be the corresponding reverse plan.

Now compose: first transport B to A, then A to A, then A back to B.

$$\gamma_{B\to B}(x,\omega) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \gamma_{B\to A}(x,y)\,\frac{\chi_{\rho_A>0}(y)}{\rho_A(y)}\,\gamma_{A\to A}(y,z)\frac{\chi_{\rho_A>0}(z)}{\rho_A(z)}\,\gamma_{A\to B}(z,\omega)\,dy\,d$$

Qualitative theory, N=2

Minimize $\int_{\mathbb{R}^6} \frac{1}{|x-y|} d\gamma(x,y)$ subject to: γ has equal marginals ρ.

Theorem (Cotar/GF/Klueppelberg, arXiv 2011/CPAM 2013) For $\rho \in \mathcal{P}(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$,

- unique minimizer γ
- Minimizer of 'Monge form', $\gamma(x,y) = \mu(x)\delta_{T(x)}(y)$ for some map $T : \mathbb{R}^d \to \mathbb{R}^d$
- $T(x) = x + \frac{\nabla v(x)}{|\nabla v(x)|^{3/2}}$ for some potential $v : \mathbb{R}^3 \to \mathbb{R}$

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Similar statements on physical grounds in Seidl 99, Seidl/Gori-Giorgi/Savin 07
Similar rigorous results: Buttazzo/Gori-Giorgi/DePascale 12

Why $T(x) = x + \frac{\nabla v(x)}{|\nabla v(x)|^{3/2}}$?

Optimal transport answer: Generalize $1/|x-y| \longrightarrow$
$c(x,y) = \ell(x-y) = k(|x-y|)$

$\ell^* :=$ generalized Legendre transform of ℓ
– Extend k to all of $\mathbb{R}$ via $k(r) := +\infty$ if $r < 0$
– k^* ordinary Leg.trf. of k, i.e. $k^*(p) := \sup_p (p \cdot r - k(r))$
– $\ell^*(z) := k^*(-|z|)$

Gangbo-McCann theory for opt.map: $T(x) = x - \nabla \ell^*(\nabla v(x))$

Check that theory (originally for convex costs) generalizes to Coulomb; advice by Robert McCann gratefully acknowledged

Explicit computation: $\ell(x-y) = 1/|x-y| \Longrightarrow \ell^*(z) = -2\sqrt{|z|}$

Physics answer: (Seidl 1999)

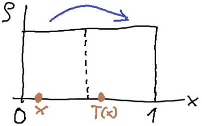
$\nabla v(x)$=Coulomb force on electron at x by electron at $T(x)$,
i.e. $\nabla v(x) = \frac{T(x)-x}{|T(x)-x|^3}$.

Exact solution, 2 particles in 1D

Special case of results in Cotar, GF, Klüppelberg, CPAM

ρ=uniform measure on [0,1]

$\gamma_{opt}(x, y) = \rho(x)\delta_{T(x)}(y)$



T rigidly switches right and left half of [0,1],

$T(x) = x + 1/2$ for $x < 1/2$, $x - 1/2$ for $x > 1/2$

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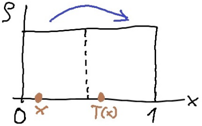

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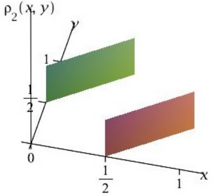

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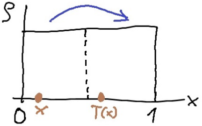

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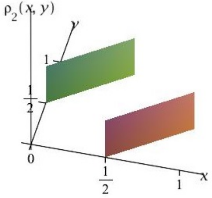
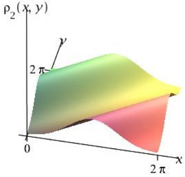
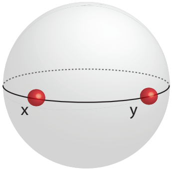


Generalization to N particles in 1D: Colombo, DePascale, DiMarino

Physical realization

Beryllium atom, angular pair density





Accurate numerics (many DOF's, no insight in mechanism)

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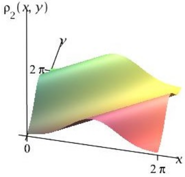

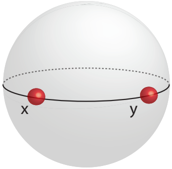

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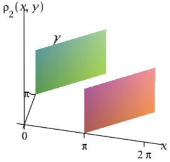
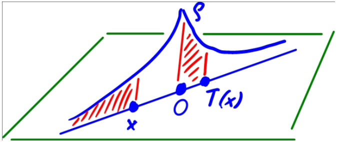


Optimal transport
Position of maxima of pair density ($x - y = \pi$) correctly captured

Exact solution, 2 particles in 3D, radial density

$\gamma_{opt}(x,y) = \rho(x)\delta_{T(x)}(y)$



Optimal map T determined by:

$\frac{T(x)}{|T(x)|} = -\frac{x}{|x|}$ (opposite direction)

$4\pi \int_{-\infty}^{-|x|} r^2 \rho(r) dr = 4\pi \int_0^{|T(x)|} r^2 \rho(r) dr$ (mass balancing).

Pf of this: 1. Coulomb cost $c(|x-y|) = 1/|x-y|$ convex, decreasing in the distance.

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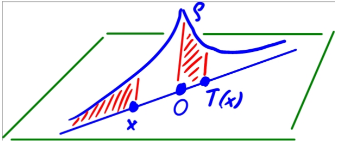

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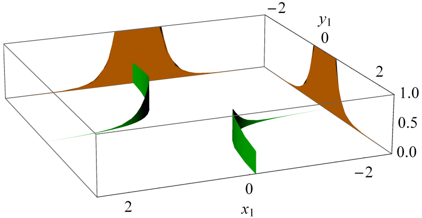

Open: 'Monge solutions' [alias sparsity] for N>2?

Recall: semiclassical limit of HK functional for N particles has form

$$\min\{\int \sum_{i<j} c(x_i, x_j)\, d\gamma \,|\, \gamma \mapsto \rho,\ \gamma \text{ symm. prob.meas.on } \mathbb{R}^{3N}\}$$

Curse of dimension (just like original Schrödinger eq.)

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I.e., only need $N-1$ maps $T_i : \mathbb{R}^3 \to \mathbb{R}^3$ instead of 1 fctn on $\mathbb{R}^{3N}$

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Open: Coulomb cost $c(x,y) = 1/|x-y|$ (Pass: ex. with 4D supp.)

Large N

Optimal transport with infinitely many particles

Theorem (Cotar, GF, Pass, arXiv 2013) a) For pair interactions

$$V_{ee}^N = \binom{N}{2}^{-1} \sum_{1 \le i < j \le N} c(x_i, x_j)$$

with a potential $c(x_1, x_2) = \ell(x_1 - x_2)$ with positive Fourier transform, and any given one-body density ρ with $\int \rho = 1$, the infinite-body energy

$$\lim_{N\to\infty} \int_{(\mathbb{R}^3)^\infty} V_{ee}^N(x_1, .., x_N) d\gamma(x_1, x_2, ...) = \int_{(\mathbb{R}^3)^\infty} c(x_1, x_2) d\gamma(x_1, x_2, ...)$$

is minimized over symmetric probability measures γ in infinitely many variables with $\gamma \mapsto \rho$ if and only if

$$\gamma(x_1, x_2, x_3, ...) = \rho(x_1)\rho(x_2)\rho(x_3)\cdots$$

(independent product measure).

b) The optimal cost per particle pair of the N-body OT problem, $\inf_{\gamma_N \mapsto \rho} \int V_{ee}^N d\gamma_N$, tends to the mean field cost $\int c(x,y)\rho(x)\,\rho(y)\,dx\,dy (= \inf_{\gamma \mapsto \rho} C_\infty[\gamma])$ as $N \to \infty$.

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Infinite-body minimizer not of 'Monge' form.

Open: thermodynamic (O(N)) correction. Note total N-body cost $O(N^2)$

Intuition, 1: reformulation via representability

GF, Mendl, Pass, Cotar, Klüppelberg, arXiv 2013/to appear in J.Chem.Phys.

Recall 1-body and 2-body marginals:

$$\begin{aligned} p_1(x_1) &= \int_{\mathbb{R}^{3(N-1)}} p_N(x_1,..,x_N)dx_2..dx_N \\ p_2(x_1,x_2) &= \int_{\mathbb{R}^{3(N-2)}} p_N(x_1,..,x_N)dx_3..dx_N \end{aligned}$$

Notation: $p_N \mapsto p_1$, $p_N \mapsto p_2$, etc.

Def. A probability measure p_2 on $\mathbb{R}^6$ is said to be *N*-density-representable, $N \geq 2$, if there exists a symmetric probability measure p_N on $\mathbb{R}^{3N}$ such that $p_N \mapsto p_2$, and infinite-density-representable if there exists a symm. p_∞ on $(\mathbb{R}^3)^\infty$ s.th. $p_\infty \mapsto p_2$.

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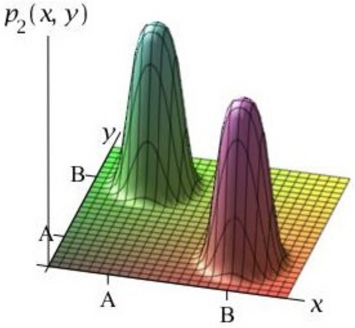
– highly nontrivial restriction
– precise characterization deep open question
– some nec.cdns were derived by physicists (Davidson, Ayers) and probabilists (under the name 'exchangeable sequences of random variables', Aldous) which to this day are unaware of each other

Example of a pair density which is not 3-representable



Violates the necessary condition of GF et al that for any partition of $\mathbb{R}^3$ into two subsets $\mathcal{A}$ and $\mathcal{B}$,

$$\int_{\mathcal{A}\times\mathcal{B}} p_2 + \int_{\mathcal{B}\times\mathcal{A}} p_2 \leq 2(\int_{\mathcal{A}\times\mathcal{A}} p_2 + \int_{\mathcal{B}\times\mathcal{B}} p_2)$$

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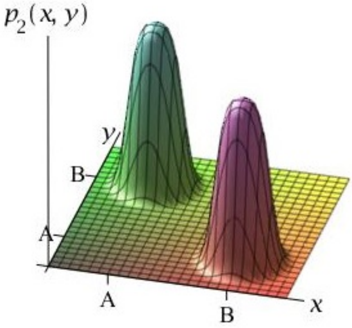

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Physically: weight of 'neutral' configurations can at most be twice as big as weight of 'ionic' configurations.

Reformulation of N-body and infinite-body OT

For any given single-particle density ρ, and any cost of two-body form $V_{ee}^N = \binom{N}{2}^{-1} \sum_{1\leq i<j\leq N} c(x_i, x_j)$ with c symmetric,

$$\min_{\gamma_N \mapsto \rho} \int_{\mathbb{R}^{3N}} V_{ee}^N d\gamma_N = \min_{\substack{\rho_2 \mapsto \rho \\ \rho_2 \ N\text{-density-rep.}}} \binom{N}{2} \int_{\mathbb{R}^6} c \, d\rho_2,$$

$$\min_{\gamma_\infty \mapsto \rho} \lim_{N\to\infty} \int_{(\mathbb{R}^3)^\infty} V_{ee}^N d\gamma = \min_{\substack{\rho_2 \mapsto \rho \\ \rho_2 \ \infty\text{-density-rep.}}} \int_{\mathbb{R}^6} c \, d\rho_2.$$

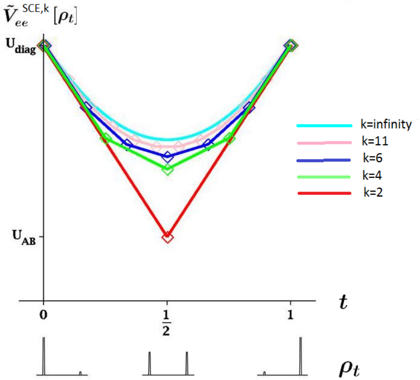
Optimal cost per particle pair as fctn of particle no.

Two-state toy model: F., Mendl, Cotar, Klüppelberg, Pass, JCP, in press

$$\tilde{V}_{ee}^{SCE,k}[\rho] := \min_{p_2 \text{ k-rep.}, p_2 \mapsto \rho} \int c(x,y)dp_2(x,y)$$

$$c(A,A) = c(B,B) = U_{diag} > c(A,B) = c(B,A) = U_{AB}$$

$$\rho = (1-t)\delta_A + t\delta_B$$



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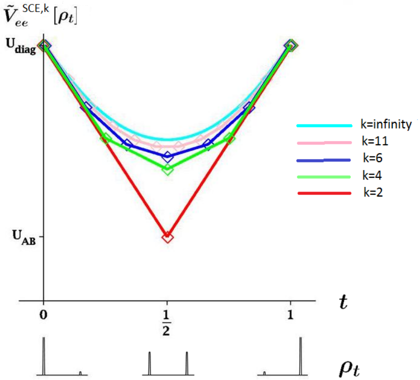
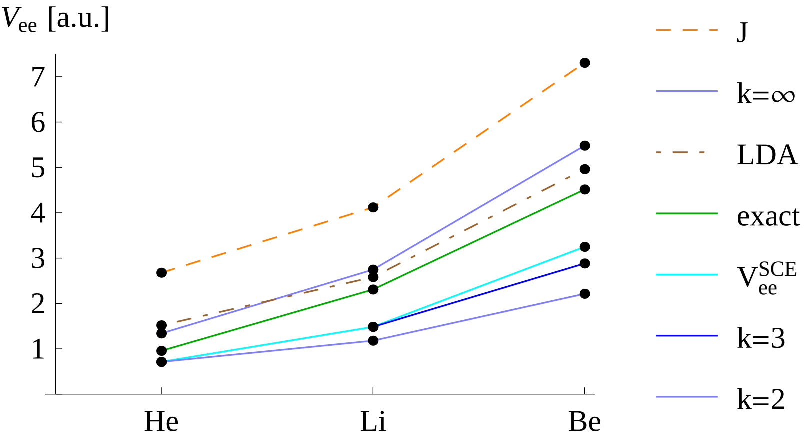


Fact: $\lim_{k\to\infty} \tilde{V}_{ee}^{SCE,k}[\rho] = \int c(x,y)\rho(x)\rho(y)\, dx\, dy$ mean field en. (!)

Comparison of OT cost to true quantum interaction energy

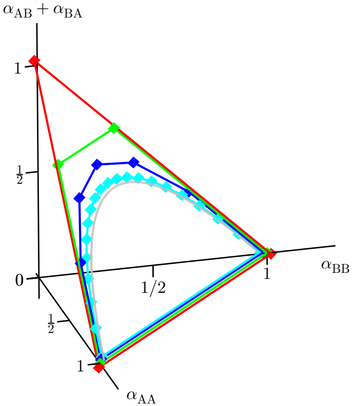
Ab-initio-densities of atoms: F., Mendl, Cotar, Klüppelberg, Pass, to appear, JCP



Infinite-dimensional geometric intuition

$\lim_{k\to\infty}$ (k-repr.ρ_2's) = convex hull of mean field measures $\rho_1 \otimes \rho_1$

2-site system: $\rho_2 = \alpha_{AA}\delta_{AA} + \alpha_{AB}\delta_{AB} + \alpha_{BA}\delta_{BA} + \alpha_{BB}\delta_{BB}$



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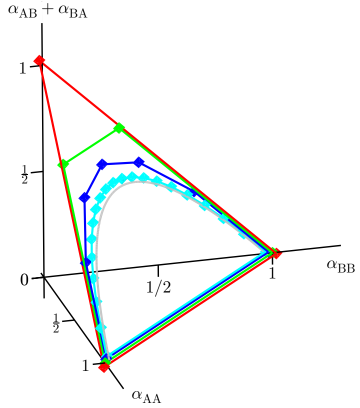
2-site system: $\rho_2 = \alpha_{AA}\delta_{AA} + \alpha_{AB}\delta_{AB} + \alpha_{BA}\delta_{BA} + \alpha_{BB}\delta_{BB}$



General: de Finetti's thm $\gamma_\infty(x_1, .., x_N, ..) = \int_{\mathcal{P}(\mathbb{R}^3)} \prod_{i=1}^{\infty} \rho_1(x_i) d\nu(\rho_1)$

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Answer, general case: novel probabilistic interpretation of infinite-body OT functional

If γ infinitely rep'ble, then by de Finetti,

$$\gamma = \int_{\mathcal{P}(\mathbb{R}^d)} Q^{\otimes\infty} d\nu(Q)$$

for some ν, and (when $\gamma \mapsto \rho$)

$$C_\infty[\gamma] = \int_{\mathbb{R}^{2d}} \ell(x-y)\, d\rho(x)\, d\rho(y) + \int_{\mathbb{R}^d} \hat{\ell}(z) \mathrm{var}_{\nu(dQ)} \hat{Q}(z) dz.$$

Variance term: $\mathrm{var}_{\nu(dQ)} \hat{Q}(z) = \int_{P(\mathbb{R}^d)} |\hat{Q}(z)|^2 d\nu(Q) - \left| \int_{P(\mathbb{R}^d)} Re(\hat{Q}(z)) d\nu(Q) \right|^2$

Minimized if and only if $\nu = \delta_\rho$

Summary

In the semiclassical limit, many-body quantum correlations reduce to (still nontrivial, strongly correlated) multivariate distributions governed by optimal transport problems.

For a large no. of particles, surprisingly, mean field/independent distributions emerge.

Open: efficient description after 'un-doing' the semiclassical limit.

http://www-m7.ma.tum.de