Quadratic fermionic interactions yield Hamiltonians with large ground-state energy gaps

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Polynomially large ground-state energy gaps are rare in many-body quantum systems, but useful in quantum information and an interesting feature of the one-dimensional quantum Ising model. We show analytically that the gap is generically polynomially large not just for the quantum Ising model, but for one-, two-, and three-dimensional interaction lattices and Hamiltonians with certain random interactions. We extend the analysis to Hamiltonian evolutions and we use the Jordan-Wigner transformation and a related transformation for spin-3/2 particles to show that our results can be restated using spin operators in a surprisingly simple manner. These results also yield a new perspective on the one-dimensional cluster state.

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I. INTRODUCTION

A typical many-body quantum Hamiltonian must fit exponentially many energy levels into a polynomial-sized energy range, so most energy gaps (the difference between two successive energy levels) must be exponentially small. It is not clear *a priori* why the ground-state energy gap should ever be larger than the rest. Nonetheless large ground-state energy gaps are important in adiabatic quantum computing (AQC) [1] and for stability when approximating graph states using local Hamiltonians [2,3]. A large ground-state energy gap is also an interesting feature of the standard example of a second-order quantum phase transition, namely, the one-dimensional quantum Ising model [4,5]. In this paper we expand the result for the one-dimensional quantum Ising model to identify broader classes of Hamiltonians that exhibit a large ground-state energy gap.

Let us be more precise. Mathematically, we can construct a Hamiltonian with any given set of 2^n energy levels. Theorem I.1, given below, establishes that large ground-state energy gaps are rare among choices of energy levels.

Theorem I.1 (Large ground-state energy gaps are rare). Consider uniform random choices of energy levels for a Hermitian operator on n two-state particles (qubits) under the restriction that the ground-state energy is zero and the energies are contained in the unit interval. The fraction of these choices with a ground-state energy gap greater than $2^{-n/2}$ tends to $e^{-2^{n/2}}$ for large n.

Proof. The ground-state energy gap is larger than some $\epsilon>0$ provided the 2^n-1 nonzero energy levels are selected from the interval $(\epsilon,1]$. Thus the fraction of choices of energy levels with a ground-state energy gap of at least ϵ is $(1-\epsilon)^{2^n-1}$. Let us choose $\epsilon=2^{-n/2}$; then we have

$$(1-2^{-n/2})^{2^n-1} = (1-2^{-n/2})^{\sqrt{2^n-1}\sqrt{2^n-1}} \tag{1}$$

$$\approx (e^{-1})^{\sqrt{2^n-1}} \tag{2}$$

$$\approx e^{-2^{n/2}}. \tag{3}$$

■

In fact, since the dimension of the problem is exponentially large in the number of qubits, it is difficult to even *determine* the minimum ground-state energy gap for large systems.

Adiabatic quantum computing is an approach to quantum computation that depends on having a ground-state energy gap bounded below by a polynomial in the inverse of the problem size. In AQC, a problem is encoded as the ground state of some Hamiltonian $\mathcal{H}_P$. It is assumed that it is feasible to prepare a physical system in the ground state of some simple Hamiltonian $\mathcal{H}_0$ and then evolve the Hamiltonian slowly from $\mathcal{H}_0$ to $\mathcal{H}_P$. Under the right conditions and if the evolution is done sufficiently slowly [6], then at the end of the evolution the state of the system is the ground state of $\mathcal{H}_P$. Measurement of this final state reveals the solution to the original problem. As an approach to quantum computing, AQC is known to be equivalent to standard gated quantum computing in that each can be efficiently simulated by the other [7,8]. Also, a simple AQC evolution achieves unsorted database search in time $O(\sqrt{N})$, where N is the database size, just as in Grover's search algorithm [9].

For the effective application of AQC, it would be useful to identify a class of Hamiltonians satisfying the following conditions:

(1) The class should have many degrees of freedom and allow many interactions between qubits, so that it represents diverse problem instances for AQC.

(2) The class should include a simple initial Hamiltonian $\mathcal{H}_0$.

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(3) It is convenient if between any two Hamiltonians in the class there is a path that stays within the class.

(4) All Hamiltonians in the class should have large ground-state energy gaps.

(5) Finally, the class must include Hamiltonians whose ground states encode the solution to difficult classical problems.

Given condition 5, condition 4 is difficult to satisfy. Overall there are few analytic results establishing large ground-state energy gaps for AQC evolutions. We seek to understand when ground-state energy gaps may be large. One known example is the one-dimensional quantum Ising model [4,5]. The key to the analysis of this model is the Jordan-Wigner transformation that maps it to a quadratic fermionic Hamiltonian [10]. We provide background on these Hamiltonians in Sec. II. It is clear that quadratic fermionic Hamiltonians satisfy conditions 1–3. In Sec. III we will show that they meet condition 4 as well. In Sec. IV we identify which lattice Hamiltonians of one, two, and three dimensions have a degenerate ground state and show that the ground-state energy gap grows quickly as we move away from these degenerate Hamiltonians. We extend these analyses to Hamiltonian evolutions in Sec. V. Finally, in Sec. VI we derive alternate representations of these Hamiltonians using the Jordan-Wigner transform and a related transform for spin-3/2 particles and relate the results to the one-dimensional cluster state.

II. BACKGROUND ON THE FERMIONIC COMMUTATION RELATIONS

For a detailed exposition on properties of the fermionic commutation relations (FCRs), see, e.g., [11–13]. Here we only highlight some essential points, mostly without proof, that are needed to develop the results in following sections.

The FCRs on a set of linear operators $\{c_j : j=1,\ldots,n\}$ are

$$\{c_j, c_k^\dagger\} = \delta_{j,k}, \quad \{c_j, c_k\} = 0, \tag{4}$$

where the bracket notation indicates the anticommutator $\{x,y\}=xy+yx$ and δ_{jk} equals the identity operator if $j=k$ and zero otherwise. The superscript dagger denotes the Hermitian adjoint. A consequence of the FCRs is that $\{c_j, c_j^\dagger : j=1,\ldots,n\}$ are creation and annihilation operators that anticommute.

Suppose we have a Hamiltonian of the form

$$\mathcal{H} = \sum_{j=1}^{n} C_j c_j^\dagger c_j, \tag{5}$$

where the coefficients C_j are positive and real. All the terms in $\mathcal{H}$ commute and the jth term has eigenvalues 0 and C_j. Now, take the sum of elements in each possible subset (including the empty set) of $\{C_j : j=1,\ldots,n\}$. The 2^n resulting values are the eigenvalues of $\mathcal{H}$. In particular, the ground-state energy of $\mathcal{H}$ is zero and the ground-state energy gap is the least nonzero coefficient C_j. To decide whether an arbitrary value is an eigenvalue of $\mathcal{H}$ for arbitrary coefficients is nondeterministic polynomial-time (NP)-complete however, as it is equivalent to the subset-sum problem (also known as the knapsack problem) [11].

We can write many Hamiltonians in the form of Eq. (5) using Theorem II.1 (below), originally due to Lieb *et al.* [10]. Suppose we have a *quadratic fermionic Hamiltonian* $\mathcal{H}$ defined as

$$\mathcal{H} = \sum_{j,k=1}^{n} A_{j,k}(c_j^\dagger c_k - c_j c_k^\dagger) + B_{j,k}(c_j^\dagger c_k^\dagger - c_j c_k) \tag{6}$$

for some set of real coefficients $A_{j,k}$ and $B_{j,k}$. For convenience, we gather the coefficients $A_{j,k}$ and $B_{j,k}$ into real $n \times n$ matrices that we label A and B. If $B=0$, then $\mathcal{H}$ represents a Hubbard model with no on-site interactions, for instance, electrons in metals [14] or graphene [15]. If A and B are tridiagonal, then $\mathcal{H}$ represents, under the Jordan-Wigner transform [10], a one-dimensional chain of spin-1/2 particles with nearest-neighbor interactions. If A and B have three nonzero super- and subdiagonals, then $\mathcal{H}$ represents a chain of spin-3/2 particles with nearest-neighbor interactions [16]. Also, we can see using the FCRs that different choices of A and B may represent the same Hamiltonian. In particular, for any given Hamiltonian, A can be chosen to be symmetric and B antisymmetric.

Theorem II.1 establishes that we can write Eq. (6) in the form of Eq. (5), added to a multiple of the identity operator. Thus we can easily find the first few eigenvalues of $\mathcal{H}$ and in particular the ground-state energy gap.

Theorem II.1 (Lieb et al. [10]). Consider a quadratic fermionic Hamiltonian as in Eq. (6), where A is an $n \times n$ real symmetric matrix, B is an $n \times n$ real antisymmetric matrix, and the operators $\{c_k : k=1,\ldots,n\}$ satisfy the FCRs. Then we can find Λ^2 diagonal and X unitary so that $X(A-B)(A+B) = \Lambda^2 X$, and Y unitary so that $Y(A+B)(A-B)=\Lambda^2 Y$. Define the operators $\{\eta_j : j=1,\ldots,n\}$ by

$$\eta_j = \frac{1}{2}\sum_{k=1}^{n} (X_{jk}+Y_{jk})c_k + (X_{jk}-Y_{jk})c_k^\dagger. \tag{7}$$

Then $\{\eta_j : j=1,\ldots,n\}$ satisfy the FCRs and

$$\mathcal{H} = \sum_{j=1}^{n} 2\Lambda_j \eta_j^\dagger \eta_j - \left(\sum_{j=1}^{n} \Lambda_j\right) I_{2^n}, \tag{8}$$

where Λ_j denotes the jth entry on the diagonal of the matrix Λ and I_{2^n} is the identity operator.

Proof. See the Appendix. ■

Theorem II.1 was used initially by Lieb *et al.* [10] to find the spectrum of the one-dimensional XY model and subsequently has been used, for instance, in the analysis of the one-dimensional model of free electron transport [12]. Quadratic fermionic Hamiltonians as in Eq. (6) have also sparked recent interest because of their application to quantum complexity theory. If one takes a set of gates defined by $U = \exp(i\mathcal{H}t)$ for some t and a constant quadratic fermionic Hamiltonian $\mathcal{H}$ in the form of Eq. (6), then one obtains a set of gates that resembles a universal set, but in fact may be classically simulated [17]. Broader sets of gates that can be classically simulated have been identified [18,19]. To classically simulate an evolving Hamiltonian, it has been shown [8] that Hamiltonian evolutions may be efficiently approximated by discretizing the evolution into a sequence of short,

constant Hamiltonians. Theorem II.1 has also been used to find efficient sets of quantum gates for computing properties of quadratic fermionic Hamiltonians in the form (6) [20]. Further, the relationship between a vanishing energy gap and discontinuity in the ground state has been studied for these Hamiltonians [21].

The Jordan-Wigner transformation applied to the Hamiltonian evolution

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n} \sigma_j^z + s\sum_{j=1}^{n-1} \sigma_j^x \sigma_{j+1}^x \tag{9}$$

transforms $\mathcal{H}(s)$ into a quadratic fermionic Hamiltonian in the form of Eq. (6), thus providing a means for determining the spectrum for any $s \in [0,1]$. In fact, this evolution exhibits a second-order quantum phase transition and a ground-state energy gap that decreases as $\Omega(1/n)$ [4,5], which is surprisingly large. The notation $\Omega(1/n)$ means that the ground-state energy gap is larger than ϵ/n for n greater than some n_0 and some constant factor ϵ.

Since $(A+B)^\dagger = A-B$ and since the singular values of a matrix M are the square roots of the eigenvalues of $M^\dagger M$, we see that Λ_j from Eq. (8) is a singular value of $A+B$. Further, C_j in Eq. (5) can be defined to be $2\Lambda_j$. Thus, if $A+B$ is nonsingular, then twice the least singular value is the ground-state energy gap of $\mathcal{H}$. If $A+B$ is singular, then $\mathcal{H}$ has a degenerate ground state and the least nonzero singular value is the energy gap between the ground-state subspace and the higher energy levels of the Hamiltonian. In any case, since $A+B$ has only n dimensions, in contrast to $\mathcal{H}$ which has 2^n, we might expect that often the least singular value of $A+B$ is not exponentially small in n. Then the ground-state energy gap of $\mathcal{H}$ would not be exponentially small. In Sec. III we state and prove more precise formulations of this claim.

III. QUADRATIC FERMIONIC HAMILTONIANS WITH RANDOM INTERACTIONS

To establish that the ground-state energy gaps are large for quadratic fermionic Hamiltonians, we provide two theorems. In Theorem III.1 (below), we take a particular distribution of coefficient matrices A and B under the restriction $\|A+B\|_2 \leq 1$, where $\|A+B\|_2$ denotes the largest singular value of $A+B$ and establish that the ground-state energy gap is $\Omega(1/n)$. Then, in Theorem III.3, we show that the ground-state energy gap is $\Omega(1/\sqrt{n})$ for Gaussian-distributed interaction coefficients.

Theorem III.1 (Ground-state energy gaps of quadratic fermionic Hamiltonians with bounded coefficients). Choose a real diagonal $n \times n$ matrix Σ uniformly at random with entries in the unit interval and choose U and V according to any probability distribution over orthogonal $n \times n$ matrices. Then $C = U\Sigma V^\dagger$ represents a distribution over all real matrices with $\|C\|_2 \leq 1$. Take A to be the symmetric part of C and B to be the antisymmetric part of C, i.e., $A=(C+C^\dagger)/2$ and $B=(C-C^\dagger)/2$, and let $\mathcal{H}$ be defined as in Eq. (6). The probability that the ground-state energy gap of $\mathcal{H}$ is greater than $2x/n$, for any $x>0$, tends to e^{-x} for large n.

Proof. If the ground-state energy gap $\mathcal{H}$ is greater than $2x/n$, then the singular values of C are contained in the interval $(x/n,1)$. The fraction of choices for Σ where this is true is

$$\left(1-\frac{x}{n}\right)^n = \left[\left(1-\frac{x}{n}\right)^{n/x}\right]^x, \tag{10}$$

which tends to e^{-x} for large n. ■

To determine the ground-state energy gap for Gaussian-distributed interaction coefficients, we first need the following theorem about random matrices due to Edelman ([22], Corollary 3.1).

Theorem III.2 (Edelman [22]). Let C be an $n \times n$ matrix whose elements have independent Gaussian distributions with mean zero and unit variance. We denote such distributions as $N(0,1)$. Let ζ be the least singular value of C. Then for large n, $n\zeta^2$ converges in distribution to

$$\rho(x) = \frac{1+\sqrt{x}}{2\sqrt{x}} e^{-(x/2+\sqrt{x})}. \tag{11}$$

Since $n\varsigma^2$ has a probability distribution that is asymptotically independent of n, it follows that $\varsigma = \Omega(1/\sqrt{n})$. Also, Eq. (11) implies that $\varsigma \neq 0$ with probability 1. Similar results for other ensembles of random matrices are known [23]. Let us now apply Theorem III.2 to quadratic fermionic Hamiltonians.

Theorem III.3 (Ground-state energy gaps of quadratic fermionic Hamiltonians with Gaussian coefficients). Let C be an $n \times n$ matrix with independent $N(0,1)$ coefficients, let A be the symmetric part of C, and let B be the antisymmetric part of C, so

$$A = \frac{C+C^\dagger}{2}, \quad B = \frac{C-C^\dagger}{2}, \tag{12}$$

and $C=A+B$. Define

$$\mathcal{H} = \sum_{j,k=1}^{n} A_{j,k}(c_j^\dagger c_k - c_j c_k^\dagger) + B_{j,k}(c_j^\dagger c_k^\dagger - c_j c_k) \tag{13}$$

and let γ be the ground-state energy gap of $\mathcal{H}$. Then, for large n, $n\gamma^2/4$ converges in distribution to $\rho(x)$ defined in Eq. (11).

Proof. By Theorem III.2, if $\gamma/2$ is the least singular value of C, then $n\gamma^2/4$ converges in distribution to $\rho(x)$ for large n. Theorem III.2 also implies that C is nonsingular with probability one, so γ is the ground-state energy gap. ■

Since $n\gamma^2/4$ has a probability distribution that is asymptotically independent of n, $\gamma = \Omega(1/\sqrt{n})$. Recalling Theorem I.1, we see this is a remarkable property: since there must be 2^n distinct energy levels in an energy range of $O(n^2)$, most of the energy gaps must be exponentially small.

In fact the Hamiltonians in Theorem III.3 are also nondegenerate with probability 1. Degeneracies occur if two distinct subsets of singular values of C have the same sum. Such linear dependencies are measure-zero events, and since the joint probability density function for the singular values of C exists and is continuous [22], the probability of any measure-zero event is zero.

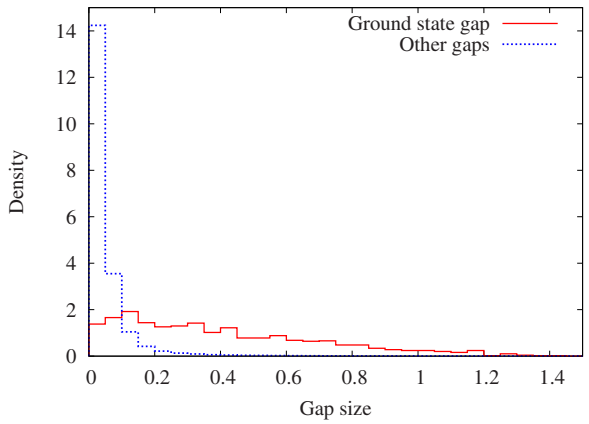


FIG. 1. (Color online) The ground-state energy-gap distribution is compared to the distribution for the other energy gaps, in reduced units. All the energy levels are computed for 1000 random $n=10$ (ten-qubit) Hamiltonians. Each Hamiltonian is chosen randomly as described in Theorem III.3. As predicted by Theorem III.3, the ground-state energy gaps are much larger than the other gaps.

Figure 1 illustrates the difference between the distribution of the ground-state energy gaps and the rest of the gaps for 1000 randomly generated ten-qubit Hamiltonians, and indeed the ground-state energy gaps are typically much larger than the other gaps.

In the next section we will move on from random interactions and instead analyze Hamiltonians of interactions on one-, two-, and three-dimensional lattices.

IV. LATTICE INTERACTIONS IN ONE, TWO, AND THREE DIMENSIONS

The one-dimensional quantum Ising model is expressed with A and B matrices ([10], p. 413)

$$A=\frac{1}{2}\begin{pmatrix} 0 & 1 & & & 1 \\ 1 & 0 & 1 & & \\ & 1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ 1 & & & 1 & 0 \end{pmatrix},$$

$$B=\frac{1}{2}\begin{pmatrix} 0 & 1 & & & -1 \\ -1 & 0 & 1 & & \\ & -1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ 1 & & & -1 & 0 \end{pmatrix}, \tag{14}$$

where omitted entries are zero. The ground state of this Hamiltonian can be found in polynomial time with AQC [4,5]. In fact, this holds for more general choices of A and B, including any instance of the one-dimensional XY model. An essential property of the definitions in Eq. (14) is that each row is a cyclic shift of the previous row. Such matrices are called *circulant*. For n qubits, it is easy to check that there are n degrees of freedom in choosing a symmetric circulant matrix A and antisymmetric circulant matrix B.

Circulant coefficient matrices other than the XY model include scenarios such as non-nearest-neighbor interactions on a one-dimensional chain of interacting fermions. The restriction that A and B are circulant imposes the requirement that the interaction strengths depend only on relative positions and it imposes periodic boundary conditions.

Theorem IV.1 (Ground-state energy gaps for circulant A and B matrices). Let

$$\mathcal{H}=\sum_{j,k=1}^{n} A_{j,k}(c_j^\dagger c_k - c_j c_k^\dagger) + B_{j,k}(c_j^\dagger c_k^\dagger - c_j c_k), \tag{15}$$

where A is a real circulant $n\times n$ symmetric matrix and B is a real circulant antisymmetric $n\times n$ matrix. Let $C=A+B$ and label the entries in the first column of C as $\hat{C}$, which determine the rest of the matrix entries of C.

(i) The ground state is degenerate if $\hat{C}$ lies in one of n linear subspaces.

(ii) One (or two, for n even) of those linear subspaces is $n-1$ dimensional and the rest are $n-2$ dimensional.

(iii) Under an orthogonal perturbation away from these subspaces, the ground-state energy gap grows as $\Omega(\sqrt{n})$.

Proof. The ground-state energy gap of $\mathcal{H}$ is twice the least singular value of C, so let us find the singular values of C. Circulant matrices form a commutative ring ([24], p. 201), so if A and B are circulant, then so are C and $C^\dagger$. Circulant matrices also have the nice property that they are diagonalized by the discrete Fourier transform matrix ([25], p. 124)

$$F_n=\frac{1}{\sqrt{n}}\begin{pmatrix} e^{(0\cdot 0)2\pi i/n} & e^{(0\cdot 1)2\pi i/n} & \cdots \\ e^{(1\cdot 0)2\pi i/n} & e^{(1\cdot 1)2\pi i/n} & \cdots \\ e^{(2\cdot 0)2\pi i/n} & e^{(2\cdot 1)2\pi i/n} & \cdots \\ \vdots & & \\ e^{((n-1)\cdot 0)2\pi i/n} & e^{((n-1)\cdot 1)2\pi i/n} & \cdots \end{pmatrix}. \tag{16}$$

So C and $C^\dagger$ commute and thus the singular values of C, which are the square roots of the eigenvalues of $C^\dagger C$, are equal to the magnitudes of the eigenvalues of C. Further, since the first column of F_n is constant, the first column of the equation $F_nC=\Lambda F_n$ yields the following expression for the eigenvalues of C:

$$F_n\hat{C}=\frac{1}{\sqrt{n}}\begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \vdots \\ \lambda_n \end{pmatrix}. \tag{17}$$

Evidently $\mathcal{H}$ has a degenerate ground state if $\lambda_k=0$ for some k. Let us define vectors f_k^R and f_k^I from the real and imaginary parts of the kth row of F_n. Since C is real, setting the real and imaginary parts of λ_k to zero yields the following two equations:

$$0=\mathrm{Re}[\lambda_k]=\sqrt{n}f_k^R\hat{C}, \tag{18}$$

$$0 = \mathrm{Im}[\lambda_k] = \sqrt{n} f_k^I \hat{C}. \tag{19}$$

Since the first element of f_k^R is $1/\sqrt{n}$ and the first element of f_k^I is zero, the only way these two equations are dependent is if Eq. (19) is trivially zero. That only occurs for $k=1$, and if n is even, for $k=(n/2)+1$; in those cases, λ_k is zero if and only if $\hat{C}$ lies in the $(n-1)$-dimensional subspace defined by Eq. (18). Otherwise, $\lambda_k=0$ if and only if $\hat{C}$ lies in an $(n-2)$-dimensional subspace defined by Eqs. (18) and (19). The first two parts of the theorem are thus proved.

Now let us assume that $\hat{C}$ lies in the kth degenerate subspace (i.e., $\lambda_k=0$) and consider a perturbation $\Delta\hat{C}$ that is orthogonal to that subspace. We want to know how fast the ground-state energy gap grows, so we need to find $|\Delta\lambda_k|$.

If $\Delta\hat{C}$ is orthogonal to the subspace, then $\Delta\hat{C}=\alpha f_k^R+\beta f_k^I$ for some α and β. Then we can substitute into Eq. (17) and multiply both sides by $\sqrt{n}$. Using the double-angle formula for sine, we see that f_k^R and f_k^I are orthogonal, yielding

$$\mathrm{Re}[\Delta\lambda_k] = \alpha\sqrt{n}\|f_k^R\|^2, \tag{20}$$

$$\mathrm{Im}[\Delta\lambda_k] = \beta\sqrt{n}\|f_k^I\|^2. \tag{21}$$

For $k\neq 1$ and $k\neq(n/2)+1$, it can be shown using trigonometry identities that $\|f_k^R\|^2=\|f_k^I\|^2=1/2$, and so we have

$$|\Delta\lambda_k| = \frac{\sqrt{n}}{2}\sqrt{\alpha^2+\beta^2}. \tag{22}$$

Otherwise we have $\|f_k^R\|=1$, $\|f_k^I\|=0$, and so

$$|\Delta\lambda_k| = \sqrt{n}|\alpha|. \tag{23}$$

Thus the final part of the theorem is proved. ■

It should be noted that while circulant matrices yield to elegant analysis, similar results could be obtained for interaction matrices derived from other boundary conditions. For instance, if C is symmetric Toeplitz tridiagonal (Toeplitz matrices are those with constant diagonals), then its eigenvalues may be found analytically ([26], p. 158). Analyses of the two- and three-dimensional interaction grids would then build on the one-dimensional analysis in exact analogy to the circulant case.

Now let us consider the case of a two-dimensional lattice of interacting fermions with periodic boundary conditions. The A and B matrices then have a block structure such as

$$A = \begin{pmatrix} A_0 & I & & & I \\ I & A_0 & I & & \\ & \cdot & \cdot & \cdot & \\ & & I & A_0 & I \\ I & & & I & A_0 \end{pmatrix},$$

$$B = \begin{pmatrix} 0 & B_0 & & & B_0 \\ B_0 & 0 & B_0 & & \\ & \cdot & \cdot & \cdot & \\ & & B_0 & 0 & B_0 \\ B_0 & & & B_0 & 0 \end{pmatrix}, \tag{24}$$

where B_0 and A_0 are as in Eq. (14). Notice that B is antisymmetric even though it is block symmetric because B_0 is antisymmetric. Evidently, each block is circulant and A and B are circulant in the blocks. Such matrices are called "block circulant with circulant blocks" (BCCB). Let us assume that the blocks are $p\times p$ and there are q blocks per row, so $n=pq$.

Theorem IV.2 (Ground-state energy gaps for BCCB A and B matrices). Let A and B be $n\times n$ BCCB matrices with $p\times p$ blocks and q blocks per row, so $pq=n$. Assume A is real symmetric and B is real antisymmetric. Define the quadratic fermionic Hamiltonian $\mathcal{H}$ with A and B as in Eq. (6). Let $C=A+B$ and label the first column of C as $\hat{C}$. Then the ground state is degenerate if $\hat{C}$ lies in one of n linear subspaces. A perturbation in A or B from these subspaces results in a $\Omega(\sqrt{n})$ increase in the ground-state energy gap.

Proof. It is easy to check that $C=A+B$ is BCCB. Then $TCT^\dagger$ is diagonal [27], where

$$T = \begin{pmatrix} F_p & & \\ & F_p & \\ & & \ddots \end{pmatrix} P_y \begin{pmatrix} F_q & & \\ & F_q & \\ & & \ddots \end{pmatrix}, \tag{25}$$

and P_y is a permutation matrix that reorders the columns as $(1, p+1, 2p+1, \ldots, (q-1)p+1, 2, p+2, 2p+2, \ldots)$. The matrix T diagonalizes C by first diagonalizing the blocks of C, then reordering the rows and columns so that the matrix is block diagonal with circulant blocks, and finally diagonalizing those blocks. Geometrically, this procedure can be thought of as a Fourier transform first along the horizontal axis of the lattice and then along the vertical axis.

Also, since $C^\dagger$ is BCCB with $p\times p$ blocks and q blocks per row, $C^\dagger$ is diagonalized by the same matrix and thus commutes with C. So the singular values of C are the magnitudes of the eigenvalues of C.

We can check that each entry of the first column of T is $1/\sqrt{n}$. So, in analogy to Eq. (17), a linear transform T applied to the first column of C yields the eigenvalues of C. The rest of the argument is essentially identical to the proof of Theorem IV.1. ■

We can even analyze a three-dimensional lattice of interacting fermions. Then the A and B matrices are as in Eq. (24), but A_0 and B_0 are BCCB instead of circulant. Let us call these matrices "block circulant with BCCB blocks" or $(\mathrm{BC})^2\mathrm{CB}$.

Theorem IV.3 (Ground-state energy gaps for $(\mathrm{BC})^2$CB A and B matrices). Let A and B be $n\times n$ $(\mathrm{BC})^2$CB matrices. Let the number of blocks be r and the BCCB blocks contain q circulant sub-blocks each $p\times p$, so $n=pqr$. Define the quadratic fermionic Hamiltonian $\mathcal{H}$ with A and B as in Eq. (6). Let $C=A+B$ and label the first column of C as $\hat{C}$. Then the

ground state is degenerate if $\hat{C}$ lies in one of n linear subspaces. A perturbation in A or B away from these subspaces results in a $\Omega(\sqrt{n})$ increase in the ground-state energy gap.

Proof. The proof is analogous to that of Theorem IV.2, but we set

$$T = \begin{pmatrix} F_p & & \\ & F_p & \\ & & \ddots \end{pmatrix} P_y \begin{pmatrix} F_q & & \\ & F_q & \\ & & \ddots \end{pmatrix} P_z \begin{pmatrix} F_r & & \\ & F_r & \\ & & \ddots \end{pmatrix}, \tag{26}$$

where P_z is a permutation matrix that reorders the columns as $(1, pq+1, 2pq+1, \ldots, (r-1)pq+1, 2, pq+2, 2pq+2, \ldots)$. This transformation first diagonalizes the BCCB blocks, then permutes rows and columns to obtain a block-diagonal matrix with circulant blocks and diagonalizes the remaining blocks. ■

V. EVOLUTIONS OF QUADRATIC FERMIONIC HAMILTONIANS

In this section we show how the previous results on quadratic fermionic Hamiltonians can be extended to Hamiltonian evolutions. For the case of circulant A and B matrices, we discuss how to perturb an evolution to ensure that the minimum ground-state energy gap is large. We analytically derive the minimum ground-state energy gap of the one-dimensional Ising model.

We choose, as our simple initial Hamiltonian,

$$\mathcal{H}_0 = \sum_{j=1}^{n} (2c_j^\dagger c_j - I_{2^n}) = \sum_{j=1}^{n} (c_j^\dagger c_j - c_j c_j^\dagger). \tag{27}$$

The ground state of this Hamiltonian is easy to construct. For example, for electrons in a metal, c_j is the annihilation operator for electron occupation at site j, and then the ground state of $\mathcal{H}_0$ is the state with each site unoccupied. Written in the form of Eq. (6), we have $A=I_n$ and $B=0$. As an example, let us define the Hamiltonian evolution $\mathcal{H}(s)$, where

$$\mathcal{H}(s) = (1-s)\mathcal{H}_0 + s \sum_{j,k=1}^{n} [A_{j,k}(c_j^\dagger c_k - c_j c_k^\dagger) + B_{j,k}(c_j^\dagger c_k^\dagger - c_j c_k)]. \tag{28}$$

Then $\mathcal{H}(s)$ is a quadratic fermionic Hamiltonian for all $s \in [0,1]$. To find the ground-state energy gap of $\mathcal{H}(s)$, we define

$$\breve{A}(s) = (1-s)I_n + sA,$$

$$\breve{B}(s) = sB. \tag{29}$$

Then we can rewrite Eq. (28) as

$$\mathcal{H}(s) = \sum_{j,k=1}^{n} \breve{A}_{j,k}(s)(c_j^\dagger c_k - c_j c_k^\dagger) + \breve{B}_{j,k}(s)(c_j^\dagger c_k^\dagger - c_j c_k), \tag{30}$$

and twice the least nonzero singular value of $\breve{A}(s)+\breve{B}(s)$ is the ground-state energy gap of $\mathcal{H}(s)$. We cannot directly use Theorem III.3 to establish that the ground-state energy gap of $\mathcal{H}(s)$ in Eq. (28) is large for all s, since Theorem III.3 is a probabilistic result for a single random Hamiltonian.

Observe that since the identity matrix I_n is circulant, then if A and B are circulant then so are $\breve{A}(s)$ and $\breve{B}(s)$, and the analysis in Theorem IV.1 can be applied to the whole evolution. Analogous results hold for the BCCB and BC^{2}CB cases. In the case of the one-dimensional Ising model with periodic boundary conditions, we have

$$\breve{C}(s) = \breve{A}(s) + \breve{B}(s) = \begin{pmatrix} 1-s & s & & & & \\ & 1-s & s & & & \\ & & \ddots & \ddots & & \\ & & & & & s \\ s & & & & & 1-s \end{pmatrix}.$$

We want to find twice the least singular value of $\breve{C}(s)$. Following the proof of Theorem IV.1, we define the first column of $\breve{C}(s)$ as $\hat{C}$ and then the singular values of $\breve{C}(s)$ are the magnitudes of the components of $\sqrt{n}F_n\hat{C}$, which can be written explicitly as

$$\lambda_k(s) = (1-s) + s\left[\cos\left(\frac{2\pi(k-1)(n-1)}{n}\right) + i\sin\left(\frac{2\pi(k-1)(n-1)}{n}\right)\right]. \tag{31}$$

Then we have

$$|\lambda_k(s)|^2 = (1-s)^2 + s^2 + 2(1-s)s\cos\left(\frac{2\pi(k-1)(n-1)}{n}\right). \tag{32}$$

Evidently $|\lambda_k(s)|^2 > (1-s)^2+s^2-0.5$ for $s \in [0,1]$. So for $s \neq 0.5$, as n increases, we have that $\lambda_k(s)$ is bounded below by a constant independent of n and k. Thus we only need to consider $s=0.5$, where

$$|\lambda_k(s)|^2 = \frac{1}{2}\left[1 + \cos\left(\frac{2\pi(k-1)(n-1)}{n}\right)\right]. \tag{33}$$

We get zero, and thus a level crossing at $s=0.5$, if the argument to cosine is an odd multiple of π. For n even, that happens for $k-1=n/2$. For n odd, it is impossible—the numerator is always even and the denominator always odd—so no level crossing occurs. Since the argument to cosine is restricted to a lattice of spacing $2\pi/n$, for n odd the argument may not get closer than $2\pi/n$ to an odd integer multiple of π. It follows from Taylor expansion of cosine that $|\lambda_k(s)|^2$ is at least $\Omega(1/n^2)$ and so the ground-state energy gap is at least $\Omega(1/n)$.

In general, it is only the $(n-1)$-dimensional subspaces where the Hamiltonians have degenerate ground states that pose any difficulty for adiabatic evolution, for those subspaces divide the space of Hamiltonians in two and no evolution may cross the divide without encountering a ground-state degeneracy. For n odd, the only $(n-1)$-dimensional subspace is defined by $C_{n,1}=-\Sigma C_{j,1}$. This subspace can be avoided: if the final Hamiltonian lies on the same side of the

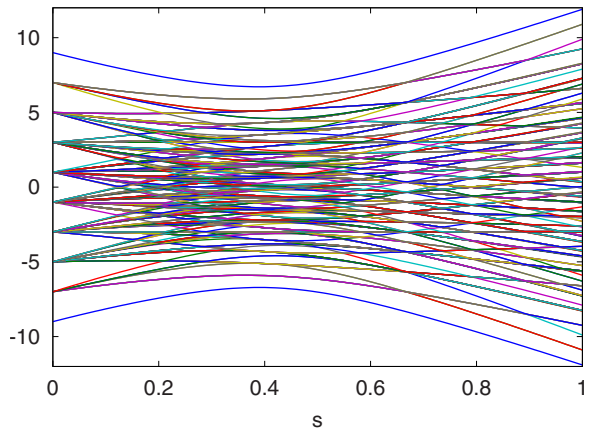


FIG. 2. (Color online) Energy spectrum as a function of s for a two-dimensional lattice of interacting fermions, using the A and B matrices from Eq. (24), in reduced units. The minimum ground-state energy gap is larger than most of the other minimum-energy gaps.

divide as $\mathcal{H}_0$, nothing needs to be done. Otherwise, use $-\mathcal{H}_0$ as an initial Hamiltonian instead. The $(n-2)$-dimensional subspaces effectively represent "strings" in the space and can be avoided, if necessary, by using a non-straight-line path [28–30].

Also, suppose the ground-state energy gap is small because of a close approach to the kth degenerate subspace. Then we can perturb the evolution to increase the minimum ground-state energy gap by adding multiples of f_k^R and f_k^I to $\hat{C}(s)$.

Figure 2 shows the evolution of the spectrum from $\mathcal{H}_0$ to an example nine-qubit Hamiltonian with BCCB interactions. Evidently the ground-state energy gap is much larger than most of the other gaps.

VI. REPRESENTATIONS OF THE HAMILTONIANS

Using the Jordan-Wigner transformation, we can define Hamiltonians using other kinds of particle operators that also have large ground-state energy gaps. In the Hubbard model of free electrons, interaction terms such as $c_j^\dagger c_k^\dagger - c_j c_k$ do not occur because they do not conserve the number of electrons. However, they may occur in spin systems transformed into fermionic representations. The best-known example is the Hamiltonian resulting from the Jordan-Wigner transformation applied to the XY model [10]. Let us first identify *all* the Hamiltonians that, under the Jordan-Wigner transformation [31]

$$c_j = (-1)^{j-1}\sigma_1^z\sigma_2^z\cdots\sigma_{j-1}^z\left(\frac{\sigma_j^x - i\sigma_j^y}{2}\right),$$

$$c_j^\dagger = (-1)^{j-1}\sigma_1^z\sigma_2^z\cdots\sigma_{j-1}^z\left(\frac{\sigma_j^x + i\sigma_j^y}{2}\right), \tag{34}$$

yield a quadratic fermionic Hamiltonian in the form of Eq. (6). Theorem VI.1 is equivalent to the result in ([32] p. 4), but using a different basis representation.

Theorem VI.1 (Quadratic fermionic Hamiltonians represented with Pauli operators). There is a bijection between Hamiltonians on n qubits of the form

$$\mathcal{H} = \sum_{j=1}^{n} W_{j,j}\sigma_j^z + \sum_{k>j} W_{j,k}\sigma_j^x\sigma_{j+1}^z\cdots\sigma_{k-1}^z\sigma_k^x + \sum_{k>j} W_{k,j}\sigma_j^y\sigma_{j+1}^z\cdots\sigma_{k-1}^z\sigma_k^y, \tag{35}$$

where the coefficients $W_{j,k}$ are real, and Hamiltonians of the form

$$\mathcal{H} = \sum_{j,k=1}^{n} A_{j,k}(c_j^\dagger c_k - c_j c_k^\dagger) + B_{j,k}(c_j^\dagger c_k^\dagger - c_j c_k), \tag{36}$$

where $\{c_j : j = 1,\ldots,n\}$, defined by Eq. (34), satisfy the FCRs, A is a real symmetric $n\times n$ matrix, and B is a real antisymmetric matrix. The bijection is given by the invertible transformation

$$A_{j,j} = W_{j,j},$$

$$A_{j,k\neq j} = A_{k,j} = \frac{(-1)^{k-j+1}}{2}(W_{j,k} + W_{k,j}),$$

$$B_{j,k\neq j} = -B_{k,j} = \frac{(-1)^{k-j+1}}{2}(W_{j,k} - W_{k,j}). \tag{37}$$

Proof. Apply Eq. (34) to Eq. (36) and use the commutation relations for Pauli operators to simplify the result. ■

Using Theorem VI.1, we can restate earlier results in a surprisingly simple manner. First, observe that application of Theorem VI.1 to $\mathcal{H}_0$ defined in Eq. (27) yields

$$\mathcal{H}_0 = \sum_{j=1}^{n} \sigma_j^z. \tag{38}$$

The ground state of $\mathcal{H}_0$ is the configuration with each particle in a spin-down eigenstate of σ^z. If $\mathcal{H}_P$ is in the form of Eq. (35), then so is the Hamiltonian evolution

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n} \sigma_j^z + s\mathcal{H}_P \tag{39}$$

for $0 \le s \le 1$.

Next, observe that, up to sign, the elements of the matrix W are the same as those of $A+B$. So to find the ground-state energy gap for a Hamiltonian that can be written in the form of Eq. (35), we only need to apply the necessary sign changes to the elements of W, find the least nonzero singular value of the resulting matrix, and multiply by 2. Thus Theorem III.3 can be applied to the Hamiltonians in Eq. (35) yielding a simple result:

Theorem VI.2 (Ground-state energy gaps of Hamiltonians defined using Pauli operators with Gaussian coefficients). Let $\mathcal{H}$ be defined by Eq. (35), where the elements of W are $N(0,1)$ and independent. Let γ be the ground-state energy gap of $\mathcal{H}$. Then, for large n, $n\gamma^2/4$ converges in distribution to the probability density function

$$\rho(x) = \frac{1+\sqrt{x}}{2\sqrt{x}} e^{-(x/2+\sqrt{x})}. \tag{40}$$

Proof. Observe that the entries of W are, up to sign, those of $A+B$ as defined by Theorem VI.1. Thus $A+B$ has independent $N(0,1)$ entries, so we have the same proof as Theorem III.3. ■

The one-dimensional cluster state, while not universal for quantum computing, is useful for gaining intuition about cluster states [33]. It is known that the Hamiltonian whose ground state is the one-dimensional cluster state can be mapped onto the one-dimensional Ising model [33]. However, the results in this section and Sec. V give an alternative proof that the one-dimensional cluster state can be realized in polynomial time using AQC.

The third-order interaction terms in Eq. (35) are exactly the stabilizers of the one-dimensional cluster state [34]. In fact,

$$\mathcal{H} = -\sum_{j=1}^{n-2} \sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^x + (-1)^{n-1} \sigma_1^y \sigma_2^z \sigma_3^z \cdots \sigma_{n-2}^z \sigma_{n-1}^y + (-1)^{n-1} \sigma_2^y \sigma_3^z \sigma_4^z \cdots \sigma_{n-1}^z \sigma_n^y \tag{41}$$

is a Hamiltonian whose ground state is the one-dimensional cluster state. By Theorem VI.1, A and B matrices corresponding to $\mathcal{H}$ are circulant and so Theorem IV.1 applies. The discussion of Sec. V implies the existence of an adiabatic evolution from $\mathcal{H}_0$ to $\mathcal{H}$ with a large minimum ground-state energy gap.

In general, we can define Fermi operators using spin-S operators provided $2S+1=2^n$ for some n [16]. For instance, using n spin-3/2 particles, we can define $2n$ Fermi operators by

$$c_{1,j} = \frac{-1}{\sqrt{3}} S_j^- S_j^z S_j^- \prod_{k<j} \left[\frac{5}{4} - (S_k^z)^2 \right], \tag{42}$$

$$c_{2,j} = \frac{1}{\sqrt{3}} \left(\frac{1}{2} + S_j^z \right)^2 S_j^- \prod_{k<j} \left[\frac{5}{4} - (S_k^z)^2 \right], \tag{43}$$

where S^x, S^y, and S^z are spin-3/2 operators and $S^{\pm} = S^x \pm iS^y$. While the standard Jordan-Wigner transform applied to a one-dimensional chain of spin-1/2 particles results in a tridiagonal B matrix, the spin-3/2 transform applied to a one-dimensional chain of spin-3/2 particles yields a pentadiagonal B matrix.

VII. CONCLUSION

We showed that polynomially large ground-state energy gaps are rare in many-body quantum Hermitian operators, but the gap is generically polynomially large for quadratic fermionic Hamiltonians. In addition to Hamiltonians with random interactions, we derived analytic results for the ground-state energy gap of lattices in one, two, and three dimensions. We extended the analysis to Hamiltonian evolutions. Our results on fermionic lattices, under the Jordan-Wigner transformation, imply that the ground states of certain nonlocal Hamiltonians may be found efficiently, including the one-dimensional cluster state.

Since quadratic fermionic Hamiltonian evolutions are classically simulatable, the adiabatic quantum computations in this article are simulatable. Thus we have provided a polynomial-time classical algorithm for finding properties of the ground states of certain random-interaction Hamiltonians and fermionic interaction lattices in one, two, and three dimensions.

It should be noted that the Jordan-Wigner transformation can be generalized to higher dimensions, e.g., [35]. Interesting results may follow from application of these alternate transformations to our theorems.

Some fermionic systems may only approximately decouple into "noninteracting quasiparticles," unlike the exact decouplings studied here. These systems may be "approximately" classically simulatable and have "approximately" polynomially large ground-state energy gaps. This may be interesting to explore.

In the Hamiltonians studied here the decoupling transformation is both known to exist and easy to find explicitly. Perhaps similar results could be obtained for systems where the transformation is known to exist but difficult to find explicitly.

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APPENDIX: PROOF OF THE LIEB *et al.* THEOREM

For completeness we include a proof of Theorem II.1. We first need the property that the fermionic commutation relations are preserved under certain unitary transformations.

Theorem A.1 (Unitary transformations). Suppose the operators $\{c_j : j=1,\ldots,n\}$ obey the FCRs. Let

$$T = \begin{pmatrix} U & V \\ V & U \end{pmatrix}, \tag{A1}$$

where U and V are real $n \times n$ matrices and suppose T is unitary. Define the set of operators $\{\eta_j : j=1,\ldots,n\}$ by

$$\begin{pmatrix} \eta_1 \\ \vdots \\ \eta_n \\ \eta_1^\dagger \\ \vdots \\ \eta_n^\dagger \end{pmatrix} = T \begin{pmatrix} c_1 \\ \vdots \\ c_n \\ c_1^\dagger \\ \vdots \\ c_n^\dagger \end{pmatrix}, \tag{A2}$$

where Eq. (A2) denotes the transformation

$$\eta_j = \sum_{i=1}^{n} T_{j,i} c_i + T_{j,i+n} c_{i+n}^\dagger. \tag{A3}$$

Then $\{\eta_j : j=1,\ldots,n\}$ also obey the FCRs.

Proof. The proof follows from substituting the definitions of $\{\eta_j : j=1,\ldots,n\}$ into the FCRs, and using the known commutation relations on $\{c_j, c_j^\dagger : j=1,\ldots,n\}$. ■

Now we are ready to prove Theorem II.1.

Proof of Theorem II.1. We write Eq. (6) as

$$\mathcal{H} = (c_1^\dagger \ \cdots \ c_n^\dagger \ c_1 \ \cdots \ c_n) \begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_n \\ c_1^\dagger \\ \vdots \\ c_n^\dagger \end{pmatrix}. \tag{A4}$$

The theorem is equivalent to showing there are solutions to

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} = \frac{1}{2}\begin{pmatrix} (X+Y) & (X-Y) \\ (X-Y) & (X+Y) \end{pmatrix}^\dagger \begin{pmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{pmatrix} \times \frac{1}{2}\begin{pmatrix} (X+Y) & (X-Y) \\ (X-Y) & (X+Y) \end{pmatrix} \tag{A5}$$

for some non-negative real $n \times n$ diagonal matrix Λ, where X and Y are unitary. If so, then substituting Eq. (A5) into Eq. (A4) and using the definition of η_k, we get

$$\mathcal{H} = \sum_{k=1}^{n} (\Lambda_k \eta_k^\dagger \eta_k - \Lambda_k \eta_k \eta_k^\dagger). \tag{A6}$$

Further, by Theorem A.1, $\{\eta_k : k=1,\ldots,n\}$ satisfy the FCRs. So we can apply the FCRs to the second term in each summand to get Eq. (8).

Now we set about finding solutions to Eq. (A5). We rewrite it for convenience as

$$\begin{pmatrix} X+Y & X-Y \\ X-Y & X+Y \end{pmatrix}\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} = \begin{pmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{pmatrix}\begin{pmatrix} X+Y & X-Y \\ X-Y & X+Y \end{pmatrix}. \tag{A7,A8}$$

Equation (A8) is equivalent to the following four equations:

$$(X+Y)A - (X-Y)B = \Lambda(X+Y), \tag{A9}$$

$$(X+Y)B - (X-Y)A = \Lambda(X-Y), \tag{A10}$$

$$(X-Y)A - (X+Y)B = -\Lambda(X-Y), \tag{A11}$$

$$(X-Y)B - (X+Y)A = -\Lambda(X+Y). \tag{A12}$$

Evidently only two of the equations are independent. Adding and subtracting Eqs. (A9) and (A11) yield

$$X(A-B) = \Lambda Y, \tag{A13}$$

$$Y(A+B) = \Lambda X. \tag{A14}$$

We can left multiply by Λ to get

$$\Lambda X(A-B) = \Lambda^2 Y, \tag{A15}$$

$$\Lambda Y(A+B) = \Lambda^2 X, \tag{A16}$$

and then substitute Eq. (A14) into Eq. (A15) and Eq. (A13) into Eq. (A16) to get the pair of eigendecomposition equations

$$Y(A+B)(A-B) = \Lambda^2 Y, \tag{A17}$$

$$X(A-B)(A+B) = \Lambda^2 X. \tag{A18}$$

Since A is real symmetric and B is real antisymmetric, $(A+B)^\dagger = A-B$ and so $(A-B)(A+B)$ and $(A+B)(A-B)$ are symmetric positive semidefinite. So there is always a unitary X and Y with non-negative diagonal Λ^2 satisfying Eqs. (A17) and (A18). ■

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