

Title: Quantum codes give counterexamples to the unique pre-image conjecture of the N-representability problem

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Abstract: It is well known that the ground state energy of many-particle Hamiltonians involving only 2- body interactions can be obtained using constrained optimizations over density matrices which arise from reducing an N-particle state. While determining which 2-particle density matrices are 'N-representable' is a computationally hard problem, all known extreme N-representable 2-particle reduced density matrices arise from a unique N-particle pre-image, satisfying a conjecture established in 1972. We present explicit counterexamples to this conjecture through giving Hamiltonians with 2-body interactions which have degenerate ground states that cannot be distinguished by any 2-body operator. We relate the existence of such counterexamples to quantum error correction codes and topologically ordered spin systems.

Quantum codes give counterexamples to the  
unique pre-image conjecture of the  
 $N$ -representability problem

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# Motivation

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- Energy of a state in 2-body Hamiltonian is completely determined by its 2-particle RDM.
- Find the lowest energy density matrix; solve Hamiltonians quickly and easily.

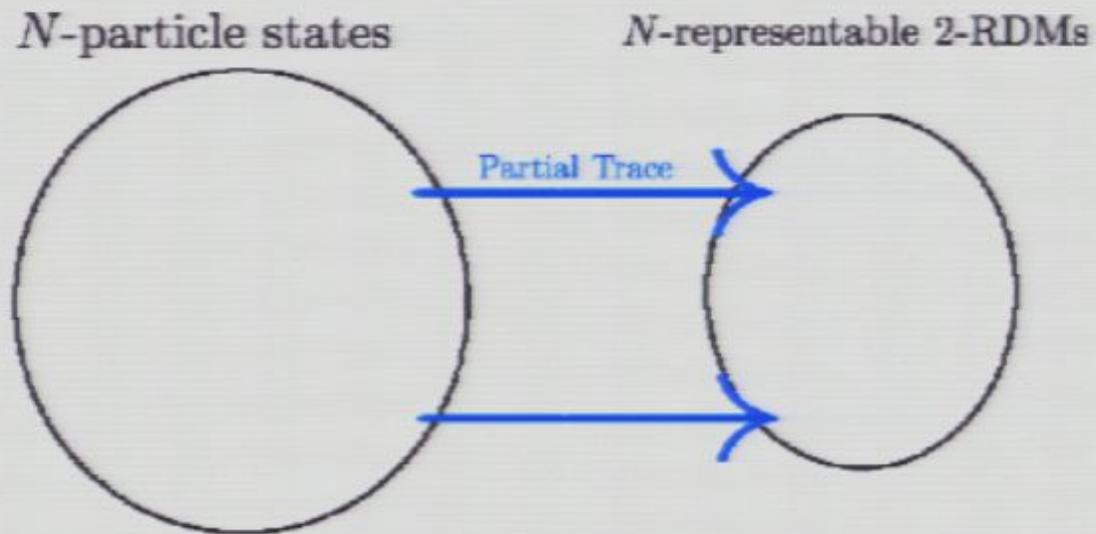
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**Problem:** Not all density matrices are the reduced density matrices of some  $N$ -particle state!

# N-Representability Problem:



What density matrices are the *reduced density matrices* of an  $N$ -particle state?

An  $N$ -particle state is called the **pre-image** of the state it maps to.

## Importance and Connections to Quantum Information

If we could solve the  $N$ -representability problem, we could solve for the ground states of 2-body Hamiltonians!

Originally there was a hope the the  $N$ -representability problem would be solved.

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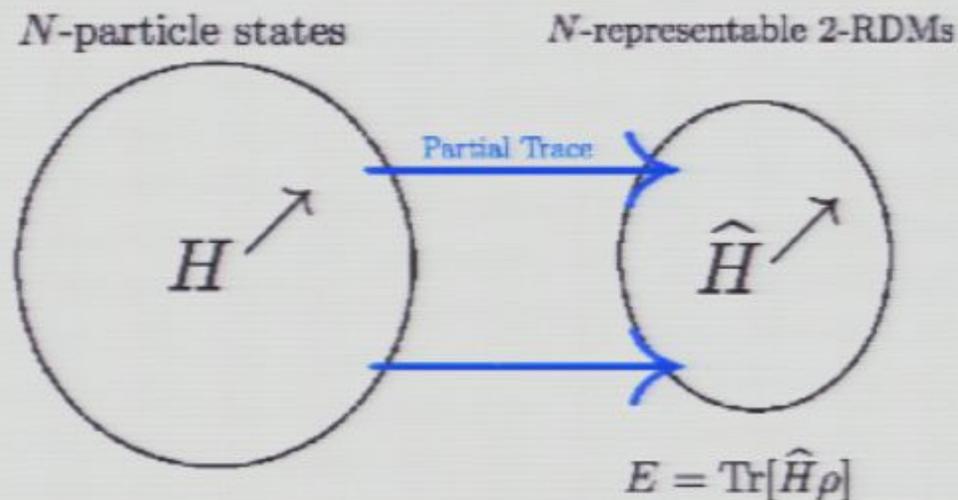
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(Liu et al., 2007): Deciding whether an arbitrary density matrix is  $N$ -representable is **QMA-complete**; hard even with a quantum computer, **no exact solution possible**.

## Avenues of Attack

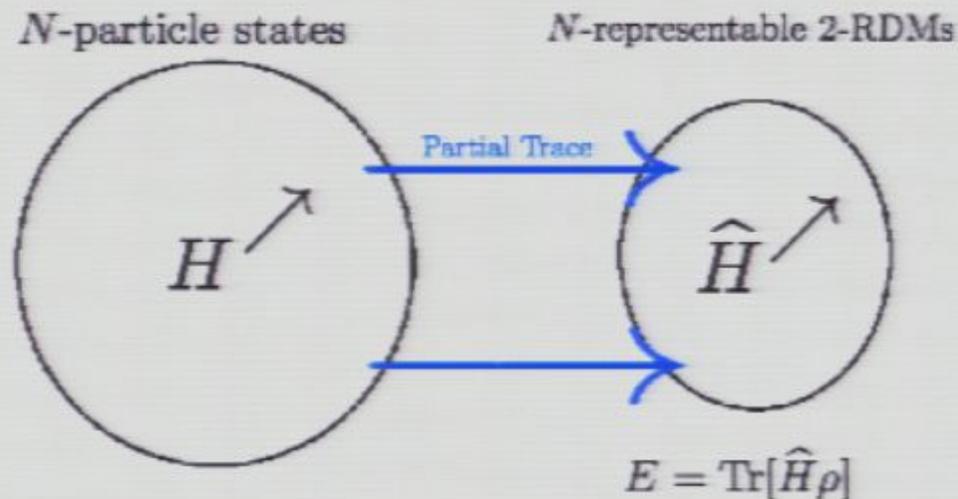
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- Form a convex set; the average of two is also  $N$ -representable.
- Energy( $\text{Tr} \hat{H}\rho$ ) is a linear function of both RDM and Hamiltonian (like a dot product with proper choice of basis).

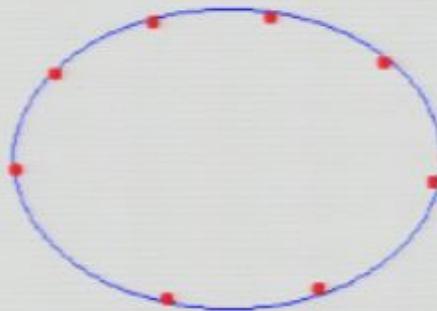
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- Energy( $\text{Tr} \hat{H}\rho$ ) is a linear function of both RDM and Hamiltonian (like a dot product with proper choice of basis).
- **Linear optimization problem constrained to convex set.**

# Extreme Points



- Not average of any two points in set.
- Unique lowest energy point for some 2-body Hamiltonian.
- Completely characterize set; every other point is some weighted average of extreme points

Therefore important in linear optimization.

## Unique Pre-Image Conjecture

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- Seems natural for systems in quantum chemistry, where  $H = -\nabla^2 + V$ .
- Similar observations have been made for translationally invariant spin systems.
- Proven for  $m$ -body density matrices where  $m \geq N/2$ .

## Main Result

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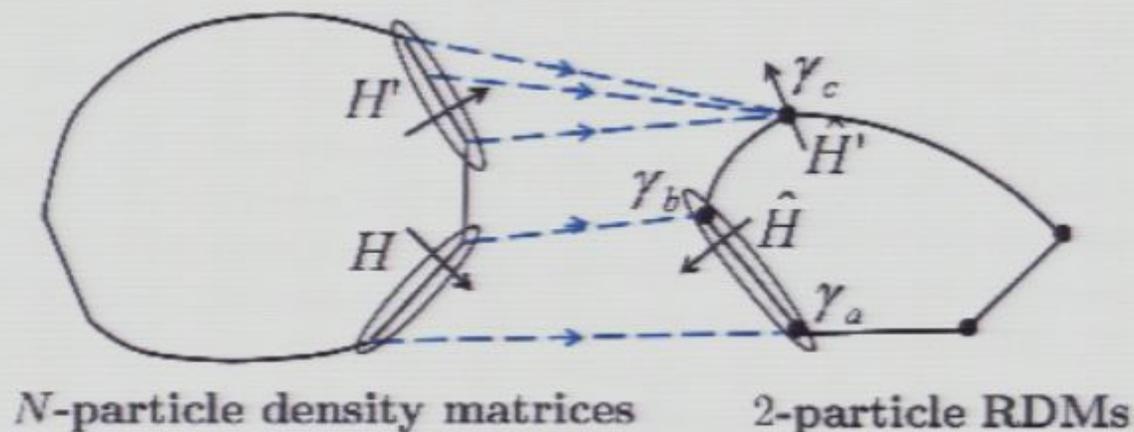
-Set of extreme points is much more complex than previously believed.

# Roadmap

- 1 Translate Erdahl's conjecture into the language of Hamiltonians.
- 2 Present spin lattice Hamiltonian.
- 3 Map spin lattice case to fermionic case-disprove conjecture.
- 4 Connect to quantum coding theory.

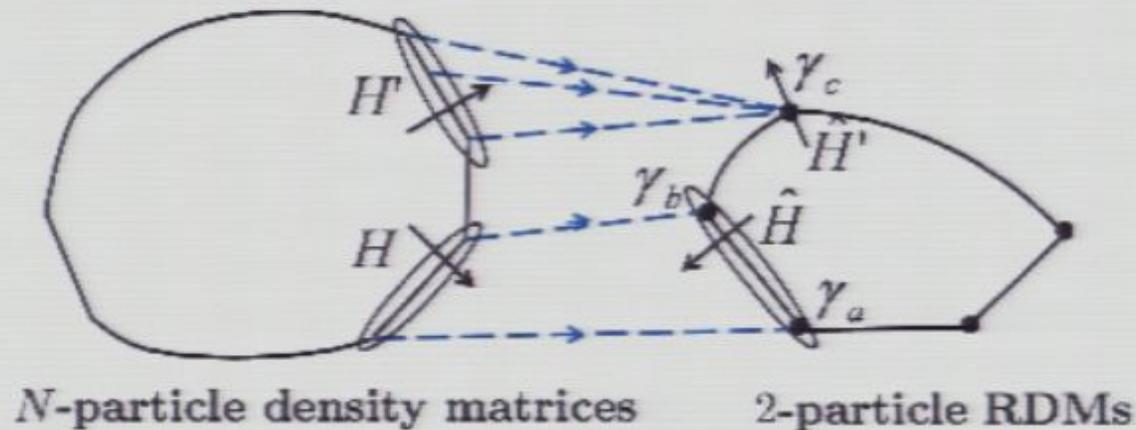
# Translating into Hamiltonian Language

Every extreme point  $\gamma$  corresponds to the ground space of some 2-body Hamiltonian.



- Consider a 2-body Hamiltonian  $H'$  whose ground states can't be distinguished by 2-body operators.
- All ground states have the same 2-particle RDM; otherwise 2-body operators would distinguish them.
- We define such a Hamiltonian to be **2-blind**.

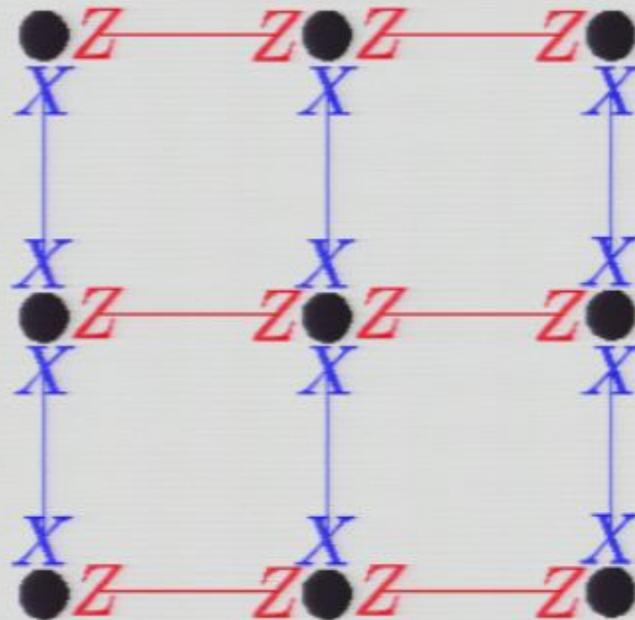
# Translation cont.



- 2-blind  $H'$  has a **unique lowest-energy reduced density matrix**  $\gamma$ , which is therefore extreme.
- Since multiple ground states of  $H'$  map to  $\gamma$ ,  $\gamma$  is an extreme point with multiple pre-images.
- **Erdahl's conjecture, translated, is that there's no 2-blind fermionic Hamiltonian.**

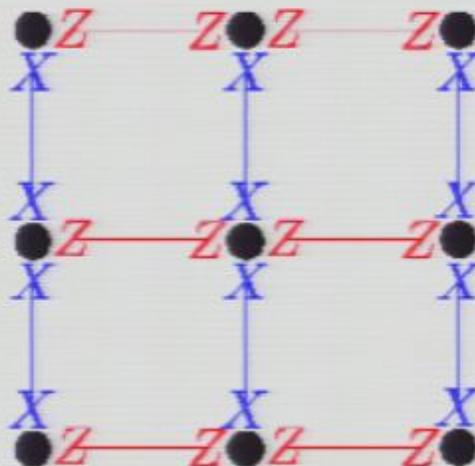
# Bacon-Shor Code: A Simple 2-Blind Spin Hamiltonian

Subsystem code with gauge generators:



$$H_{BS} \equiv \sum_{jk} (-X_{j,k}X_{j+1,k} - Z_{j,k}Z_{j,k+1})$$

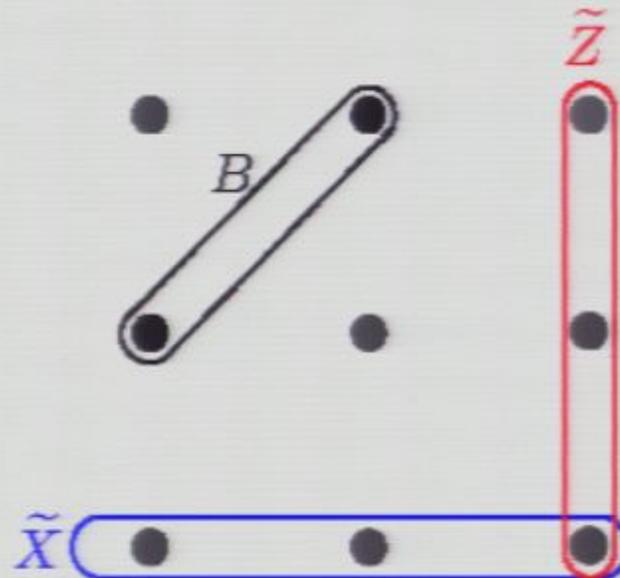
# Bacon-Shor Code: Ground States(Codewords)



- $H_{BS}$  has 2 ground states, each stabilized by stabilizer group (all columns have same parity).
- Ground states have even parity( $|C_0\rangle$ ) or odd parity( $|C_1\rangle$ ).

# Proof of Indistinguishability by 2-Body Operators:

Given any operator  $B$  acting on two qubits, we can define logical operators  $\tilde{X}, \tilde{Z}$  which don't touch the same qubits;



Therefore, Bacon-Shor Hamiltonian is 2-blind.

## Mapping to Fermions

Replace system of  $N$  spins with system of  $N$  fermions and  $N$  sites.  
Map each direct product state to a Slater determinant:

$$V : |s_1\rangle \otimes \dots \otimes |s_N\rangle \mapsto a_{1,s_1}^\dagger \dots a_{N,s_N}^\dagger |\Omega\rangle$$

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May “fermionize” one-body and two-body spin operators:

$$Z_j \mapsto Z_j^{\text{ferm}} = a_{j,\uparrow}^\dagger a_{j,\uparrow} - a_{j,\downarrow}^\dagger a_{j,\downarrow}, \quad X_j \mapsto X_j^{\text{ferm}} = a_{j,\uparrow}^\dagger a_{j,\downarrow} + a_{j,\downarrow}^\dagger a_{j,\uparrow}$$

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Fermionized spin operators have the same algebra and expectation values on fermionized states that spin operators have on spin states:

$$Z_j^{\text{ferm}} a_{j,\uparrow}^\dagger |\Omega\rangle = a_{j,\uparrow}^\dagger |\Omega\rangle, \quad Z_j^{\text{ferm}} a_{j,\downarrow}^\dagger |\Omega\rangle = -a_{j,\downarrow}^\dagger |\Omega\rangle, \text{ etc.}$$

# Fermionizing the Hamiltonian

- Fermionize  $H_{BS} \mapsto H_{BS}^{\text{ferm}}$
- Fermionize ground states  $|C_0\rangle, |C_1\rangle \mapsto V|C_0\rangle, V|C_1\rangle$
- Since ground states of  $H_{BS}$  can't be distinguished by 2-body spin operators, ground states of  $H_{BS}^{\text{ferm}}$  can't be distinguished by 2-body fermionic operators; map to same 2-RDM.
- $H_{BS}^{\text{ferm}}$  is 2-blind and gives an extreme point with multiple pre-images (it's ground space), disproving Erdahl's conjecture.

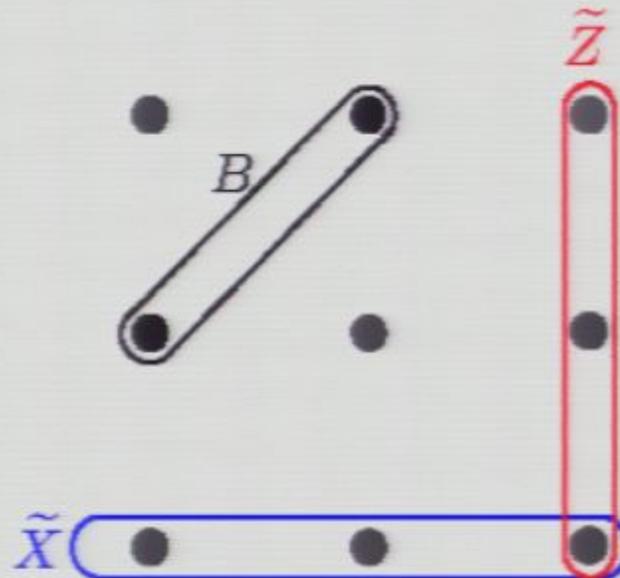
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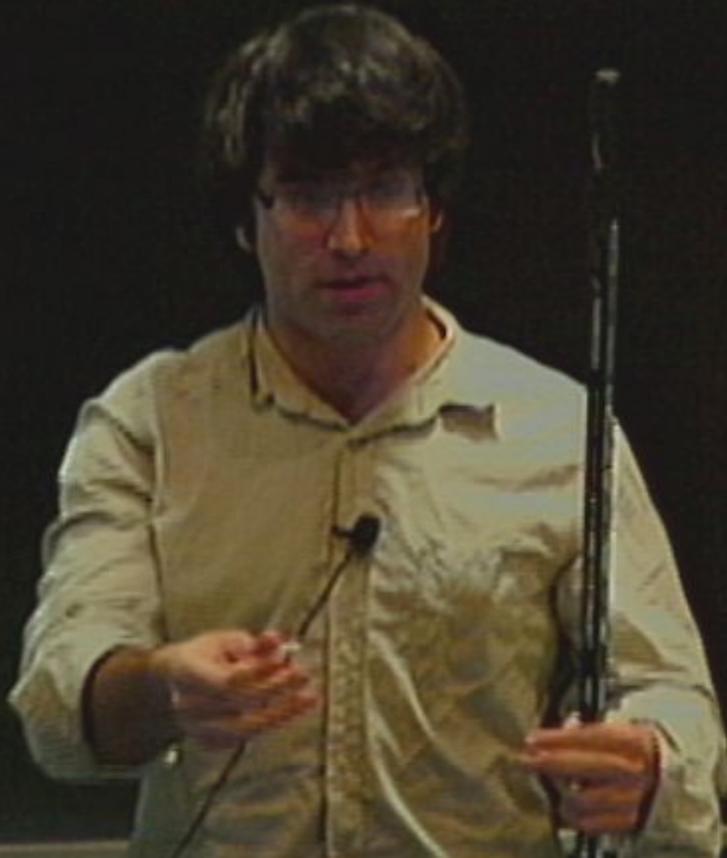
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$$n_j = a_{j\pi}^+ a_{j\pi} + a_{j\downarrow}^+ a_{j\downarrow} \quad n_j = 1 \quad \sum v_j (n_j - \frac{1}{2})^2$$



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## Connection to Quantum Coding Theory

- Want to encode qubit using codewords  $|C_p\rangle$ .
- If an error from set  $\{E_m\}$  is applied, we want to identify and correct the error without disturbing the encoded state:

$$\langle C_p | E_\ell^\dagger E_m | C_q \rangle = \delta_{pq} Q_{\ell m}.$$

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- When  $\{E_m\}$  consists of all single-bit errors,  $E_\ell^\dagger E_m$  is basis for all 2-body operators.
- QECC criteria = indistinguishability criteria;  
 Code corrects 1-bit errors  $\iff$  all codespace has same 2-RDMs (Bravyi et al. 2010).

Only a few codes form the ground space of 2-blind Ham (Bacon 2006, Bombin et al. 2010, etc. )

## Generalization to $m$ -Body RDMs

Original conjecture was that all extreme  $N$ -representable  $m$ -particle RDMs have unique pre-images.

- $m$ -blind Hamiltonians give extreme  $m$ -body RDM with multiple pre-images (toric code, topological stabilizer codes, etc.)
- Ground space gives a code which can correct  $\lfloor \frac{m}{2} \rfloor$  errors.

## Future Work: Tightening the Rules of the Game

- Intuition behind conjecture came from Hamiltonians with Laplacians:  $H = -\nabla^2 + V$ .
- Our 2-blind Hamiltonian has no Laplacian term, each site has exactly one fermion at all times.

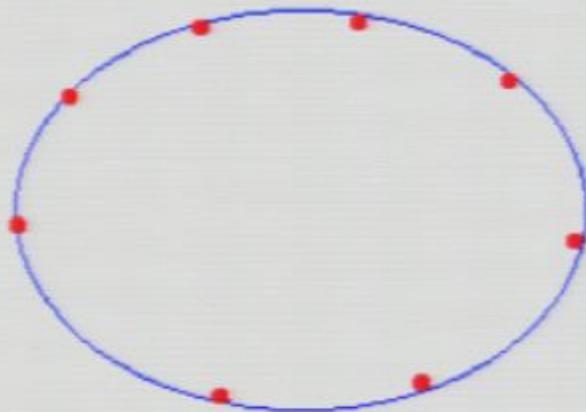
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What classes of fermionic Hamiltonians can be 2-blind?

# Quantum Chemistry

- Extreme  $N$ -representable RDMs much different than previously believed.
- What are the implications for  $N$ -representability?
- Can we find a better set of extreme points for variational calculations?



# Holonomic Quantum Computation

Curved boundaries represent states which can be transformed adiabatically as ground states of 2-body Hamiltonians.

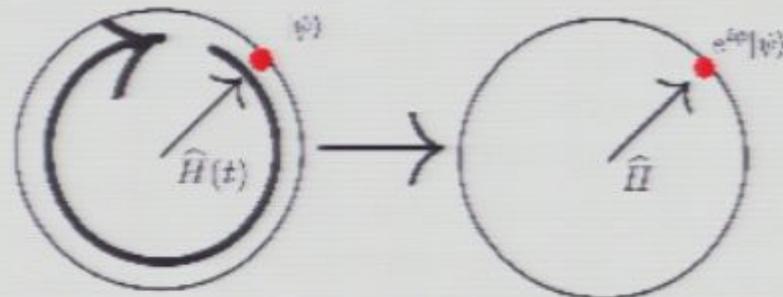


Figure: Extreme points have unique pre-images

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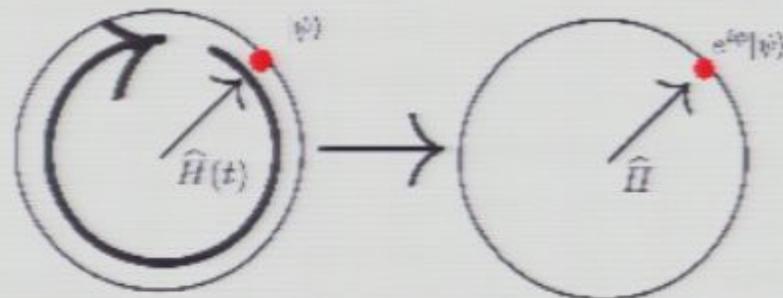


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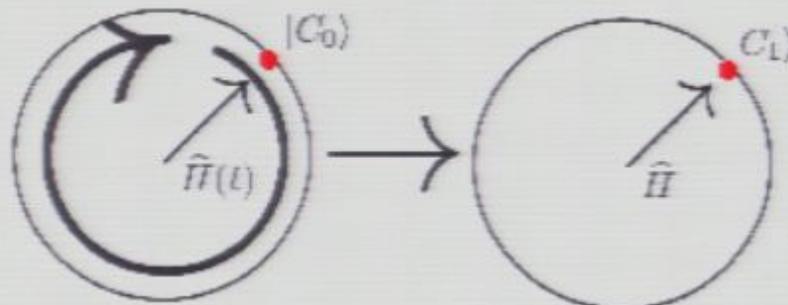


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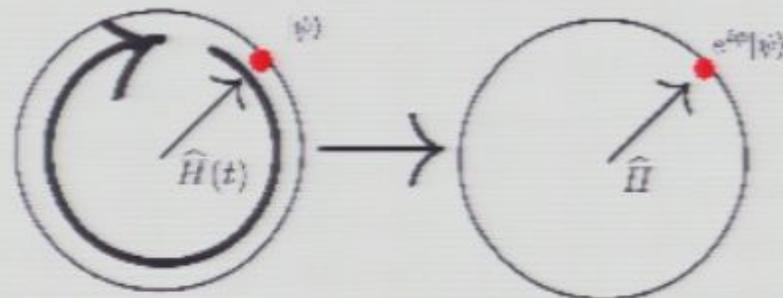


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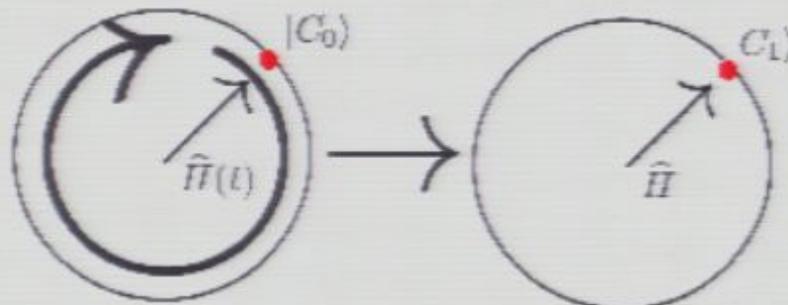


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Universal Holonomic quantum computation from time-evolving 2-blind Hamiltonian? (Oreshkov et al. 2009)

# Topological Quantum Codes

- Bacon-Shor code, other CSS subsystem codes give 2-blind Hamiltonians. Not believed to be gapped in the thermodynamic limit.
- How can we get topological quantum codes from 2-body interactions? (Kitaev, Bombin et al., Brell et al. ...)
- 2-body topologically ordered Hamiltonians with exactly solvable ground states and low-energy excitations? (Ocko and Yoshida, in preparation)