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

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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-body state. While determining which 2-body density matrices are "N-representable" is a computationally hard problem, all known extreme N-representable 2-body reduced density matrices arise from a unique N-body 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.

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For all known systems of identical particles, which have Hamiltonians restricted to symmetric (bosonic) or anti-symmetric (fermionic) states, the Hamiltonians contain, at most, two-body interactions. Therefore, for many purposes, in particular energy calculations, an N-body state can be replaced by its 2-body reduced density matrix (RDM). In doing so, one might hope to reduce complex N-body calculations by simpler 2-body ones. Early efforts gave absurdly low energies until it was realized that it was necessary to restrict to 2-body density matrices which, in fact, come from the reduction of an N-body state of the appropriate symmetry (its *pre-image*). Characterizing these 2-body RDMs is a fascinating question known as the N-representability problem [1–3].

In the 1960's, the N-representability problem was solved for one-body RDMs [1]. However, finding a solution for 2-body RDMs is so challenging that most of those who tried concluded that it was intractable. This intuition was recently validated with a quantum information theoretic proof that N-representability for the 2-body RDM belongs to the complexity class called QMA complete [4], i.e., the worst cases would be hard even with a quantum computer.

Surprisingly, this coincided with a revival of interest in the N-representability problem from several directions. A number of groups have obtained good approximations to the ground state energy in special situations [5]. New eigenvalue bounds for the 1-body RDM have been found for pure N-body fermion states [6]. For both fermions and bosons the first improvements on expectation value bounds since 1965 were obtained in [7]. Moreover, the map from an N-body state to a m-body RDM is a special type of quantum channel, which found an important application involving Renyi entropy in [8].

A widely held property about the convex set of N-representable 2-body RDMs is that all the extreme RDMs arise from a unique N-body pre-image. *Extreme N-representable RDMs* are fundamental; every N-representable 2-body RDM comes from a weighted average of extreme points, and because energy is a linear function of the RDM, its minimum must lie on the set of extreme points. The unique pre-image property holds for the best known extreme points, which come from generalizations of BCS states [3, 9]. It is also true for the few other known extreme RDMs, and similar observations [10] have been made for RDMs of translationally symmetric spin lattice systems. In 1972, Erdahl [9, Section 6] formally conjectured that all extreme RDMs have a unique pre-image, and it has been widely believed to hold since then.

Erdahl's conjecture has been proven for m-body extreme RDMs when $2m > N$ [9]. Moreover, if the conjecture were false, there would exist an unusual 2-body Hamiltonian, whose ground state degeneracy is "blind" to, i.e. undetectable by, 2-body operators. All ground states of such a "2-blind" Hamiltonian would have the same 2-body RDM, and thus the degeneracy cannot be broken without at least a 3-body interaction; 2-body perturbations would only shift the energy.

In this paper, we give explicit counterexamples to Erdahl's conjecture. To do so, we first exhibit a class of 2-blind *spin lattice* Hamiltonians, whose ground states are quantum error correction codes. Extended to fermions, these examples provide extreme N-representable 2-body RDMs with multiple pre-images, which are thus the desired counterexamples. We then directly relate the general conditions for quantum error correction to the existence of such counterexamples. Our results imply that the set of N-representable RDMs is much larger and very different from what has long been the prevailing wisdom. In addition, the Hamiltonians we use [11] play a pivotal role in the study of topological quantum error correction [12, 13].

N-representability and the unique pre-image conjecture: We begin with a brief description of the N-representability problem and its generalization beyond fermionic symmetries. For fermions, a symmetric 2-body Hamiltonian H_N acts on antisymmetric states $|\psi^-\rangle$ for which the 2-body RDM is $\rho_{12}^- = \mathrm{Tr}_{3\ldots N}|\psi^-\rangle\langle\psi^-|$. A 2-body RDM ρ_{12}^- is called *N-representable* if it has a *pre-image* Λ, i.e. $\rho_{12}^- = \mathrm{Tr}_{3\ldots N}\Lambda$, where $\Lambda = \sum p_{\psi^-}|\psi^-\rangle\langle\psi^-|$ is an N-body state of appropriate symmetry. The critical interplay between the one and two-body terms of H_N is captured by

$$H = H_N - E_0 = \sum_j T_j + \sum_{j<k} V_{jk} \; - E_0 = \sum_{j<k} \widehat{H}^N_{jk}, \quad (1)$$

where E_0 is the ground state energy of H_N, and $\widehat{H}^N_{jk} \equiv V_{jk} + \frac{1}{N-1}(T_j + T_k) - \binom{N}{2}^{-1} E_0$ is known as the reduced Hamiltonian. One can verify the energy of Λ is determined by its 2-body RDM ρ_{12}^- by

$$\binom{N}{2} \mathrm{Tr}\, \widehat{H}^N_{12}\, \rho_{12}^- = \mathrm{Tr}\, H\Lambda \geq 0, \quad (2)$$

with equality if and only if Λ is a ground state of H_N.

Although H is positive semidefinite by construction, $\widehat{H}^N_{12}$ is *not* positive semidefinite in general; however, it acts as if it were on the set of N-representable RDMs. Thus it acts as a "witness" for N-representability, a special case of a general duality concept known as the polar cone of a convex set.

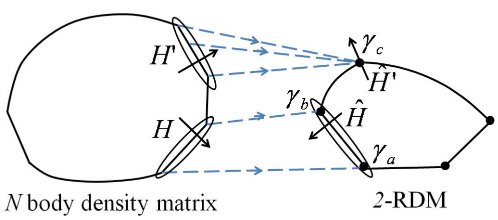

FIG. 1. Mapping of N-body density matrices to N-representable 2-body RDMs. γ_a, γ_b are extreme 2-body RDMs with unique pre-images. γ_c is an extreme 2-body RDM with multiple pre-images.

N-representable 2-body RDMs form a convex set, as the average of two is also N-representable. The set of N-representable RDMS, like any convex set, is characterized by its extreme points, which are not the average of any two points in the set (Fig. 1). Erdahl [9, Section 3] showed that in finite dimensions every extreme N-representable RDM γ_{12} is also *exposed* in the sense that there is some Hamiltonian $\widehat{H}^N_{12}$ for which γ_{12} is the unique lowest energy N-representable RDM. Every extreme point thus corresponds to the ground state eigenspace of at least one two-body Hamiltonian H_N.

When the ground state of H_N is non-degenerate, it is the unique pre-image of its 2-body RDM. A degenerate ground state eigenspace defines a convex subset of the N-representable 2-body RDMs, which typically corresponds to a flat (exposed) region on the boundary. In exceptional cases, this region is a single extreme point with multiple pre-images; this happens when the Hamiltonian is 2-blind, meaning that all degenerate ground states have the same 2-body RDM.

It is useful to extend the concept of N-representability to the complete absence of symmetry. This leads to the closely related *quantum marginal* problem which asks if there is a pre-image $\Lambda = \sum p_\psi |\psi\rangle\langle\psi|$ consistent with the reduction to $\{\rho_{jk}\} \equiv (\rho_{12}, \rho_{13}, \ldots, \rho_{1N}, \rho_{23}, \ldots, \rho_{N-1,N})$, where $\{\rho_{jk}\}$ is expressed in vector form to emphasize that those which are consistent form a convex set. The reduced spin lattice Hamiltonian $\{\widehat{H}_{jk}\}$ is also written in vector form, and Eq.(2) becomes $\sum_{j<k} \mathrm{Tr}\, \widehat{H}_{jk}\rho_{jk}$.

Erdahl's conjecture is equivalent to the statement that there is no 2-blind *fermionic* Hamiltonian. We first present a 2-blind *spin lattice* Hamiltonian which gives an extreme quantum marginal $\{\rho_{jk}\}$ with multiple pre-images. We then explain how to extend this to fermions to disprove Erdhal's conjecture.

Lattice example: We consider the Hamiltonian for the two-dimensional quantum compass model used in condensed matter physics [14]. It has a doubly degenerate ground state eigenspace, known as the Bacon-Shor code [11] in quantum information theory, for which the 2-body RDMs $\{\rho_{jk}\}$ are independent of the choice of eigenstate.

Let X_{jk} and Z_{jk} denote the Pauli operators σ_x and σ_z, respectively, acting on the site (j,k) in a square $n \times n$ spin lattice, and define

$$H_{n^2} \equiv -\sum_{jk} \big(J_x X_{j,k} X_{j+1,k} + J_z Z_{j,k} Z_{j,k+1}\big), \quad (3)$$

where $J_x, J_z > 0$, and subscript addition is mod n, corresponding to cyclic boundary conditions.

For $n = 3$, define the even parity columns

$$v_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad v_1 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad v_3 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}.$$

The odd parity columns are obtained by flipping all spins $0 \leftrightarrow 1$. Symmetry considerations can be used to show that H_{n^2} is block diagonal, including two blocks spanned by states where all columns have even parity or all columns have odd parity.

It can be shown that the lowest energy eigenvalues of these blocks are unique and those of other blocks strictly larger [11, 15]. (In fact it is not hard to verify that $E_0 \leq -9J_Z$ on these blocks and that for $J_Z \gg J_x$ the

Hamiltonian is $\gtrsim -5J_Z$ on the other blocks.) Therefore, this Hamiltonian has a pair of ground states which can be distinguished by even and odd parity. Let

$$
\begin{aligned}
|A_1\rangle &= \tfrac{1}{2}\sum_{j=0}^{3}(v_j, v_j, v_j),\\
|A_2\rangle &= \tfrac{1}{6}\sum_{j\neq k}\left[(v_j, v_k, v_k) + (v_k, v_j, v_k) + (v_k, v_k, v_j)\right],\\
|A_3\rangle &= \tfrac{1}{\sqrt{24}}\sum_{i\neq j\neq k\neq i}(v_i, v_j, v_k).
\end{aligned}
$$

The even parity ground state of Eq.(3) is

$$|C_0\rangle = a_1|A_1\rangle + a_2|A_2\rangle + a_3|A_3\rangle, \tag{4}$$

and the odd parity ground state $|C_1\rangle$ can be obtained by flipping all spins.

To verify that all ground states $u|C_0\rangle + v|C_1\rangle$ have the same 2-body RDMs, it is both necessary and sufficient to show that for all 2-body operators B,

$$\langle C_p|B|C_q\rangle = \delta_{pq} b \tag{5}$$

for some constant b. To prove that $\langle C_p|B|C_p\rangle = b$ for all p, we introduce the operators $\widetilde{X}_j = \prod_i X_{j,i}$, which act equivalently on the ground space; $\widetilde{X}_j|C_p\rangle = |C_{1-p}\rangle$ for all j. Given any two-body operator B which acts on sites (j_1, k_1) and (j_2, k_2), an $\widetilde{X}_j$ may be chosen which does not affect the same sites as B; $j \neq j_1, j_2$. Therefore:

$$\langle C_0|B|C_0\rangle = \langle C_0|\widetilde{X}_j B \widetilde{X}_j|C_0\rangle = \langle C_1|B|C_1\rangle = b. \tag{6}$$

One can similarly show $\langle C_0|B|C_1\rangle = 0$ using $\widetilde{Z}_k = \prod_i Z_{i,k}$.

Therefore, because H_{n^2} is a two-body Hamiltonian where all degenerate ground states have the same 2-body RDMs, it follows that H_{n^2} is 2-blind and $\widehat{H}_{n^2}$ gives an exposed, and therefore extreme $\{\rho_{jk}\}$ with no unique pre-image. This fact is already surprising and interesting. We show next that this can be mapped to fermions to give a counterexample to Erdahl's conjecture.

From spin lattices to fermions: To extend our example to fermions we replace our spin lattice of N sites with a system of N fermions. Each fermion has both a spatial (site) and an internal (spin) degree of freedom. To map a spin state $|\psi\rangle$ to a fermionic state $|\psi^-\rangle$, we map each computational basis state to a Slater determinant with exactly one fermion per site (half-filled orbitals) by

$$V : |s_1\rangle \otimes \ldots \otimes |s_N\rangle \mapsto a^\dagger_{1,s_1} \ldots a^\dagger_{N,s_N}|\Omega\rangle, \tag{7}$$

where $a^\dagger_{j,s_j}$ creates a fermion at site j with spin s_j and $|\Omega\rangle$ is the vacuum state. The map V satisfies $V^\dagger V = I_{\text{latt}}$ and $VV^\dagger = P_{\mathcal{H}_{\text{Half}}}$, the projection onto fermionic states with half-fillled orbitals. We may map non-trivial(Trace zero) one-body spin operators to corresponding one-body "fermionized" operators:

$$W_j = \sum w_{st}|s_j\rangle\langle t_j| \mapsto W_j^{\text{ferm}} = \sum w_{st} a^\dagger_{j,s_j} a_{j,t_j}. \tag{8}$$

It can be verified that the fermionized operators have the same algebra and expectation values on states with half-filled orbitals that the original spin operators have on spin states:

$$W_j^{\text{ferm}}|\psi^-\rangle = W_j^{\text{ferm}} \cdot V|\psi\rangle = V \cdot W_j|\psi\rangle. \tag{9}$$

Therefore, we can see a similar correspondence between quantum marginals and 2-body RDM of states with half-filled orbitals:

$$\{\rho_{jk}\} \mapsto \binom{N}{2}^{-1} \cdot \sum_{1\leq j<k\leq N} V_{jk}\rho_{jk}V_{jk}^\dagger = \rho_{12}^-,$$

where $V_{jk} : |s_j s_k\rangle \mapsto a^\dagger_{j,s_j} a^\dagger_{k,s_k}|\Omega\rangle$ acts similarly on pairs of sites. This gives us the full correspondence:

$$
\begin{array}{ccc}
|\psi\rangle & \longleftrightarrow & |\psi^-\rangle \\
\downarrow & & \downarrow \\
\{\rho_{jk}\} & \longleftrightarrow & \rho_{12}^-
\end{array}
$$

Since there is a linear, one-to-one correspondence $\{\rho_{jk}\} \longleftrightarrow \rho_{12}^-$, it follows that ρ_{12}^- is extreme with multiple pre-images if and only if $\{\rho_{jk}\}$ is extreme with corresponding pre-images. Applying this procedure to the Bacon-Shor code gives an extreme fermionic 2-body RDM with multiple pre-images, disproving Erdahl's conjecture. Moreover, because every extreme N-representable 2-body RDM is exposed, we know that there exists a "2-blind" fermionic Hamiltonian which exposes this extreme point.

We can explicitly construct such a Hamiltonian by applying Eq.(8) to all terms in the spin Hamiltonian. Because of Eq.(9), the eigenstates and energies in the invariant subspace of half-filled orbitals, i.e. $n_j = a^\dagger_{j\uparrow}a_{j\uparrow} + a^\dagger_{j\uparrow}a_{j\uparrow} = 1$ for all j, correspond to those of the spin Hamiltonian by $|\psi_E^-\rangle = V|\psi_E\rangle$. To ensure that all ground states have half-filled orbitals, we must add a penalty term $\sum_j U_j\,(n_j - 1)^2$ with U_j sufficiently large to ensure that states with $n_j \neq 1$ have higher energy. Moreover, there is a threshold M such that $U_j > M$ defines an n^2-parameter family of exposing Hamiltonians.

These procedures also work for bosonic systems.

Quantum error correction codes: The counterexample given above is a special case of a much more general connection between RDMs with multiple pre-images, m-blind Hamiltonians, and quantum error correction codes. In quantum coding theory [16], a quantum state is encoded into a subspace of a larger system in a way such that errors can be identified and corrected without disturbing the encoded state. This subspace is spanned by an orthonormal basis of codewords $|C_p\rangle$, and a necessary and sufficient condition for a quantum code to be able to correct a set of single particle errors $\mathcal{E} = \{E_m\}$ is that [16]

$$\langle C_p|E_\ell^\dagger E_m|C_q\rangle = \delta_{pq} Q_{\ell m}. \tag{10}$$

$\mathcal{E}$ contains the operators $\{F_{1,a}, \ldots F_{N,a}\}$ for all a, where $F_{j,0}, F_{j,1} \ldots F_{j,d^2-1}$ is a basis of for single-particle operators on site j. Therefore, since $E_\ell^\dagger E_m = F_{j,a}^\dagger F_{k,a'}$ forms a basis for the set of two-body operators, the criteria for a code to be able to correct all single-particle errors $\langle C_p|E_\ell^\dagger E_m|C_q\rangle = \delta_{jk} Q_{\ell m}$, is *exactly* the criteria of Eq.(5) for all states in the code space $\{|C_p\rangle\}$ to have the same set of 2-body RDMs.

This set of 2-body RDMs will be extreme if and only if the code space is the ground space of some Hamiltonian with at most 2-body interactions. The Bacon-Shor code has this property and yields extreme points with multiple pre-images. However, most quantum codes, including stabilizer codes and non-stabilizer CWS codes [16, 17], do not have this property and simply yield interior points with multiple pre-images.

Erdahl's general conjecture was for m-body RDMs, with $m \geq 2$. While counterexamples for $m > 2$ can come from the Bacon-Shor code defined on larger lattices, they also come from m-blind Hamiltonians whose ground states define a quantum code that can correct any $\lfloor \frac{m}{2} \rfloor$-particle errors. Topological quantum codes can have this property; for example, Kitaev's toric code [12] is a 4-blind Hamiltonian which gives an extreme N-representable 4-body RDM with multiple pre-images. Other topological quantum codes exhibit the same properties [13, 18]. Indeed, similar relationships between topological quantum codes and RDMs have been observed in [19, 20].

Extensions and open issues: The fermionic extreme points constructed here, which come from N-body states with half-filled orbitals, are quite different from those one encounters for atomic and molecular systems, and also differ from the best known extreme points which come from generalizations of BCS states [3, 9]. The critical issue is not whether the states described here – or their associated Hamiltonians – arise in practical applications. Our results demonstrate that the class of extreme points is much larger and more complex than previously believed. From the standpoint of quantum chemistry, the challenge is to characterize a class of extreme points which will lead to useful new computational algorithms.

The 2-blind fermionic Hamiltonians we used to disprove Erdahl's conjecture are quite different from fermionic Hamiltonians that physicists usually encounter, which have two-body potential terms as well as one-body terms having the form of a Laplacian. This leads to a question of fundamental importance in developing physically realizable quantum codes; can Hamiltonians with physically reasonable Laplacian and local potential terms, including realistic spin and magnetic interactions, be 2-blind?

Some of these counterexamples are closely related to topologically ordered spin systems. Stabilizer topological codes are counterexamples for $m > 2$, and subsystem [21] topological codes [22] are candidates of counterexamples for $m = 2$. Further work along these directions will undoubtedly continue to forge new connections between quantum information, condensed matter physics, and quantum chemistry.

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