Constrained Search in Imaginary Time

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Aim of the Method

Find

$$\inf_{\Psi} \langle \hat{A} \rangle_{\Psi}$$

under constraints

$$\begin{aligned} \|\Psi\| &= 1, \\ \langle \hat{B}_i \rangle_{\Psi} &= b_i \in \mathbb{R}, \qquad i = 1, 2, \ldots, M \end{aligned}$$

Part 1: Generalized Discrete Functional Theory

General Assumptions

$\mathcal{H}$ ... finite-dimensional Hilbert space
$\hat{A}, \hat{B}_0 = \mathbb{1}, \hat{B}_1, \ldots, \hat{B}_M$ ... self-adjoint operators
(= Hermitian matrices), all linearly independent
$\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_M) \in \mathbb{R}^M$ ... external "potential", coupled to $\hat{B}_i$
$\boldsymbol{b} = (b_0 = 1, b_1, \ldots, b_M) \in \mathbb{R}^M$ ... "density" constraints,
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static setting:

$$\hat{H}(\boldsymbol{\beta}) = \hat{A} + \sum_{i=1}^{M} \beta_i \hat{B}_i$$

"N"-Representability of $\boldsymbol{b}$?

$$\mu(\Psi) := (\langle \mathbb{1} \rangle_\Psi, \langle \hat{B}_1 \rangle_\Psi, \ldots, \langle \hat{B}_M \rangle_\Psi) \stackrel{?}{=} \boldsymbol{b} \in \mathbb{R}^{M+1}$$

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If also all $\hat{B}_i$ <u>commute</u>, $\exists$ orthonormal basis $\{\Phi_k\}$ of $\mathcal{H}$ in which they are all simultaneously diagonal,

$$\hat{B}_i \Phi_k = \Lambda_{ik} \Phi_k \quad \text{and} \quad \mu(\Phi_k) = (\Lambda_{0k}, \Lambda_{1k}, \dots, \Lambda_{Mk}).$$

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$$\mu(\Psi) = \sum_k \lambda_k \mu(\Phi_k), \quad \lambda_k \geq 0, \sum_k \lambda_k = 1$$

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Proposition

Let $\mathcal{B}$ be the convex hull of $\{\mu(\Phi_k)\}$. For every $\boldsymbol{b} \in \mathcal{B}$ there is a $\Psi \in \mathcal{H}$ such that $\mu(\Psi) = \boldsymbol{b}$. (Just take $c_k = \sqrt{\lambda_k}$ above.)

"v"-Representability of $\boldsymbol{b}$?

$$E(\boldsymbol{\beta}) := \inf_{\Psi}\{\langle \hat{H}(\boldsymbol{\beta})\rangle_\Psi \mid \|\Psi\| = 1\}$$

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$$\tilde{F}(\boldsymbol{b}) := \begin{cases} \inf_\Psi\{\langle \hat{A}\rangle_\Psi \mid \mu(\Psi) = \boldsymbol{b}\} \leq \|\hat{A}\| & \text{if } \boldsymbol{b} \in \mathcal{B} \\ \infty & \text{else} \end{cases}$$

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But this means that F is convex and finite on $\mathcal{B}$
$\Rightarrow \underline{\partial}F(\boldsymbol{\beta}) \neq \emptyset$ if $\boldsymbol{b} \in \operatorname{int}\mathcal{B}$ and F even <u>differentiable</u> almost everywhere.

Hohenberg–Kohn Theorem

Definition

A $\boldsymbol{b} \in \mathcal{B}$ is called <u>regular</u> if for all $\Psi \in \mathcal{H}$ with $\mu(\Psi) = \boldsymbol{b}$ the $\hat{B}_i \Psi$ are linearly independent ($i = 0, \ldots, M$).

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Proof: For fixed $\boldsymbol{b}$ and $\boldsymbol{\beta}, \boldsymbol{\beta}'$ the ground-state energies are $E(\boldsymbol{\beta}^{(\prime)}) = \inf_{\Psi \mapsto \boldsymbol{b}} \{\langle \hat{A} \rangle_\Psi\} + \boldsymbol{\beta}^{(\prime)} \cdot \boldsymbol{b}$. Since the 'inf' is independent of $\boldsymbol{\beta}^{(\prime)}$, we can take the same Ψ for both Hamiltonians. Subtracting both Schrödinger equations $\hat{H}(\boldsymbol{\beta}^{(\prime)})\Psi = E(\boldsymbol{\beta}^{(\prime)})\Psi$ gives

$$\sum_{i=1}^{M} (\beta_i - \beta_i') \hat{B}_i \Psi = (\overbrace{E(\boldsymbol{\beta})}^{-\beta_0} - \overbrace{E(\boldsymbol{\beta}')}^{-\beta_0'})\Psi \Rightarrow \sum_{i=0}^{M} (\beta_i - \beta_i') \hat{B}_i \Psi = 0.$$

Since all $\hat{B}_i \Psi$ are linearly independent, it follows $\beta_i = \beta_i'$.

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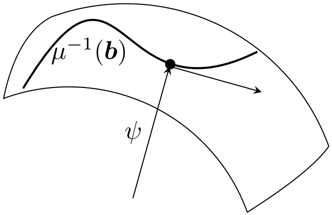

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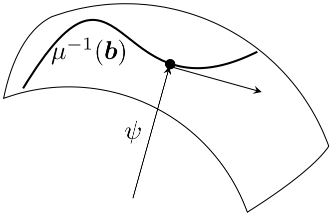

Theorem

The set of critical $(b_1, \ldots, b_M)$ *have measure zero in* $\mathbb{R}^M$*.*

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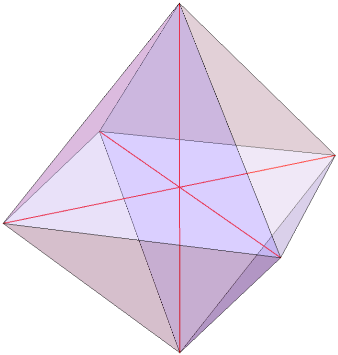
Example: $N = 2$ fermionic particles on $M = 4$ sites. 6-dim $\mathcal{H}$ and $\{\Psi, \hat{\rho}_1 \Psi, \hat{\rho}_2 \Psi, \hat{\rho}_3 \Psi\}$ (or $\{\hat{\rho}_1 \Psi, \hat{\rho}_2 \Psi, \hat{\rho}_3 \Psi, \hat{\rho}_4 \Psi\}$) linear independent.



critical:

- 6 corners
- 15 lines between 2 corners
- 11 planes between 3 corners

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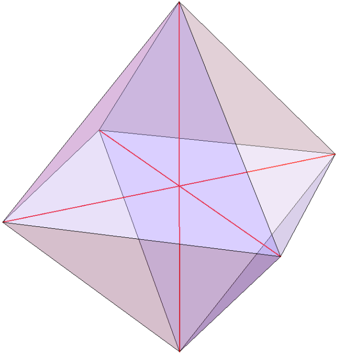

critical:
all possible HK counterexamples (ground-state densities from multiple potentials (v_1, v_2, v_3) while $v_4 = 0$)

Constraint Manifold Patches

For $\boldsymbol{b}$ regular $\mu^{-1}(\boldsymbol{b}) \subset \mathcal{H}$ is a closed manifold, but does not need to be connected.

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Example: 6-dim $\mathcal{H}$ from before, $\Psi = \sum_k c_k \Phi_k$ with fixed density, $\rho_1 = |c_1|^2 + |c_2|^2 + |c_3|^2$, $\rho_2 = |c_1|^2 + |c_4|^2 + |c_5|^2$ etc.

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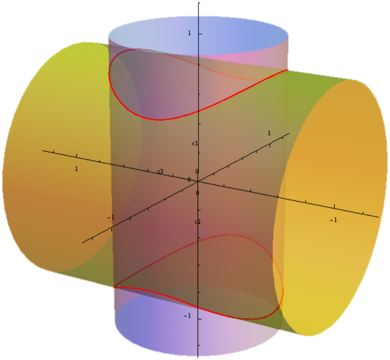

Wrap-up

What we have:

- Representability sets for $\boldsymbol{b}$.
- Hohenberg–Kohn (almost everywhere) if $\boldsymbol{b}$ is from a pure ground state.
- Geometric picture.

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What we don't have:

- Hohenberg–Kohn for $\boldsymbol{b}$ from mixed ground states.
- $\mathcal{B}$ for non-commuting matrices $\hat{B}_i$.
- Infinite dimensional setting.

Part 2: Imaginary Time Evolution

Autonomous Evolution

$$\hat{H} = \hat{A} + \sum_{i=1}^{M} \beta_i \hat{B}_i \qquad \text{(time-independent)}$$

Now, let $\{\phi_k\}$ be an orthonormal eigenbasis of $\hat{H}(\boldsymbol{\beta})$ with ordered eigenvalues $E_0 = 0 < E_1 \leq E_2 \leq \ldots$, and

$$\Psi_0 = \sum_{k=1}^{\infty} c_k \phi_k.$$

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Then the autonomous evolution equation (Schrödinger equation in imaginary time $t = \mathrm{i}\tau$)

$$-\partial_\tau \Psi(\tau) = \hat{H}\Psi(\tau)$$

with initial state Ψ_0 for $\tau > 0$ is solved by

$$\Psi(\tau) = \mathrm{e}^{-\tau\hat{H}}\Psi_0 = \mathrm{e}^{-\tau\hat{H}} \sum_{k=0}^{\infty} c_k \phi_k = \sum_{k=0}^{\infty} \mathrm{e}^{-\tau E_k} c_k \phi_k.$$

Ground-state Convergence

In the limit $\tau \to \infty$ this means ($E_0 = 0$, $E_k > 0$ for $k = 1, 2, \ldots$)

$$\Psi(\tau) = \sum_{k=0}^{\infty} \mathrm{e}^{-\tau E_k} c_k \phi_k = c_0 \phi_0 + \sum_{k=1}^{\infty} \mathrm{e}^{-\tau E_k} c_k \phi_k \longrightarrow c_0 \phi_0.$$

$\Rightarrow$ method for finding the ground state
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The restriction $E_0 = 0$ can easily be lifted by sporadically renormalizing $\Psi(\tau)$ to 1 <u>or</u> by including a chemical potential of strength $\beta_0 = -E_0$.

Non-autonomous Evolution

Idea: Choose $\beta_i(\tau)$, $i = 0, 1, \ldots, M$, such that all constraints ($\|\Psi\| = 1, \langle \hat{B}_i \rangle_\Psi = b_i$) are always fulfilled and perform imaginary-time evolution

$$-\partial_\tau \Psi(\tau) = \hat{G}(\tau)\Psi(\tau)$$

with generator

$$\hat{G}(\tau) = \hat{H}(\tau) + \beta_0(\tau)\mathbb{1}, \quad \hat{H}(\tau) = \hat{A} + \sum_{i=1}^{M} \beta_i(\tau)\hat{B}_i.$$

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Determine $\boldsymbol{\beta}(\tau)$ from

$$\partial_\tau \langle \hat{B}_i \rangle_{\Psi(\tau)} = 0.$$

$\boldsymbol{b}$ condition $\to$ $\boldsymbol{\beta}$ condition

$$\begin{aligned}
\partial_\tau \langle \hat{B}_i \rangle_\Psi &= \partial_\tau \langle \Psi, \hat{B}_i \Psi \rangle \\
&= -\langle \Psi, \hat{G}\hat{B}_i \Psi \rangle - \langle \Psi, \hat{B}_i \hat{G} \Psi \rangle = -\langle \{\hat{G}, \hat{B}_i\} \rangle_\Psi \\
&= -\langle \{\hat{A}, \hat{B}_i\} \rangle_\Psi - \sum_{j=0}^{M} \beta_j \langle \{\hat{B}_j, \hat{B}_i\} \rangle_\Psi \\
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Note: In real-time evolution the 1[st] derivative gives the continuity equation and no access to $\boldsymbol{\beta}$.

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$\boldsymbol{B}$ is the Gram matrix of vectors $\hat{B}_i \Psi$ and positive definite ($\leftrightarrow$ invertible) if the vectors are linearly independent ($\leftrightarrow$ regular).

Asymptotic Evolution

Observe

$$
\begin{aligned}
\partial_\tau \langle \hat{H} \rangle_\Psi &= -\langle \{\hat{G}, \hat{H}\} \rangle_\Psi + \langle \partial_\tau \hat{H} \rangle_\Psi \\
&= -2\langle \hat{H}^2 \rangle_\Psi + 2\langle \hat{H} \rangle_\Psi^2 + \sum_{i=1}^{M} \langle \partial_\tau (\beta_i \hat{B}_i) \rangle_\Psi \\
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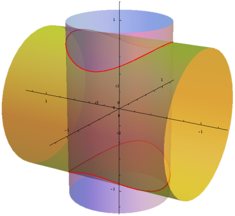
\end{aligned}
$$

so $\langle \hat{A} \rangle_{\Psi(\tau)} \searrow 0$ and stops in an eigenstate of $\hat{H}(\boldsymbol{\beta})$.

Process Getting Stuck

The evolution gets stuck...

- On the wrong constraint manifold patch (since it is continuous).



- If steered into an eigenstate of $\hat{H}(\boldsymbol{\beta})$ that is not the ground state.

Restarting the Process

In basis $\{\Phi_k\}$ that diagonalizes $\hat{B}_i$:

$$\Psi = \sum_k c_k \Phi_k \Rightarrow b_i = \langle \hat{B}_i \rangle_\Psi = \sum_{kl} c_k^* c_l \langle \Phi_k, \hat{B}_i \Phi_l \rangle$$
$$= \sum_{kl} c_k^* c_l \Lambda_{il} \langle \Phi_k, \Phi_l \rangle = \sum_k |c_k|^2 \Lambda_{ik}$$

so sign/phase of c_k can be changed freely without affecting the constraint $\boldsymbol{b}$.

Restarting the Process

In basis $\{\Phi_k\}$ that diagonalizes $\hat{B}_i$:

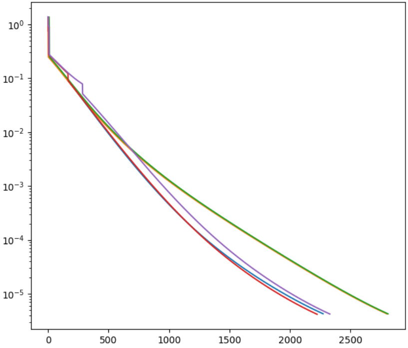
$$\begin{aligned}\Psi = \sum_k c_k \Phi_k \Rightarrow b_i = \langle \hat{B}_i \rangle_\Psi &= \sum_{kl} c_k^* c_l \langle \Phi_k, \hat{B}_i \Phi_l \rangle \\ &= \sum_{kl} c_k^* c_l \Lambda_{il} \langle \Phi_k, \Phi_l \rangle = \sum_k |c_k|^2 \Lambda_{ik}\end{aligned}$$

so sign/phase of c_k can be changed freely without affecting the constraint $\boldsymbol{b}$.

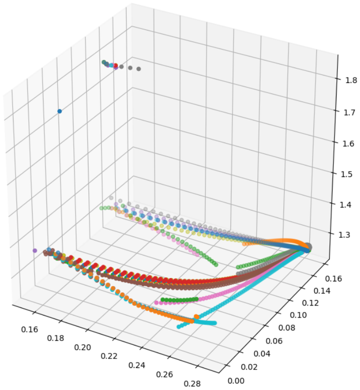
If process gets stuck $\Rightarrow$ restart in Ψ' with randomized phases that has $\langle \hat{A} \rangle_{\Psi'} \leq \langle \hat{A} \rangle_\Psi$.

Numerical Runs

Lattice with $M = 7$ sites and $N = 2$ particles: $v \mapsto \rho$ used as constraint



$\langle \hat{A} \rangle_{\Psi(\tau)}$



$x = \left| \sum_{i \in I_x} c_i \right|, y = \ldots, z = \ldots$
with c_i coefficients w.r.t. lattice basis

Summary of the Method

Find $\inf_\Psi \langle \hat{A} \rangle_\Psi$ under constraints

$$\|\Psi\| = 1,$$
$$\langle \hat{B}_i \rangle_\Psi = b_i \in \mathbb{R}, \qquad i = 1, 2, \ldots, M$$

by doing imaginary-time steps with the evolution equation

$$-\partial_\tau \Psi(\tau) = \hat{G}(\tau)\Psi(\tau)$$

with generator

$$\hat{G}(\tau) = \hat{H}(\tau) + \beta_0(\tau)\mathbb{1}, \quad \hat{H}(\tau) = \hat{A} + \sum_{i=1}^{M} \beta_i(\tau)\hat{B}_i.$$

and $\beta_i(\tau)$ determined (with an implicit time stepping) from $\langle\{\hat{A}, \hat{B}_i\}\rangle$ and $\langle\{\hat{B}_j, \hat{B}_i\}\rangle$.

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- Never needs diagonalization of operators on $\mathcal{H}$, only continued application of the operators. The equation to get $\boldsymbol{\beta}(\tau)$ can be of much lower dimension ($M+1$).
- Converges slowly; includes random element to escape if getting stuck.