Topology and phases in fermionic systems

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Abstract. There can exist topological obstructions to continuously deforming a gapped Hamiltonian for free fermions into a trivial form without closing the gap. These topological obstructions are closely related to obstructions to the existence of exponentially localized Wannier functions. We show that by taking two copies of a gapped, free fermionic system with complex conjugate Hamiltonians, it is always possible to overcome these obstructions. This allows us to write the ground state in matrix product form using Grassmann-valued bond variables, and show insensitivity of the ground state density matrix to boundary conditions.

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The distinction between different phases of matter is one of the most basic ideas in condensed matter and statistical physics. In general, following Landau, to go between two states of different symmetry in a classical system requires a phase transition, unless a symmetry breaking field is turned on. In the case of quantum systems, similar ideas about symmetry hold. Suppose there exist two local Hamiltonians, $H_0$ and $H_1$, which both have an energy gap, $\Delta E$, between a sector of approximately degenerate ground states and the rest of the spectrum. Then we ask: can one find a family of local Hamiltonians, $H_s$, which depend continuously on $s$ and interpolate between $H_0$ and $H_1$ such that the gap remains open?

If so, then it is possible to go from $H_0$ to $H_1$ without a quantum phase transition. However, if so, then the technique of quasi-adiabatic [1] continuation can be applied and leads, in certain cases, to a proof that there must be a phase transition due to an obstruction. For example in a ferromagnetic transverse field Ising model, $H = J \sum_{i,j,n.n.} S_i^z S_j^z + B \sum_i S_i^y$, one can show that it is not possible to continue from a Hamiltonian with $J \gg B$ in the ferromagnetic phase to one with $B \gg J$ in the paramagnetic phase without a phase transition unless one violates the Ising symmetry: one cannot have all of the $H_s$ invariant under a global flip of all the spins. This is a case of a symmetry obstruction.

However, there can be even worse obstructions. In the case of a topological obstruction, such as in the fractional quantum Hall effect, where $H_0$ has a multiply degenerate ground state on a torus, any path in parameter $H_s$, if it includes only local Hamiltonians, can only produce an exponentially small splitting in the ground state sector [1,2] unless the gap to the rest of the spectrum is closed. Here, symmetry does not play a role. A generalization of this kind of topological obstruction was presented in [3], where it was shown that if all local operators have exponentially small matrix elements between the ground states for $H_0$, then this is preserved under quasi-adiabatic continuation.

In general, we will take the ability to interpolate between two different Hamiltonians, while preserving appropriate symmetries, without closing the gap as a definition of what it means to be in the same phase. Our main result here is the construction of such a path in parameter space for a simple but important class of systems: free fermion systems. These systems in some cases possess topological obstructions to continuation back to a trivial system, where we call a system trivial if there are no terms in the Hamiltonian coupling different sites. Examples of such topological obstructions include Majorana number and Chern number [4]. The key idea of the construction in this paper is to evade these obstructions by doubling the system, taking two copies which are time reverses of each other. This approach will always work, as we show, for non-interacting systems; for interacting systems it will work if the interacting system can be continued to a non-interacting system, but it will fail in cases of strong interaction when topological order causes the ground state degeneracy to depend on the topology of the system.

Then, given the path in parameter space $H_s$, for $s = 0$ to $1$, between the original Hamiltonian $H_0$ and a trivial Hamiltonian $H_1$, we use quasi-adiabatic continuation to write the ground state of the original system in a matrix product form [5] and show insensitivity to boundary conditions, a question naturally raised by work in [6] and [7] where similar results were found for bosonic systems; another, less efficient, way to write the ground state in a matrix product form is using thermal operators following [12].
be the free fermionic lattice Hamiltonian. The Hilbert space on each site \( i \) has two possible states, and \( \Psi_i^\dagger, \Psi_i \) are the creation and annihilation operators. \( \mathcal{H} \) is a many-body operator, while the \( H_{ij} \) represent the matrix elements of a Hermitian \( V \)-by-\( V \) matrix \( \hat{H} \) and \( \Delta_{ij} \) are the matrix elements of an antisymmetric \( V \)-by-\( V \) matrix \( \Delta \). Let \( \text{dist}(i,j) \) be a metric on the lattice. Assume that the spectrum of the many-body Hamiltonian \( \mathcal{H} \) has a gap \( \Delta E \) between the ground state and the first excited state. Note that if \( \Delta = 0 \), then the ground state is definite filling fraction, obtained by occupying all the negative energy eigenstates, and leaving all the positive energy eigenstates open; this filling fraction can be tuned by adding a chemical potential term, which is simply a constant shift in the matrix \( \hat{H} \), and in this case the gap \( \Delta E \) is non-vanishing precisely when the chemical potential lies in a gap in the single-particle spectrum. When \( \Delta \neq 0 \), we can still express the requirements of a gap in \( \mathcal{H} \) in terms of the single-particle spectrum as follows: let \( A \) be the matrix

\[
A = \begin{pmatrix}
\hat{H} & \hat{\Delta} \\
\hat{\Delta}^\dagger & -\hat{H}^\dagger
\end{pmatrix},
\]

so that

\[
\mathcal{H} = \frac{1}{2} (\Psi, \Psi^\dagger) \cdot A \cdot (\Psi, \Psi^\dagger),
\]

where \( (\Psi, \Psi^\dagger) \) is the 2\( V \)-dimensional vector \((\Psi_1, \Psi_2, \ldots, \Psi_V, \Psi_1^\dagger, \Psi_2^\dagger, \ldots, \Psi_V^\dagger)\). This implies that the eigenvalue of \( A \) which is smallest in absolute value is equal to the gap \( \Delta E \) in absolute value.

We assume that \( \mathcal{H} \) is local in the following sense: for some constant \( \mu > 0 \), and for some constant \( s_1 \), then for all \( i \), we have the bound \( 2 \sum_j \exp[\mu \text{dist}(i,j)] \sqrt{|H_{ij}|^2 + |\Delta_{ij}|^2} \leq s_1 \). This implies the existence of a Lieb–Robinson bound [8]–[10]: there are some velocity \( v \) and some constant \( c \) depending only on \( \mu, s_1 \) such that for any operators \( O_X, O_Y \) with support on sets \( X, Y \) we have \( \| [O_X(t), O_Y] \| \leq c \times |X| \| O_X \| \| O_Y \| \exp[-\mu \text{dist}(X,Y)] (\exp(v|t|) - 1) \).

We introduce a system defined on two copies of the original lattice, with the same two-state Hilbert space on each site of each copy. We label sites on this system by \((i, a)\), where \( i \) has \( V \) possible values and \( a = \uparrow, \downarrow \), and \( \Psi_{i,a}^\dagger, \Psi_{i,a} \) are the creation and annihilation operators. We use the metric \( \text{dist}'(\{(i, a), (j, b)\}) = \text{dist}(i, j) + (1 - \delta_{a,b}) \).

We set \( \mathcal{H}_0 \) to be the sum of \( \mathcal{H} \) on the first copy and \( \mathcal{H}^* \) on the second copy. We now define the continuous family of Hamiltonians with this Hilbert space:

\[
\mathcal{H}_s = \sqrt{1 - s^2} \mathcal{H}_0 + s \Delta E \sum_i \left( \Psi_{i,\uparrow}^\dagger \Psi_{i,\uparrow} + \text{h.c.} \right).
\]
The results that we now show are that: (1) for all \( s, 0 \leq s \leq 1 \), the Hamiltonian \( \mathcal{H}_s \) has a gap equal to \( \Delta E \); (2) for all \( s, 0 \leq s \leq 1 \), the Hamiltonian \( \mathcal{H}_s \) obeys the same Lieb–Robinson bound as \( \mathcal{H} \), namely \( 2\sqrt{1-s^2} \sum_j \exp[\mu \text{dist}(i,j)] \sqrt{|H_{ij}|^2 + |\Delta_{ij}|^2 + s^2 \Delta E} \leq s_1 \leq \infty \); (3) the ground state of \( \mathcal{H}_1 \) is a product wavefunction of the form

\[
|\Psi\rangle = \left( \prod_i \left( \frac{1}{\sqrt{2}} \Psi^\dagger_{i,1} \Psi^\dagger_{i,1} + \frac{1}{\sqrt{2}} \right) \right) |0\rangle,
\]

where \(|0\rangle\) is the state where all sites are empty. The proof of (3) is immediate. To prove (2), note that \( \Delta E \) is bounded above by \( s_1 \) so that we may estimate the operator norm of \( s\Delta E(\Psi^\dagger_{i,1} \Psi^\dagger_{i,1} + \text{h.c.}) \).

We finally consider (1). Define the matrix \( C_s \) by

\[
C_s = \begin{pmatrix} \sqrt{1-s^2}A & s\Delta E \mathbb{I} \\ s\Delta E \mathbb{I} & \sqrt{1-s^2}A \end{pmatrix},
\]

where \( \mathbb{I} \) is the unit 2\( \times \)2 matrix.

Then,

\[
\mathcal{H}_s = \frac{1}{2}(\Psi_1, \Psi^\dagger_1, \Psi^\dagger_1, \Psi_1)^\dagger \cdot C_s \cdot (\Psi_1, \Psi^\dagger_1, \Psi^\dagger_1, \Psi_1).
\]

For each eigenvalue \( \lambda \) of \( A \), \( C_s \) has two eigenvalues equal to \( \pm \sqrt{(1-s^2)\lambda^2 + s^2 \Delta E^2} \). Since the smallest eigenvalue of \( A \) was equal to \( \Delta E \) in absolute value, the same holds for \( C_s \) and hence (1) follows.

Finally, we comment on the reason for doubling the system, presenting two examples of topological obstructions. The first example is a one-dimensional example based on the idea of Majorana number [4]. We consider a periodic chain of \( V \) sites, labeled \( j = 1 \ldots V \). We define the operators \( c_{2j-1} = \Psi_j + \Psi^\dagger_j \) and \( c_{2j} = (\Psi_j - \Psi^\dagger_j)/i \), thus giving Majorana operators \( c_k \) defined for \( k = 1 \ldots 2V \). A quadratic Hamiltonian for a Majorana system is defined by a matrix \( A \) as in equation (2), while the ground state \( \Psi_0 \) of the Hamiltonian has correlators given by

\[
\langle \Psi_0 | c_j c_k | \Psi_0 \rangle = \delta_{jk} - iB_{jk},
\]

where the antisymmetric matrix \( B \) obeying \( B^2 = -1 \) is given by \( B = -\text{isgn}(A) \). Consider the state \( \Psi_{\text{odd}} \) defined by the matrix \( B_{\text{odd}} \) with \( (B_{\text{odd}})_{ij} = \delta_{i+1,j} \) if \( i = 1 \) mod 2 and \( (B_{\text{odd}})_{ij} = \delta_{i-1,j} \) if \( j = 1 \) mod 2. This state is the state in which every site is occupied: \( \langle \Psi_{\text{odd}} | \Psi^\dagger_1 | \Psi_{\text{odd}} \rangle = 1 \). Now consider the state \( \Psi_{\text{even}} \) defined by \( (B_{\text{even}})_{ij} = (B_{\text{odd}})_{i+1,j+1} \). Kitaev defines a Majorana number for any antisymmetric matrix \( B \) obeying \( B^2 = -1 \) such that \( B_{jk} \) decays sufficiently rapidly in \( \text{dist}(j,k) \). The Majorana number is an integer equal to \( \pm 1 \) for an infinite chain, and is close to \( \pm 1 \) for a finite chain depending on how the chain length compares to the rate at which the coefficients decay.

The Majorana number has opposite signs for the states \( \Psi_{\text{odd}}, \Psi_{\text{even}} \). This means that there is no way to find a family of free fermion Hamiltonians \( \mathcal{H}_s \) which are local and gapped which have ground state \( \Psi_{\text{even}} \) for \( s = 0 \) and \( \Psi_{\text{odd}} \) for \( s = 1 \). To show this, suppose that such a family did exist. Then, given a gapped Hamiltonian, the matrix \( B_s \) has matrix elements \( (B_s)_{ij} \) decaying exponentially rapidly in \( |i-j| \) due to locality of correlation functions [11] and hence has a well-defined Majorana number up to corrections.
which tend to zero as \( V \) becomes large compared to the correlation length, and hence the Majorana number cannot change sign in this evolution.

However, doubling the chain evades this topological obstruction as the Majorana number is always even for the doubled system. The second example is in two dimensions [4]. Consider a matrix \( P \) such that \( P^2 = P \) and such that \( P_{jk}^2 \) is sufficiently rapidly decaying in \( \text{dist}(j, k) \). Then Kitaev defines a quantity \( \nu(P) \) for such a matrix which generalizes the notion of Chern number. This quantity \( \nu(P) \) is shown to be equal to an integer in an infinite system, and to be close to an integer in a finite system, the error depending on how the decay of the coefficients in \( \text{dist}(j, k) \) compares to the system size.

For any gapped local Hamiltonian of the form \( H = \Psi_1^\dagger H \Psi_j \) (so that there are no pairing terms: \( \Delta = 0 \)), we can define a projector \( P_{jk} = \langle \Psi_0 | \Psi_j^\dagger \Psi_k | \Psi_0 \rangle \). Since the Hamiltonian is gapped, the correlations in the ground state \( \Psi_0 \) will be short range, and hence \( P_{jk} \) will decay exponentially rapidly in \( \text{dist}(j, k) \). Hence, if the system size is sufficiently large compared to the correlation length, \( \nu(P) \) will be close to an integer. A factorized wavefunction has \( \nu(P) = 0 \), so therefore there is no way to continue from a gapped Hamiltonian with non-vanishing \( \nu(P) \) to a Hamiltonian with a factorized ground state without either closing the gap or violating locality. However, by doubling the system, and using the complex Hamiltonian for the second of the two copies, we evade this obstruction, since the total Chern number of the \( P \) defined by the ground state of \( H \), system vanishes for all \( s \): at \( s = 0 \) it cancels between the two copies.

**Quasi-adiabatic continuation and matrix product ground state**—The existence of a family of Hamiltonians (4) implies that the ground state of \( H_0 \) can be represented as a matrix product state as follows. The results that follow are valid for arbitrary families of local Hamiltonians \( H_s \), which have a gap for all \( 0 \leq s \leq 1 \) and which have a trivial ground state at \( s = 1 \), so we develop them in generality. Let \( l \) be some arbitrary length scale. Let us write an arbitrary local Hamiltonian \( H_s \) as \( \sum_{Z} H_Z(s) \), where \( H_Z(s) \) has support only on set \( Z \); in this specific problem of free fermions, \( Z \) will always be a set of one or two sites. Using the technique of quasi-adiabatic continuation, we can define a Hermitian operator \( D \) such that \( \partial_s \Psi_0(s) = iD_Z(s) + \sum_{Z} \mathcal{O}([Z] \exp[\sqrt{1/\xi}||\partial_s H_Z(s)||/[\Delta E]) \), where the correlation length \( \xi = 2\nu/\sqrt{\Delta E} + \mu \). The operator \( D_Z(s) \) has support on the set of sites within distance \( l \) of \( Z \), and has \( ||D_Z(s)|| \leq \sqrt{1/\xi}||\partial_s H_Z(s)||/[\Delta E] \). For a free fermion system, as here, the operator \( D_Z(s) \) is a bilinear in the fermion operators.

Then, for sufficiently large \( l \), we can get a good approximation to the \( \Psi_0(0) \) with

\[
\Psi_0(0) \approx \exp \left[ i \int_1^0 D_s \, ds \right] \Psi_0(1), \tag{9}
\]

and then we can approximate the exponential by a matrix product operator of some given bond dimension, so that we can approximate \( \Psi_0 \) as a matrix product state. It remains only to estimate the errors involved in the particular case to determine how large the bond dimension of the matrix product state must be. For (4), we have \( |Z| \leq 2 \) and \( ||\partial_s H_Z(s)|| \leq s_1 \), so for some \( c_1 \) which is a numeric constant of order unity, then for \( l = c_1 \log(Vs_1/[\Delta E]) + c_2 \xi \), equation (9) gives an approximation to \( \Psi_0(0) \) with error of order \( \exp[-c_2] \). The unitary operator \( \exp[i \int_1^0 D_s \, ds] \) can be regarded as time evolution under an effective time dependent Hamiltonian \( D_s \). This effective Hamiltonian has a Lieb–Robinson group velocity which we denote \( \xi' \) which is bounded by a constant of order

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unity times $s_1 l / \Delta E$. Then, for the given $l$, we can approximate $\exp[i \int_{-1}^0 D_s ds']$ with error $\epsilon$ by a matrix product operator $U_{\text{mps}}$ as follows.

This kind of approximation was discussed for one-dimensional spin systems in [13]. The construction of [13] proceeds by breaking the one-dimensional system into short intervals labeled 1, 2, ..., and showing that the unitary operator can be approximately written as a quantum circuit: $V_{1,2} V_{2,3} \ldots U_1 U_2 \ldots$, where the operators $U_1, U_2, \ldots$ act only on each interval 1, 2, ... and the unitary operators $V_{i,i+1}$ act only on the right half of interval $i$ and the left half of interval $i+1$, so that $[U_i, U_j] = [V_{i,i+1}, V_{j,j+1}] = 0$. This construction can be directly generalized to higher dimensions [14]. As a next step, auxiliary bond variables are introduced to write the operators $V_{i,i+1}$ as a sum of product of operators on interval $i$ and interval $i+1$.

In our problem, in order to decompose the operator $V_{i,i+1}$ into a sum of products of operators, we must introduce Grassmann-valued bond variables. In order to approximate the unitary evolution to an error $\epsilon$, we need the number of Grassmann-valued bond variables on each bond to be logarithmically large in $\xi$ (for the spin system, the bond dimension is exponentially large in this quantity). Thus, we can approximate $\Psi(0)$ by a matrix product state $\Psi_{\text{mps}} = U_{\text{mps}} \Psi(0)$ with Grassmann-valued bond variables. We note that the bond dimension required for this free fermion system is much smaller than that for quasi-adiabatic continuation of a general interacting system, where a bond dimension polylogarithmically large in $V$ may be required, because $D_Z$ is a fermion bilinear.

Sensitivity to boundary conditions—The final question that we consider is the sensitivity of such a gapped fermion system (4) to boundary conditions at $s = 0$. Consider two systems with Hamiltonians $\mathcal{H}, \mathcal{H}'$ which agree on some set of sites $X$ in the following sense: for any operator $O$ with support on $X$, $[O, \mathcal{H}] = [O, \mathcal{H}']$. Now, let $Y$ be some subset of $X$ such that the set of all points $i$ with $\text{dist}(i, Y) \leq l$ is a subset of $X$. We then consider the difference between the reduced density matrices, $\rho_Y, \rho_Y'$, of the two systems. We will show that as $l$ gets large, the difference between the two density matrices converges to zero in trace norm. Physically, this may be viewed as a statement about insensitivity to boundary conditions: even if two systems differ at the ‘boundary’ (that is, outside $X$), far enough away from the boundary (that is, inside $Y$ for large enough $l$) the physical properties will be the same.

We again use quasi-adiabatic continuation. We take two copies of each system, and define a continuous family of Hamiltonians $\mathcal{H}_s, \mathcal{H}_s'$ as above, so that $\mathcal{H}_1 = \mathcal{H}_1'$. Let $\Psi_0(s), \Psi'_0(s)$ be the ground states of these Hamiltonians. Then [1] for any operator $O$ with support on $Y$ we can define an operator $O(s)$ such that $O(s)$ is supported on $X_1(\Psi_0(1)|O(1)|\Psi_0(1)) - (\Psi_0(0)|O|\Psi_0(0))) | \leq \epsilon$ where the error $\epsilon$ is exponentially small in $l$ [1]. Since $\mathcal{H}_s, \mathcal{H}_s'$ agree on $X$, we find that also $| \langle \Psi_0(1)|O(1)|\Psi_0(1)\rangle - \langle \Psi_0(0)|O|\Psi_0(0)\rangle | \leq \epsilon$. However, since $\mathcal{H}_1 = \mathcal{H}_1'$, we have $\langle \Psi_0(1)|O(1)|\Psi_0(1)\rangle = \langle \Psi_0'(1)|O(1)|\Psi_0'(1)\rangle$, and so $| \langle \Psi_0(0)|O|\Psi_0(0)\rangle - \langle \Psi_0'(0)|O|\Psi_0'(0)\rangle | \leq 2\epsilon$ for any $O$ with support on $Y$. Therefore, we can bound the trace norm distance between $\rho_Y$ and $\rho_Y'$: $\text{tr}(|\rho_Y - \rho_Y'|) \leq 2\epsilon$. We can estimate $\epsilon$ in the specific case of a $d$-dimensional free fermionic system to get

$$\text{tr}(|\rho_Y - \rho_Y'|) \leq \text{const} \times |Y| \sqrt{l/v \Delta E s_1} \exp[-l/\xi'] \xi'^d. \quad (10)$$

Discussion and Wannier functions—Can there be topological obstructions to continuing a time reversal symmetric undoubled system back to a trivial system? One
possible example is the spin Hall state [15], but by turning on an external magnetic field, breaking the time reversal symmetry, it is possible to continuously deform the undoubled Hamiltonian to a trivial Hamiltonian.

In order to understand possible obstructions in time reversal symmetric systems better, we consider Wannier functions. We say that a system has exponentially localized Wannier functions if one can find a basis of states $|\phi_n\rangle$ which span the occupied states of the free fermion system (so that the Green’s function is equal to $G = \sum_n |\psi_n\rangle \langle \phi_n|$) and which are exponentially localized in real space. Such functions have long been considered for periodic systems, as well as more recently for disordered systems [17].

If a free fermion Hamiltonian $H_0$ can be continued to a trivial Hamiltonian $H_1$, then exponentially localized Wannier functions exist: the Hamiltonian $H_1$ has Wannier functions $|\phi_n\rangle$, where each $|\phi_n\rangle$ has support on a single site. Then, by quasi-adiabatically continuing from $H_1$ to $H_0$, we can find exponentially localized Wannier functions for $H_0$. Only very recently [16] was it shown that for time reversal symmetric, periodic systems in two and three dimensions exponentially localized Wannier functions do exist, in that case without any doubling required. On the other hand, the proof in [16] suggests that there exist time reversal symmetric, four-dimensional, periodic systems for which exponentially localized Wannier functions do not exist. These systems would be in a different topological phase from a trivial Hamiltonian, and even by adding a magnetic field it is not possible to continue back to the trivial Hamiltonian without closing a gap.

An interesting open question is when such exponentially localized Wannier functions must exist for gapped, undoubled, time reversal symmetric, disordered systems. In one dimension, with open boundary conditions, this can be shown as follows: let $X$ be the position operator. Then, $GXG$ is a Hermitian operator and can be diagonalized; because $G$ is short range due to the gap [11], the eigenvectors of $GXG$ are exponentially localized in real space and hence can be used as Wannier functions. In two dimensions, we consider the pair of operators $GXG, GYG$. These operators almost commute, since $\| [GXG, GYG] \| \sim O(1) \ll \| GXG \| \sim L$, where $L$ is the linear size of the system. If these operators are close to a pair of commuting operators we could simultaneously diagonalize those operators and use their eigenfunctions as Wannier functions. The question of when almost commuting operators are close to commuting operators is well studied [18], and those results can be used to show that given a family of systems of increasing size $L$ and constant gap, then for any $\delta > 0$ for sufficiently large $L$ we can define Wannier functions localized on a scale $\delta L$. In three dimensions, we have three almost commuting operators $GXG, GYG, GZG$, which need not be close to commuting operators as shown in [19].

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