Orthogonalization of Fermion k-Body Operators and Representability

Joint work with V. Bach (arXiv:1807.05299)

R. Rauch, Montréal, July 21, 2018

Section 1

Motivation: The Representability Problem

Quantum Systems in Theoretical Chemistry

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  - **Hamiltonian:** a *2-body operator* $\mathbb{H} = \mathbb{H}^* = \bigoplus_{N \geqslant 0} \mathbb{H}_N$, e.g.

$$\mathbb{H}_N = \underbrace{\sum_{i=1}^{N} \left(-\Delta_i - \sum_{j=1}^{K} \frac{Z_j}{|x_i - R_j|} \right)}_{\text{1-particle “free part”}} + \underbrace{\sum_{1 \leqslant i < j \leqslant N} \frac{1}{|x_i - x_j|}}_{\text{2-particle “interaction part”}} . \tag{2}$$

Computing the Ground State Energy

Key Problem: Compute the ground state energy

$$E_0 = \inf_{\rho \in \mathcal{DM}} \operatorname{tr}\{\rho \mathbb{H}\}, \quad \mathcal{DM} \doteq \{\text{density matrices on } \mathcal{F}\}. \tag{3}$$

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- **More generally:** practically all physical relevant information can be obtained by 2-body expectation values.

Reducing Density Matrices

Idea: Replace density matrix $\rho \in \mathcal{B}(\mathcal{F})'$ by its 2-*body reduction*

$$R_2(\rho) \doteq \rho|_{\mathcal{O}_2(\mathcal{F})} \in \mathcal{O}_2(\mathcal{F})'. \tag{4}$$

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- **Drawback:** We need an efficient way of varying over $R_2(\mathcal{DM})$.

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Representability Problem (for $R_2(\mathcal{DM})$)

Find a *computationally efficient* characterization of $R_2(\mathcal{DM})$:

$$\textit{Given } r \in \mathcal{O}_2(\mathcal{F})', \textit{ is there } \rho \in \mathcal{DM} \textit{ with } r = R_2(\rho)?$$

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- **Generalization:** $\mathcal{DM} \rightsquigarrow \mathcal{S} \subseteq \mathcal{B}(\mathcal{F})'$ and $k = 2 \rightsquigarrow k \in \mathbb{N}_0$: *representability problem for $R_k(\mathcal{S})$*.

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- **Representability conditions** (i.e. necessary conditions for representability) yield lower bounds on E_0.

Geometric Interpretation

Note: If $\dim \mathfrak{h} < \infty$, then $R_k : \mathcal{B}(\mathcal{F})' \to \mathcal{O}_k(\mathcal{F})'$ can be interpreted as the *orthogonal projection*

$$\pi_k : \mathcal{L}^2(\mathcal{F}) \to \mathcal{O}_k(\mathcal{F}) \subseteq \mathcal{L}^2(\mathcal{F}). \tag{6}$$

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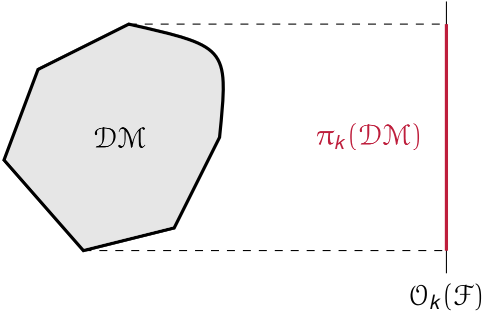

Some History of Representability Methods

- **1940:** Idea to replace $\mathcal{DM}$ by $R_2(\mathcal{DM})$ (Husimi)
- **1950/60s:** First systematic analysis (Coleman, Coulson, Garrod, Percus, Löwdin, Yang)
  - GPQ-conditions lead to inaccurate lower bounds
  - solved Representability Problem for $R_1(\mathcal{SD}_N)$
- **1978:** T_1- and T_2-conditions (Erdahl)
- **2005:** Representability of $R_1(\mathcal{P}_N)$ solved (Klyachko)
- **2006:** Highly accurate lower bounds exploiting Erdahls T_1- and T_2-conditions (Cancés, Lewin, Stoltz)
- **2012:** Derivation of HF error estimates from G- and P-condition (Bach, Bretaux, Knörr, Menge)

Section 2

Orthogonalization of *k*-body Operators

Goal of Present Work

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- **Approach:**
  1. Apply Gram-Schmidt orthogonalization in low dimensions
  2. Find and prove a general conjecture

Main Result

Theorem 1 (Bach and Rauch 2018)

Let $\dim \mathfrak{h} \doteq n < \infty$ *and* $\varphi_1, \ldots, \varphi_n$ *an ONB of* $\mathfrak{h}$. *Then an orthogonal basis of* $\mathcal{L}^2(\mathcal{F})$ *is given by*

$$\mathfrak{B} \doteq \left\{ \left(\prod_{k \in K} [c_k, c_k^*] \right) c_I^* c_J \;\middle|\; \begin{array}{c} I, J, K \subseteq \{1, \ldots, n\} \\ \text{mutually disjoint} \end{array} \right\}, \tag{7}$$

where for $I = \{i_1 < \cdots < i_l\} \subseteq \{1, \ldots, n\}$ *we define*

$$c_I^* \doteq c^*(\varphi_{i_1}) \cdots c^*(\varphi_{i_l}), \qquad c_I \doteq (c_I^*)^* = c(\varphi_{i_l}) \cdots c(\varphi_{i_1}). \tag{8}$$

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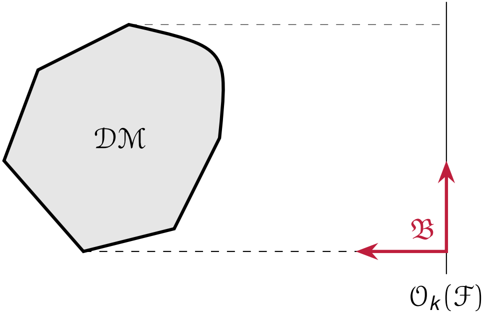
Theorem 2 (Bach and Rauch 2018)

An orthogonal basis of $\mathcal{O}_k(\mathcal{F})$ *is given by* $\mathfrak{B} \cap \mathcal{O}_k(\mathcal{F})$.

Main Result: Geometric Interpretation

- **To Summarize:** We have constructed an ONB $\mathfrak{B}$ of $\mathcal{L}^2(\mathcal{F})$ adapted to the study of representability and related questions.



Current Research

1. Characterize $\pi_k(\mathcal{DM}) \subseteq \mathcal{O}_k(\mathcal{F})$ using the ONB $\mathfrak{B} \cap \mathcal{O}_k(\mathcal{F})$
2. Identify classical representability conditions as boundary conditions
3. Obtain new representability conditions
4. Study action of Bogoliubov transformations on representability conditions

Possible Application

- Consider a 2-body Hamiltonian $\mathbb{H}$, fix an ONB $\varphi_1, \ldots, \varphi_n$ of $\mathfrak{h}$ and write

$$\mathbb{H} = \sum_{i,j} t_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ij;kl} c_i^* c_j^* c_l c_k, \tag{9}$$

- Let $\mathfrak{B}$ be the associated ONB of $\mathcal{L}^2(\mathcal{F})$ as given by Theorem 1
- For $\mathfrak{A} \subseteq \mathfrak{B}$ define $P_{\mathfrak{A}} \doteq \sum_{\theta \in \mathfrak{A}} |\theta\rangle\langle\theta| \leqslant 1_{\mathcal{L}^2(\mathcal{F})}$.
- Then, under suitable positivity requirements on V,

$$\mathbb{H} \geqslant \sum_{i,j} t_{ij} c_i^* c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ij;kl} c_i^* c_j^* P_{\mathfrak{A}} c_l c_k \doteq \mathbb{H}_{\mathfrak{A}}. \tag{10}$$

- **Idea:** by a suitable choice of the orbital basis $\varphi_1, \ldots, \varphi_n$ and $\mathfrak{A} \subseteq \mathfrak{B}$ one obtains nontrivial lower bound $E_0(\mathbb{H}_{\mathfrak{A}})$ of $E_0(\mathbb{H})$.

Section 3

Appendix

k-Body Operators

Definition 3

A *k-body operator* on $\mathcal{F}$ is a $\mathbb{C}$-linear combination of elements of the form

$$c^\sharp(f_1)\cdots c^\sharp(f_{2l}) \qquad f_1,\ldots,f_{2\ell}\in\mathfrak{h} \text{ and } 0\leqslant\ell\leqslant k, \tag{11}$$

with $c^*(f), c(f)\in\mathcal{B}(\mathcal{F})$ the *creation-* and *annihilation operators* on $\mathcal{F}$.

Representability of $R_2(\mathcal{DM}_N)$

Let $\rho \in \mathcal{DM}_N \doteq \{\rho \in \mathcal{DM} \mid \hat{\mathbb{N}}\rho = N\rho\}$. Then $R_2(\rho) \in \mathcal{O}_2(\mathcal{F})'$ is characterized by

$$\gamma_\rho \in \mathcal{B}(\mathfrak{h}), \tag{1-RDM}$$

$$\Gamma_\rho \in \mathcal{B}(\mathfrak{h} \wedge \mathfrak{h}). \tag{2-RDM}$$

- ***N*-Representability Problem**: Given $\gamma \in \mathcal{B}(\mathfrak{h})$ and $\Gamma \in \mathcal{B}(\mathfrak{h} \wedge \mathfrak{h})$, is there $\rho \in \mathcal{DM}$ with $\hat{\mathbb{N}}\rho = N\rho$ such that

$$\gamma = \gamma_\rho \qquad \Gamma = \Gamma_\rho \tag{12}$$

- Examples of ***N*-Representability conditions**:

$$0 \leqslant \gamma_\rho \leqslant 1, \quad \mathrm{tr}\{\gamma_\rho\} = N, \quad \Gamma_\rho \geqslant 0. \tag{13}$$

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