Uniqueness of Pre-images of Quantum Marginals and Convex Structure of Reduced Density Matrices

Mary Beth Ruskai
ruskai@member.ams.org

delocalized

joint with Bei Zeng, Jianxin Chen, Sam Ocko, and many others

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Story of my Life

- 1969 – Phd thesis (quant chem) on N-Rep for 2-body RDM

  Hope: Reduce messy 100-electron calc to simpler 2-elec ones.

  Concluded no free lunch – left to postdoc math physics Geneva

- 1971-72 — postdoc with E. Lieb at MIT

  proved Strong Subadditivity (SSA) of Quantum entropy

  1973 gave talk at IUPAP meeting and session chair asked

  "beautiful theorem, but what use is it?"

- $\approx$ next 20-25 years worked on Schrd̈ingier operators

Story (cont)

- 1997 – sabbatical at Georgia Tech

  started getting e-mail about SSA and equality conditions

  SSA in Preskill's notes and physicists began to care

  started (returned) to work in Quantum InfoTheory (QIT)

- 2006 Klyachko announced solution of pure state 1-rep

  2007 2-body N-rep shown QMA complete

  QIT interest in quantum marginals

  could use QECC to resolve 1972 open question in N-rep

- at age $\approx$ 65-70, returning to womb

Aside on Klyachko and Weyl

- 1912 Weyl raised question:

  given 3 ordered sequences $\{a_k\}, \{b_k\}, \{c_k\}$ when do $\exists$

  matrices $A, B, \geq 0$ and $C = A + B$ such that these are e-vals

- Klyachko solved in 1998

- Horn (195?) diagonal elements majorize e-vals of matrix $A \geq 0$

- Horn (1962) conjectured inequalities to solve Weyl's problem

  BUT Klyachko's inequalities not same as Horn's

- Kuntson and Tao (See Notices of AMS 2001) Honeycombs

  Showed both sets redundant and

  Klyachko and Horn inequalities both prune to same minimal set

Klyachko's contributions to N-rep and QIT

2005 solved pure state N-rep problem for 1-body RDM

based on Schubert calculus + Berenstein-Sjamaar (2000)

Recovers Borland-Dennis (1972) nasc conds for $N = 3, R = 6$

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1, \quad \lambda_1 + \lambda_2 \leq \lambda_3 + 1$$

Klyachko remarked no progress for over 30 years since.

mentioned Ruskai, though not a co-author

didn't know MBR had unpublished alternate proof

reduced to 2×2 version of Weyl's problem

encouraged by Klyachko – wrote and submitted to *J Phys A*

as comment on 1972 paper in *J Phys B*

published as Fast Track Communication (2007) in *J Phys A*

Get Serious: Structure of Talk

- Basic definitions
- Convex Structure – basics

  2-body reduced Hamiltonian
- Pure pre-images of overlapping pair of quantum marginals

  Pure pre-images of complementary pair of quantum marginals
- QECC give extreme points with non-unique pre-images
- Contributions of QIT to N-Rep
- Open Questions

Question:: How to number slides in reverse in beamer??

Defs of RDM and Quantum Marginals

N-body state $|\Psi\rangle\langle\Psi|$ or mixed $\rho_N = \sum_k \lambda_k |\Psi_k\rangle\langle\Psi_k| = \rho_{1,2\ldots N}$

$|\Psi\rangle \in \mathcal{H}_N \subseteq \mathcal{H}^{\otimes N}$ $\quad$ $\mathcal{H}$ is one-body Hilbert space

typical $\mathcal{H}_N$ symmetry restrict, e.g., fermions $\mathcal{H}_N = \mathcal{H}^{\wedge N}$ anti-sym

Def: $\rho_{1,2,\ldots m} = \text{Tr}_{m+1,\ldots N} |\Psi\rangle\langle\Psi|$ or $\text{Tr}_{m+1,\ldots N}\, \rho_{1,2\ldots N}$

more generally $\quad \rho_J = \rho_{j_1,j_2,\ldots j_m} = \text{Tr}_{J^c}\, \rho_N$

$J_m = J = \{j_1, j_2, \ldots j_m\} \qquad J^c = \{k_1, k_2 \ldots k_{N-m}\} : k_i \notin J\}$

called reduced density matrix (RDM) or quantum marginal

$\mathcal{D}(\mathcal{H}_N) =$ set of N-body density matrices $\rho_N \geq 0$, $\text{Tr}\, \rho_N = 1$.

N-Representability and Quantum Marginal problem

Quant Marg Prob: Given some set $\{\rho_{J_1}, \rho_{J_2}, \ldots\}$?

Is there a $\rho_N \in \mathcal{D}(\mathcal{H}_N)$ such that all $\rho_{J_m} = \text{Tr}_{J^c}\, \rho_N$

N-representability: Given $\rho_{1,2,\ldots m} \in \mathcal{D}(\mathcal{H}^{\wedge m})$

is there $\rho_N \equiv \rho_{1,2,\ldots N} = \sum_k \lambda_k |\Psi_k\rangle\langle\Psi_k| \in \mathcal{D}(\mathcal{H}^{\wedge N})$

such that $\rho_{1,2,\ldots m} = \text{Tr}_{m+1,\ldots N} \sum_k \lambda_k |\Psi_k\rangle\langle\Psi_k|$ anti-sym Ψ_k

only need $\rho_{1,2,\ldots m}$ get rest by symmetry

given ρ_{12} know ρ_{23}, ρ_{46} etc. all same by anti-sym

extensively studied in 1960's – esp. by quantum chemists

Pure state problem – require pre-image pure $|\Psi\rangle\langle\Psi|$

But only mixed form convex set and variation over convex set

always achieved on boundary with pure pre-image

Convex Structure

Set of N-rep m-body RDM is convex set

subset of convex set of all DM in $\mathcal{B}(\mathcal{H}^{\wedge^m})$.

Recall closed convex set intersection of half-spaces and dual cone

BLACKBOARD PICTURE

Compare entanglement witness picture

Look at polar cone in more detail for 2-body system

Reduced Hamiltonians

typical 2-body Ham

$$H_N = -\sum_k \Delta_k + \sum_k U(x_k) + \sum_{j<k} V(x_j, x_k)$$
$$= \sum_{j<k} \Big[\tfrac{1}{N-1}\big(-\Delta_j + U(x_j) - \Delta_k + U(x_k)\big) + V(x_j, x_k) \Big]$$
$$H_N - E_0 = \sum_{j<k} \Big[\tfrac{1}{N-1}\big(T_j + T_k \big) + V(x_j, x_k) - \tbinom{N}{2}^{-1} E_0 \Big] = \sum_{j<k} \widetilde{H}_{jk}$$

$$0 \le \langle \Psi, (H_N - E_0)\Psi \rangle = \sum_{j<k} \mathrm{Tr}\, \widetilde{H}_{jk}\, \rho_{jk} = \tbinom{N}{2} \mathrm{Tr}\, \widetilde{H}_{12}\, \rho_{12}$$

Hope: reduce n-body calculation to 2-body

BUT variational calcs give energy below E_0

reduced Ham $\widetilde{H}_{12}$ not nec pos semi-def in $\mathcal{B}(\mathcal{H} \wedge \mathcal{H})$

Polar cone

$X \subseteq \mathcal{H}^{\otimes N}$ typical $X = \mathcal{H}^{\wedge N}$ $\quad \mathcal{D}^m(X) =$ image of $\mathcal{D}(X)$

$\mathcal{P}\big(\mathcal{D}^m(X)\big) \equiv \{V_m \in \mathcal{B}(\mathcal{H}^{\otimes m}) : \text{Tr}\, V_m\, \rho_m \geq 0\ \forall \rho_m \in \mathcal{D}^m(X)\}$

polar cone $\quad V_m$ "witness" N-rep – compare entanglement witness

N-rep reduced Hamiltonians $\widetilde{H}_{12}$ give polar cone

Quant Marg case: $V_m = (V_{1,2\ldots m} \ldots)$ vector of m-body operators

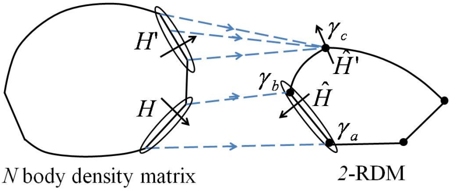
$R_m = (\rho_{1,2\ldots m} \ldots)$ a vector of all m-body quant marg

$H_N(V) = \sum_{j_1 j_2 \ldots j_m} V_{j_1 j_2 \ldots j_m}$ $\quad m$-local Ham

$$\langle \Psi, H_N(V_m)\Psi \rangle = \sum_{j_1 j_2 \ldots j_m} \text{Tr}_{j_1 j_2 \ldots j_m} \rho_{j_1 j_2 \ldots j_m} V_{j_1 j_2 \ldots j_m}$$

Reduced Ham vector of operators $\widetilde{V_m}$ with $V_{j_1 j_2 \ldots j_m} - \binom{N}{m}^{-1} E_0$

Mapping picture



Extreme for N-body need not $\mapsto$ extreme for m-body.

Many pure N-body $\mapsto$ interior of m-body.

Generic interior point has multiple pre-images

Dual Cone of 1-body RDM gives Pauli

Example: Only single slater dets $\mapsto$ extreme pts of 1-body RDM.

all other pure N-body $|\Psi\rangle\langle\Psi| \mapsto$ interior

MAPPING PICTURE

$H_N = \sum_k T_k$ non-interacting Ham. $\widetilde{T}_1 = T_1 - \frac{1}{N} E_0$

ground state e-spaces single Slater dets.

$\Rightarrow$ e-vals of extreme ρ_1 are $\frac{1}{N}$ (N-fold deg) and 0

$\Rightarrow$ nasc for N-rep is $0 \leq \lambda_k \leq \frac{1}{N}$

Recover Pauli exclusion principle

Hierarchy of ext. pts.

Example: Only single slater dets $\mapsto$ extreme its of 1-body RDM.

all other pure N-body $|\Psi\rangle\langle\Psi| \mapsto$ interior

Hierarchy: $|\Psi\rangle\langle\Psi| \mapsto$ extreme m-body RDM

$\Rightarrow |\Psi\rangle\langle\Psi| \mapsto$ extreme $(m+1)$-body RDM

In particular, Slater dets also $\mapsto$ extreme points of 2-body RDM

BUT there are many others. For Slater det e-vals $= \binom{N}{2}^{-1}$

$\exists$ extreme points of 2-body with largest e-val $\approx \frac{1}{N}$

BCS states and AGP

Open: What are extreme points of N-rep 2-body RDM ??

2-body N-rep is QMA complete

QMA-complete is quantum analogue of NP-complete

roughly means would take exponential time even on Quant Comp.

Thm: 2-body N-Rep is QMA complete

$\Rightarrow$ Really No Free Lunch but subtle glitch

BUT used CS formalism – membership error $1/\text{poly}$ in size

For ground state energy from N-rep, $O(1)$ is good enough

Need very high accuracy but need not increase with size

fluctuations across periodic table

chemical reactions – energy of same order

Pure state pre-images of overlapping pair of RDM

Essentially due to D. W. Smith (1965) and Diosi (2004)

Thm: Almost every pure state uniquely determined by two quant marginals $(\rho_J, \rho_{J'})$ with $J \cup J' \neq \emptyset, \quad J \cup J' = \{1, 2, \ldots N\}$

Rewrite $\quad \rho_J \mapsto \rho_{JK} \quad \rho_{J'} \mapsto \rho_{KL}, \qquad J \cap J' \mapsto K$

Proof Sketch: assuming non-deg e-vals

$$\rho_J = \text{Tr}_K \, \rho_{JK} = \sum_j \mu_j^2 \, |\phi_j^J\rangle\langle\phi_j^J| \text{ etc.}$$

get two "Schmidt" expansions from ρ_J, ρ_{KL} and ρ_{JK}, ρ_L

$$\sum_j e^{i\omega_j} \mu_j |\phi_j^J \otimes \phi_j^{KL}\rangle = \; |\Psi\rangle \; = \sum_k e^{i\theta_k} \nu_k |\phi_k^{JK} \otimes \phi_k^L\rangle$$

Gives lots of linear equations for unknowns $x_j = e^{i\omega_j}, y_k = e^{i\theta_k}$

Only rarely have solutions, even more rarely non-unique,

only want those with $|x_j = e^{i\omega_j}| = |y_k e^{i\theta_k}| = 1$

Uniqueness without overlap

Thm: Erdahl (1972) ρ_J and ρ_{J^c} both extreme $\Rightarrow$ unique pre-image

Intuition: Use e-vecs of ρ_J and ρ_{J^c} to write

$$|\psi\rangle = \sum_k e^{i\omega_k} \mu_k |\chi_k \otimes \phi_k\rangle = \sum_{k \in \kappa_1} \mu_k |\chi_k \otimes \phi_k\rangle + e^{i\omega} \sum_{k \in \kappa_2} \mu_k |\chi_k \otimes \phi_k\rangle$$
$$= x_1 |\psi_1\rangle + e^{i\omega} x_2 |\psi_2\rangle$$

Either $e^{i\omega_j}$ can be determined and ψ unique OR

same RDM as mixture $\Upsilon_N = x_1^2 |\psi_1\rangle\langle\psi_1| + x_2^2 |\psi_2\rangle\langle\psi_2|$ not extreme

Extend to disjoint $(J_1, J_2, \ldots)$ with $\cup_k J_k = \{1, 2, \ldots N\}$?

Conj: (Erdahl) Extreme N-rep 2-body RDM has unique pre image.

Special case $\rho_{12}, \ \rho_{34}, \ \rho_{N-1,N}$ False!

For 1-body RDM, uniqueness true, trivial – single Slater det

Is $J^c = J'$ too good to be true?

Case I: fermions (anti-symmetric) or bosons (symmetric)

$2m \geq N$ and ρ_m extreme $\Rightarrow$ pre-image unique (all, not a.e.)

$m = 2$ applies to $N = 4$ electrons, but not $N = 5$

expand using ρ_{12} and ρ_{34} anti-sym $2 \leftrightarrow 3$ gives more conds

Case II: No sym: set of RDM = all D.M on $\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} \otimes \ldots \otimes \mathcal{H}_{j_m}$.

Extreme $\Rightarrow$ pure $\rho_J = |\chi\rangle\langle\chi|$ and $\rho_{J^c} = |\phi\rangle\langle\phi|$

pre-image is unique pure product state $|\Psi\rangle\langle\Psi| = |\chi \otimes \phi\rangle\langle\chi \otimes \phi|$

Case III: Other symmetry: e.g., rotation or translational invariance

constraints less transparent, but either exist or get product

Key Lemma (Erdahl, Section 6)

Let $\mathcal{G}$ subspace of $\mathcal{H}_N$ with $d \geq 2$ assoc with unique m-body RDM

$$\rho_J = \text{Tr}_{J^c}|\Psi\rangle\langle\Psi| \qquad \forall\ \Psi \in \mathcal{G}$$

Then for any orthog pair $|\Psi_\ell\rangle, |\Psi_k\rangle$ in $\mathcal{G}$, $\quad \text{Tr}_{J^c}|\Psi_\ell\rangle\langle\Psi_k| = 0$

$$\Rightarrow\ \langle\Psi_\ell, B_J\Psi_k\rangle = \text{Tr}_J\, B_J\big(\text{Tr}_{J^c}|\Psi_\ell\rangle\langle\Psi_k|\big) = 0 \quad \text{for any } m\text{-body } B_J$$

Proof:

$$\begin{aligned} \rho_J &= \text{Tr}_{J^c}|x\Psi_k + e^{i\theta}y\Psi_\ell\rangle\langle x\Psi_k + e^{i\theta}y\Psi_\ell| \ \text{ indep of } \theta \\ \rho_J &= x^2\rho_J + \big(e^{i\theta}\text{Tr}_{J^c}|\Psi_k\rangle\langle\Psi_\ell| + e^{-i\theta}\text{Tr}_{J^c}|\Psi_\ell\rangle\langle\Psi_k|\big) + y^2\rho_J \\ &= \rho_J + e^{i\theta}\text{Tr}_{J^c}|\Psi_k\rangle\langle\Psi_\ell| + e^{-i\theta}\text{Tr}_{J^c}|\Psi_\ell\rangle\langle\Psi_\ell| \end{aligned}$$

$$\begin{aligned} &\Rightarrow\ e^{i\theta}\text{Tr}_{J^c}|\Psi_k\rangle\langle\Psi_l| + e^{-i\theta}\text{Tr}_{J^c}|\Psi_\ell\rangle\langle\Psi_k| = 0 \quad \forall\ \theta \\ &\Rightarrow\ \text{Tr}_{J^c}|\Psi_\ell\rangle\langle\Psi_k| = 0 \end{aligned}$$

Aside on QECC

Consider O.N. basis $|\psi_k\rangle$ for subspace $\psi \mapsto \rho_{J_m}$ unique

Lemma proved that for all m-body $B_{J_m} = B_{j_1, j_2, \ldots j_m}$

$$\langle \psi_\ell, B_{J_m} \psi_k \rangle = \langle \psi_\ell, B_{j_1, j_2, \ldots j_m} \psi_k \rangle = 0 \qquad j \neq k$$

$$\langle \psi_k, B_{J_m} \psi_k \rangle = \mathrm{Tr}_J \, B_{J_m} \big(\mathrm{Tr}_{J^c} |\psi_k\rangle\langle\psi_k| \big) = \mathrm{Tr}_{J_m} B_{J_m} \, \rho_{J_m} \quad \text{indep of } k$$

consider $m = 2, \; B_{j_1 j_2} = E_{j_1}^\dagger E_{j_2}$

$$\langle \psi_\ell, B_{J_m} \psi_k \rangle = \langle E_{j_1} \psi_\ell, E_{j_2} \psi_k \rangle = \delta_{k\ell} \; \mathrm{Tr} \, E_{j_1}^\dagger E_{j_2} \rho_{j_1 j_2}$$

Precisely condition for 1-bit error correction $\quad m = 2\nu$ get ν-bit

Most QECC not from ground state e-spaces of m-body Hams

stabilizer codes highly entang. states $\Rightarrow$ RDM mixed – not ext.

Non-unique pre-image of extreme points

require m-local N-body Ham with ground state degeneracy

but can not be split by any m-body perturb

For QECC which arises as ground state e-space of m-body Ham

2-body RDM of Bacon-Shor code; non-unique 9-body pre-image

4-body RDM of Kitaev toric code; non-unique pre-image

Bacon-Shor Ham: square $n \times n$ lattice with cyclic bound cond

$$H_N = \sum_{j,k} (a_x X_{j,k} X_{j+1,k} + a_z Z_{j,k} Z_{j,k+1})$$

For $n \geq 3$ have degen ground state e-space generated by

pair of states of odd and even parity $\mapsto$ same 2-body RDM

Second quantize to fermionic counter-example

Each lattice site $k \leftrightarrow$ "spatial " function f_k from O.N. set

Def: $a^\dagger_{k,s_k}|\mathrm{vac}\rangle = |f_k \otimes s_k\rangle$ satisfy CAR

Get V : lattice state $|s_1, s_2, \ldots s_N\rangle \mapsto (f_1 s_1) \wedge (f_2 s_2) \wedge \ldots (f_N s_N)$

single Slater det with all "orbitals" f_k half-filled

$$H_{\mathrm{lattice}} \mapsto H_{\mathrm{ferm}} = \begin{pmatrix} H_{\mathrm{sing\ occ}} & 0 \\ 0 & H_{\mathrm{doub}} \end{pmatrix}$$

Add "penalty" $H_{\mathrm{ferm}} \mapsto H_{\mathrm{ferm}} + \sum_k \mu_k a^\dagger_{k\uparrow} a^\dagger_{k\downarrow} a_{k\downarrow} a_{k\uparrow}$

increases energy by $\mu_k > 0$ for any state with doubly occ orbital

ensures ground state $\mapsto$ fermonic ground state

Counter-example to Erdahl's 1972 conjecture

Images and inverse images of faces

Inverse images of faces always face – but not reverse

BUT Image of degenerate ground state eigenspaces are faces

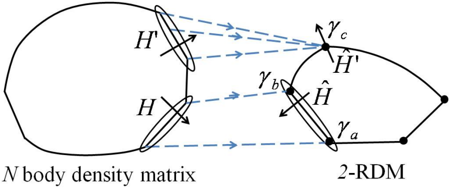


Figure: Mapping and unbreakable degeneracy – multiple preimages

Even when *m*-body corr do not uniquely determine state, can still determine subspace assoc with ground state of *m*-local Hamiltonian

m-corr subspace; max mixed state determined by *m*-cody corr.

Structure of extreme points for fermion 2-body RDM

best known: BCS and AGP very strongly paired

anti-sym 2-body state $\phi = \sum_j a_j \left[f_j(x_1)\widetilde{f}_j(x_2) - \widetilde{f}_j(x_1) f_j(x_2) \right]$

N-body $|\psi\rangle = \mathcal{A}\left[\phi(x_1, x_2) \otimes \phi(x_3, x_4) \otimes \ldots \otimes \phi(x_{2n-1}, x_{2n})\right]$

⋮

⋮ ?? terra incognito ??

⋮

new: QECC counter-ex – no pairing – half-filled

Compare: limiting cases for Hubbard model

Challenge: Find good set of ext points to obtain upper bounds.

Even if need to constuct full N-body wave function, info from study of N-rep 2-body RDM could lead to better variational methods

Proof of Erdahl Thm. for J and J^C

ρ_J extreme and pre-image unique $\Rightarrow \text{Tr}_{J^c} |\Psi_k\rangle\langle\Psi_j| = 0$

$$\begin{aligned} |\Psi_k\rangle &= \sum_t \mu_t |\chi_t \otimes \phi_t^k\rangle \\ |\Psi_\ell\rangle &= \sum_t \mu_t |\chi_t \otimes \phi_t^\ell\rangle \end{aligned}$$

and $k \neq \ell \;\Rightarrow\; \langle\phi_s^k, \phi_t^\ell\rangle = 0 \quad \forall\, s, t$

But suppose $|\Psi_k\rangle$ also have same $\rho_{J^c} = \text{Tr}_J |\Psi_k\rangle\langle\Psi_k|$ extreme

Then $\rho_{J^c} = \sum_t \mu_t^2 \, |\phi_t^k\rangle\langle\phi_t^k| = \sum_t \mu_t^2 \, |\phi_t^\ell\rangle\langle\phi_t^\ell| \quad \Rightarrow \quad |\phi_t^k\rangle = |\phi_t^\ell\rangle$

contradicts strong orthogonality above $\quad \langle\phi_t^k, \phi_t^\ell\rangle \neq 0$

So pair of extreme (ρ_J, ρ_{J^C}) have unique pre-image

Contributions of QIT to N-rep

- Klyachko

  a) Can pinning explain physical phenomena?

  b) Possible to reduce number of Slater dets in Conf. Interact

  eliminate coeff below certain threshold

- QMA complete – no free lunch

  BUT used CS formalism – membership error 1/poly in size

  For ground state energy from N-rep, $O(1)$ is good enough

  Need very high accuracy but need not increase with size

- QECC showed $\exists$ extreme point with non-unique pre-image

Need more examples of extreme points of 2-body N-rep RDM

Implications for quantum chemistry

Could be useful even viewed as "conventional" restricted variation.

Klyachko's 1-body pure state inequality might have similar use,

e.g. restrict CI from $\binom{R}{N}$ Slater dets to much smaller number

Know $N = 3, R = 6$ suffices to consider 8 instead of 20

State of art: use part set of nec. conds for lower bounds to E_0.

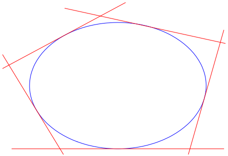


Figure: Outside optimization Inner restricted optimization

Try inside opt using suff conds from wider set of extreme points

Special challenge for QIT

- N-rep for 1-matrix depends only on eigenvalues
- N-rep for 2-matrix also depends on eigenvectors

In gen, N-rep conds don't depend on choice of 1-particle basis

N-rep conditions for m-matrix can be expressed in terms of

quantities invariant under unitaries of form $U^{\otimes m}$

$U \otimes U \otimes \ldots \otimes U$ called "local unitaries" in quantum info

Find "minimal but complete" set of invariants for 2-body N-rep?

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