

Exact Solution of Quadratic Fermionic Hamiltonians for Arbitrary Boundary Conditions

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We present a procedure for exactly diagonalizing finite-range quadratic fermionic Hamiltonians with arbitrary boundary conditions in one of D dimensions, and periodic in the remaining $D - 1$. The key is a Hamiltonian-dependent separation of the bulk from the boundary. By combining information from the two, we identify a matrix function that fully characterizes the solutions, and may be used to construct an efficiently computable indicator of bulk-boundary correspondence. As an illustration, we show how our approach correctly describes the zero-energy Majorana modes of a time-reversal-invariant s -wave two-band superconductor in a Josephson ring configuration, and predicts that a fractional 4π -periodic Josephson effect can only be observed in phases hosting an odd number of Majorana pairs per boundary.

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Developing a quantitative understanding of the physical properties of fermionic systems in the presence of non-trivial boundaries has widespread significance from both a fundamental and applied perspective. Not only has the behavior of fermions at a boundary informed leading material-characterization techniques like angle-resolved photoemission spectroscopy [1] and the revolution in metrology brought about by the integer quantum Hall effect [2]; nowadays, surface states of topological insulators and Majorana boundary modes of topological superconductors [3,4] play a central role in state-of-the-art proposals ranging from coherent spintronics [5,6] to topological quantum computation [7,8].

All of the above phenomena are linked by a common theme: topologically nontrivial band structures [4]. Band structure theory, including the topological classification of mean-field fermionic systems [9], rests on a manifestation of crystal translational symmetry, the Bloch theorem. Since translational symmetry is broken by the presence of a boundary, it is remarkable that there exists a connection between the topological nature of the bulk and the boundary physics—the bulk-boundary (BB) correspondence [4,10]. This principle states that a topologically nontrivial bulk mandates the emergence of fermionic states localized on the boundary, when boundary conditions (BCs) are changed from periodic to open, and that such states are distinguished by their *robustness* against symmetry-preserving local perturbations. While this heuristics has been numerically validated in a variety of cases, and rigorous results exist for discrete-time systems described by one-dimensional quantum walks [11], no general analytic insight is available as yet. Allowing for *arbitrary* BCs is necessary for any theory of BB correspondence to capture the robustness of the emerging localized modes to different perturbations [12]. Further motivation stems from studies of quantum quenches [13,14], where robustness against

changes of the BCs has been argued to control the (quasi) local symmetries that characterize the stationary properties in the bulk. Tackling these issues calls for a procedure to determine energy eigenstates of lattice Hamiltonians with arbitrary BCs, comparable in conceptual and computational power to what the Fourier transform accomplishes in the periodic case.

In this work, we introduce a methodology for diagonalizing in closed form finite-range quadratic fermionic Hamiltonians with translational symmetry broken by arbitrary BCs. Our central insight is a generalization of Bloch's theorem built on the recognition that a useful separation of the bulk from the boundary should be model-dependent. We identify an *indicator* for BB correspondence, that exploits both information about the bulk—encoded in “generalized Bloch states”—and the nature of the boundary—encoded in a “boundary matrix.” For periodic BCs, we prove that, generically, such indicator predicts *no* localized edge state irrespective of the bulk structure. As an application, we explore the Josephson response of an s -wave, time-reversal-invariant two-band topological superconductor (TS) introduced in [15], and show how the boundary matrix reveals that a fractional Josephson effect occurs *only* in the phase with one pair of Majoranas per boundary, consistent with the physical picture based on fermion parity switches [16]. Mathematically, our approach generalizes existing algorithms for diagonalizing banded Toeplitz matrices [17] to the block-Toeplitz case with arbitrary corner modifications, with complexity independent upon system size.

Model Hamiltonians.—Consider fermionic systems defined on a one-dimensional lattice consisting of $j = 0, \dots, L - 1$ identical cells, each containing $m = 1, \dots, d$ internal degrees of freedom, associated for instance to spin and orbital motion. Let the creation (annihilation) operator for mode labeled by (j, m) be denoted by $c_{j,m}^\dagger$ ($c_{j,m}$), and let

$\psi_j^\dagger \equiv [c_{j,1}^\dagger c_{j,2}^\dagger \cdots c_{j,d}^\dagger c_{j,1} c_{j,2} \cdots c_{j,d}]$ be the corresponding $(2d)$ -dimensional Nambu vector. We consider finite-range R , $R \ll L$, disorder-free quadratic Hamiltonians of the form

$$\hat{H} = \frac{1}{2} \sum_{r=0}^R \left(\sum_{j=0}^{L-r-1} \psi_j^\dagger h_r \psi_{j+r} + \sum_{j=L-r}^{L-1} \psi_j^\dagger g_r \psi_{j+r-L} + \text{H.c.} \right), \quad (1)$$

where the matrices h_r and g_r describe hopping and pairing among fermions situated r cells apart in the bulk and, respectively, at the boundary. In this way, standard periodic and open BCs correspond to $g_r = h_r$ and $g_r = 0$, $\forall r$. Hamiltonians of the form (1) arise ubiquitously in mean-field descriptions of fermionic systems as realized in both solid-state and cold-atom platforms [18–20].

Analyzing the single-particle sector of \hat{H} suffices to study its many-body spectrum [18]. That is, we let $\hat{H} = \frac{1}{2} \Psi^\dagger H \Psi$, with $\Psi^\dagger \equiv [\psi_0^\dagger \dots \psi_{L-1}^\dagger]$. In this way, the Hilbert space \mathcal{H} on which the single-particle Hamiltonian H acts may be conveniently factorized into the tensor product of two subsystems, $\mathcal{H} \simeq \mathbb{C}^L \otimes \mathbb{C}^{2d} \equiv \mathcal{H}_L \otimes \mathcal{H}_I$, associated with lattice and internal factors. Let the operators $c_{j,m}$ and $c_{j,m}^\dagger$ be associated with vectors $|j\rangle|m\rangle$ and $|j\rangle|m+d\rangle$, respectively. In the basis $\{|j\rangle|m\rangle | 0 \leq j \leq L-1, 1 \leq m \leq 2d\}$, H is given by

$$H = \sum_{r=0}^R [T^r \otimes h_r + (T^\dagger)^{L-r} \otimes g_r + \text{H.c.}], \quad (2)$$

where T is the left-shift operator $T|j\rangle \equiv |j-1\rangle$, $\forall j \neq 0$, $T|0\rangle \equiv 0$, and T^\dagger implements the corresponding right shift. Thus, H is a “corner-perturbed” banded block-Toeplitz matrix with $2R+1$ bands. Namely, the r th off-diagonal bands above and below the diagonal have blocks given by bulk interaction matrices h_r and h_r^\dagger , respectively, whereas boundary terms appear in the corner of the matrix. The $(L-r)$ th off-diagonal bands above and below the diagonal, which lie close to the corners, consist of blocks given by g_r^\dagger and g_r , respectively.

Periodic boundary conditions revisited.—Periodic BCs are employed in calculations of band structure and bulk topological invariants alike [4]. In this case, the single-particle Hamiltonian H in Eq. (2) is a circulant block-Toeplitz matrix, which may be expressed as $H = \sum_{r=0}^R (V^r \otimes h_r + \text{H.c.})$, in terms of the cyclic left-shift operator $V \equiv T + (T^\dagger)^{L-1}$. Crucially, translational symmetry implies that H , V , and V^\dagger form a commutative set, allowing for the eigenspectrum of H to be determined via standard discrete Fourier transform from the lattice to the momentum basis on \mathcal{H}_L . For later reference, let us introduce the generalized z -transformed lattice basis,

$$|z\rangle \equiv \frac{1}{\sqrt{N(z)}} \sum_{j=0}^{L-1} z^j |j\rangle, \quad z \in \mathbb{C}, \quad z \neq 0, \quad (3)$$

where $N(z)$ is a normalization constant, and define the “reduced bulk Hamiltonian” $h_B(z)$ as the matrix-valued symbol [21] of the block-Toeplitz matrix without boundary terms:

$$h_B(z) \equiv \sum_{r=0}^R (z^r h_r + z^{-r} h_r^\dagger). \quad (4)$$

The generalized discrete Fourier transform in Eq. (3) associates z with the pseudomomentum k , with $z \equiv e^{ik}$ and $k \equiv 2\pi q/L$, $q \in \{0, 1, \dots, L-1\}$, defining the (first) Brillouin zone. Then, the eigenvectors of H may be expressed as $|\epsilon\rangle \equiv |z\rangle|u(\epsilon, z)\rangle$, where $|u(\epsilon, z)\rangle$ is the eigenvector of the reduced bulk Hamiltonian $h_B(z)$ with eigenvalue ϵ —which is simply a reformulation of the familiar Bloch theorem. The cyclic shift symmetry restricts solutions to the Brillouin zone, and z to lie on the unit circle. Therefore, by diagonalizing $h_B(z)$ for all q , the complete quasiparticle energy spectrum and the corresponding eigenvectors may be obtained.

As lattice translation ceases to be a symmetry, the discrete Fourier transform fails to diagonalize H . In particular, the left and right shift operators T and T^\dagger do not share a common eigenbasis, calling for a different diagonalization approach. We next introduce a new diagonalization method that relies on a mapping of the Brillouin zone to the full complex plane.

Bulk-boundary separation and bulk equation.—Hamiltonians with arbitrary BCs are locally symmetric under left and right shifts in the bulk; however, these symmetries are explicitly broken at and near the boundaries. The crux of our approach consists of separating bulk from boundary subsystems. To this end, we define orthogonal projectors onto the bulk, $\mathcal{P}_B \equiv \sum_{j=R}^{L-R-1} |j\rangle\langle j|$, and onto the boundary, $\mathcal{P}_\partial \equiv \mathbb{1}_L - \mathcal{P}_B$, where $\mathbb{1}_L$ is the L -dimensional identity operator on \mathcal{H}_L . The eigenvalue equation for H then splits into a bulk and a boundary equation: $\mathcal{P}_B H |\epsilon\rangle = \epsilon \mathcal{P}_B |\epsilon\rangle$, and $\mathcal{P}_\partial H |\epsilon\rangle = \epsilon \mathcal{P}_\partial |\epsilon\rangle$. The advantage of such a separation is that one obtains *simultaneous* (relative) eigenvectors of the bulk-projected T and T^\dagger operators. The resulting eigenvalue equations are: $\mathcal{P}_B T^r |z\rangle = z^r \mathcal{P}_B |z\rangle$, $\mathcal{P}_B (T^\dagger)^r |z\rangle = z^{-r} \mathcal{P}_B |z\rangle$, $\forall r, r' \leq R$, while $\mathcal{P}_B T^r = 0 = \mathcal{P}_B (T^\dagger)^{r'}$, $\forall r, r' \geq L-R$. As for periodic BCs, it follows that these “generalized Bloch states” are of product form $|z\rangle|u(\epsilon, z)\rangle$, where as above $|u(\epsilon, z)\rangle$ is an eigenvector of $h_B(z)$ with eigenvalue ϵ .

By construction, $h_B(z)$ is a *small* matrix, of dimension $2d \times 2d$. If $\mathbb{1}_I$ denotes the $2d$ -dimensional identity operator on \mathcal{H}_I , the relevant characteristic equation establishes a functional relationship between ϵ and z , of the form

$$P(\epsilon, z) \equiv z^{2dR} \det[(h_B(z) - \epsilon \mathbb{1}_I)] = 0, \quad (5)$$

where the prefactor z^{2dR} ensures that $P(\epsilon, z)$ is a bivariate polynomial in ϵ and z , of degree at most $(2R)(2d) = 4dR$. In general, there may exist multiple generalized Bloch

states corresponding to a given value of ϵ . Let $z_\ell(\epsilon)$, $\ell = 1, \dots, n$, denote the (nonzero) distinct roots of Eq. (5) for the given ϵ , and $s_\ell(\epsilon)$ the corresponding number of linearly independent eigenvectors of $h_B(z_\ell)$ [that is, the nullity of $(h_B(z_\ell) - \epsilon \mathbb{1}_l)$]. The eigenvectors of H may then be written as linear combinations of degenerate generalized Bloch states:

$$|\epsilon\rangle \equiv \sum_{\ell=1}^n \sum_{s=1}^{s_\ell} \alpha_{\ell,s} |z_\ell(\epsilon)\rangle |u_s(\epsilon, z_\ell)\rangle, \quad \alpha_{\ell,s} \in \mathbb{C}. \quad (6)$$

In this way, the solutions of the bulk equation provide an ansatz for the eigenvectors of H , where the amplitudes $\alpha_{\ell,s}$ are yet to be determined [22]. Of particular interest is the ansatz for $\epsilon = 0$, which provides a family of *possible* zero-energy modes of the system, independent of the BCs. Notice that the solution of the bulk equation alone does *not* imply the existence of an excitation at a given value of ϵ , unless the boundary equation is simultaneously satisfied.

In general, $h_B(z)$ is *not* Hermitian, except on the unit circle $|z| = 1$. This is not surprising since such an effective Hamiltonian represents an open system, with no boundaries and no torus topology [23]. Generalized Bloch states exist for every $z \neq 0$, realizing an over-complete set of solutions of the bulk equation. Those consistent with values of z on the unit circle are in one-to-one correspondence with the solutions of the infinite periodic system. The rest correspond to solutions with exponential behavior, providing a continuation off the Brillouin zone. Thus, Eq. (6) may be regarded as a generalization of the Bloch theorem to arbitrary BCs, with Eq. (5) providing a natural analytic continuation of the dispersion relation.

Boundary equation and emergence of localized modes.—The ansatz (6) yields an eigenvector of H only if the boundary equation, $\mathcal{P}_\partial(H - \epsilon \mathbb{1})|\epsilon\rangle = 0$, is satisfied for appropriate $\alpha_{\ell,s}$, with $\mathbb{1}$ denoting the identity operator on \mathcal{H} . For notational simplicity, let us assume that $s_\ell = 1$, $\forall \ell, \epsilon$, so that $\alpha_{\ell,s} \equiv \alpha_\ell$ and $n = 4dR$ (see [22,24] for the general case). To make the action of the projector \mathcal{P}_∂ explicit, it is convenient to isolate the $4dR$ basis states in \mathcal{H} that correspond to lattice sites on the boundary, by letting $\{|b\rangle \equiv |j\rangle|m\rangle | 0 \leq j \leq R-1, L-R \leq j \leq L-1; 1 \leq m \leq 2d\}$. The above boundary equation may then be rewritten as $\sum_{\ell=1}^n \alpha_\ell B_{L,b\ell}(\epsilon) = 0$, where the “boundary matrix” $B_L(\epsilon)$ for size L and energy ϵ is the matrix with entries given by

$$[B_L(\epsilon)]_{b\ell} = B_{L,b\ell}(\epsilon) \equiv \langle b | (H - \epsilon \mathbb{1}) | z_\ell(\epsilon) \rangle | u_1(\epsilon, z_\ell) \rangle. \quad (7)$$

By construction, any set of values of $\{\alpha_\ell\}$ satisfying Eq. (7) is a vector in the kernel of $B_L(\epsilon)$. Thus, the boundary equation may be restated as $\det[B_L^\dagger(\epsilon)B_L(\epsilon)] = 0$. When this condition is obeyed, ϵ is an eigenvalue of H , with degeneracy equal to the nullity of $B_L(\epsilon)$.

For fixed BCs (fixed g_r), the localized modes of the system and their energies show asymptotic behavior in the thermodynamic limit, $L \rightarrow \infty$, which our method enables

us to characterize analytically. A localized mode in the thermodynamic limit has constituent generalized Bloch states with $|z_\ell| \neq 1$. This allows a simplification in the boundary matrix, as any L -dependent terms in $B_L(\epsilon)$ may be replaced by the appropriate limit, given by $\lim_{L \rightarrow \infty} z_\ell^L \rightarrow 0$ and $\lim_{L \rightarrow \infty} z_\ell^{-L} \rightarrow 0$ for $|z_\ell| < 1$ and $|z_\ell| > 1$, respectively. The existence check for localized modes and their calculations is then carried out in the same way as in the finite- L case.

An indicator of bulk-boundary correspondence.—The boundary matrix defined in Eq. (7) points to a natural strategy for constructing useful indicators of BB correspondence based on combined information from both the bulk and the boundary. In particular, for zero-energy modes, we propose

$$\mathcal{D} \equiv \log\{\det[B_\infty^\dagger(0)B_\infty(0)]\} \quad (8)$$

as one such indicator for an infinite system. We claim that the existence of zero-energy edge modes manifests as a singularity in the value of \mathcal{D} . Consistent with this claim, we can rigorously prove that, under generic assumptions on the matrix h_r for $r = R$, the indicator \mathcal{D} is *always finite* under periodic BCs, irrespective of the bulk properties; see [24]. We remark that other indicators are also in principle applicable to systems where translational invariance is broken (notably, based on Pfaffians [25,26]); even for clean systems as we consider, however, their numerical evaluation becomes computationally demanding for large system size.

Example.—As a first illustration, we revisit the paradigmatic case of Kitaev’s p -wave TS chain with open BCs [25] (see [24] for full detail). With reference to Eq. (2), this nearest-neighbor model corresponds to $R = 1$ and 2×2 matrices $2h_0 = -\mu\sigma_z$, $h_1 = -t\sigma_z + i\Delta\sigma_y$, $g_1 \equiv 0$, where μ , t , Δ denote chemical potential, hopping, and superconducting pairing respectively, and σ_ν , $\nu = x, y, z$, are Pauli matrices in the Nambu basis. For any ϵ , the characteristic equation for $h_B(z)$, Eq. (5), is quartic in z , which enables a closed-form solution by radicals. The roots appear as two reciprocal pairs, say, $\{z_1, z_1^{-1}, z_2, z_2^{-1}\}$, where $|z_1|, |z_2| \leq 1$. For finite chain length L , the boundary equation is satisfied if any of the two equalities $f_\pm(z_1) = f_\pm(z_2)$ hold, where $f_\pm(z) = [b(z)/(\epsilon + a(z))][(1 + z^{L+1})/(1 - z^{L+1})]^\pm$, and $a(z) = \mu + t(z + z^{-1})$, $b(z) = \Delta(z - z^{-1})$ [27]. In the thermodynamic limit, the condition for zero-energy edge modes simplifies to $a(z_1)/b(z_1) = a(z_2)/b(z_2)$, which is satisfied if and only if $|\mu| < |2t|$. This parameter regime, with phase boundary $|\mu| = |2t|$, defines the topologically nontrivial phase, hosting one Majorana mode per edge. If $\mu^2 < 4|t^2 - \Delta^2|$, (z_1, z_2) form a complex conjugate pair, whereas for $\mu^2 > 4|t^2 - \Delta^2|$, both z_1 and z_2 are real. The self-adjoint Majorana mode localized on the left edge is then given by $\gamma \equiv \sum_{j=1}^{\infty} (z_1^j - z_2^j)(c_j \mp c_j^\dagger)$, for $\mu^2 \leq 4|t^2 - \Delta^2|$.

Josephson effect in two-band s-wave superconductors.—The Kitaev chain in its topologically nontrivial phase is known to exhibit a fractional Josephson effect [25], that is, the Josephson current is 4π -periodic (more generally, $2\pi l$ -periodic, with integer $l > 1$) as a function of the superconducting phase difference ϕ , and the many-body energy $E(\phi)$ correspondingly switches parity [16]. Such an effect is regarded as both a hallmark and a leading observable signature of topological superconductivity. The simplicity of the topological phase diagram in the Kitaev chain (either 0 or 1 Majorana mode per edge) allows for an unambiguous association between a trivial (nontrivial) phase and a standard (unconventional) Josephson response; however, it is not *a priori* obvious what to expect for more complex TSs, which may support phases with different numbers of Majorana modes—or, respectively, different numbers of Majorana *pairs* per edge, if time-reversal symmetry is preserved [4]. As we show next, the existence of localized Majorana modes does *not* suffice, in general, for the system to display fractional Josephson effect.

Consider the time-reversal-invariant two-band *s*-wave TS wire introduced in [15]. Based on both the original numerical solution under open BCs and analysis of the appropriate boundary matrix $B_L(0)$ [24], phases with zero, one, or two pairs of (helical) Majorana modes localized on each boundary may exist. Using a partial Berry-phase parity as a topological indicator [15], only the phase hosting one pair of Majorana modes is predicted to be topologically nontrivial. Thanks to the present analytic approach, in particular the BB indicator \mathcal{D} defined in Eq. (8), we are now in a position to correlate this prediction with the more physical—in principle experimentally accessible—Josephson response of the system.

Our results are summarized in Fig. 1. As the insets show, a fractional Josephson effect emerges *only* in the phase that is predicted to be topologically nontrivial according to its partial Berry-phase (odd) parity [24]. Some physical insight may be gained by looking at the dependence of quasiparticle energy upon flux ϕ : as seen in the top panel, the 4π periodicity is associated with a crossing of a positive and a negative quasiparticle energy level; this crossing occurs precisely at zero energy, indicating the presence of a pair of Majorana modes for the value of flux at the crossing (solid black lines). In contrast, in the trivial phase with two pairs of Majorana modes (middle panel), the level crossing does *not* occur at zero energy, leading to the standard 2π periodicity of $E(\phi)$, also found when no Majorana mode is present (bottom panel). Since these quasiparticle energy levels lie in the gap, they are localized, and we can carry out the analysis in the thermodynamic limit [24]. This reveals that, in the nontrivial phase, the boundary equation is satisfied at $\phi = \pi, 3\pi$, confirming the presence of exact zero energy modes at those values. Even more interestingly, the proposed indicator \mathcal{D} has been numerically

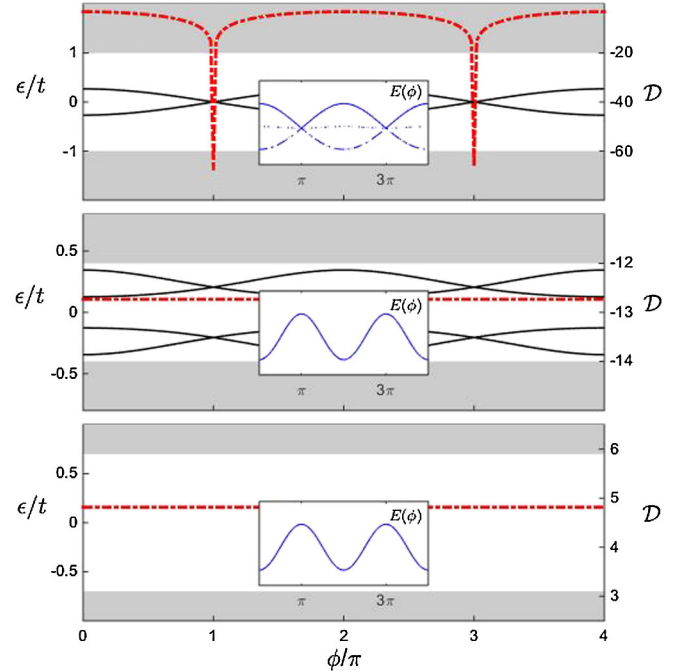


FIG. 1. Quasiparticle energies (solid black lines) and BB indicator \mathcal{D} [Eq. (8)] (dashed red line) vs flux ϕ in a phase supporting one (top), two (middle), and zero (bottom) pairs of Majorana modes per edge. The grey shaded regions indicate bulk quasiparticle energies. Insets: many-body ground state energy $E(\phi)$. With reference to [24], the parameter values are $t = \lambda = \Delta = 1$, $\mu = 0$, $w = 0.2$, $u_{cd} = 2$ (top), $u_{cd} = 0.6$ (middle), $u_{cd} = 3.7$ (bottom). In all calculations, lattice size $L = 60$ is used.

evaluated and plotted (dotted red lines): singularities clearly emerge *only* in the topologically nontrivial phase, as claimed.

Discussion.—We investigated finite-range quadratic fermionic Hamiltonians for which translational symmetry is broken only by arbitrary BCs, and showed how a Hamiltonian-dependent BB separation can make the property of the system being “almost translationally symmetric” quantitatively useful—leading to a natural generalization of the Bloch theorem. Building on this, we described an efficient diagonalization algorithm which, for $D = 1$, reduces the problem of determining the full set of eigenvalues and eigenvectors to one of finding the roots of the boundary equation. Our algorithm successfully identifies the interplay between bulk properties—captured by the generalized Bloch states $|z\rangle|u(\epsilon, z)\rangle$ —and BCs—captured by the boundary matrix, $B_L(\epsilon)$, of fixed dimension independent of L . Since the calculation of L -dependent terms in $B_L(\epsilon)$ (to fixed accuracy) may be effected in a single computation, the complexity of our algorithm is $\mathcal{O}(1)$, in contrast to $\mathcal{O}[(dL)^3]$ for generic methods of evaluating the characteristic polynomial of H .

The advantages of our algorithm extend straightforwardly to D -dimensional quadratic Hamiltonians, $D > 1$,

if the standard procedure of imposing periodic BCs in $D - 1$ directions is employed: in this way, the model reduces to a poly-sized set of $D = 1$ lattices subject to arbitrary BCs, to which our algorithm applies. We thus expect our approach to both have immediate relevance to electronic structure calculations for lattice systems, and to further elucidate gapless topological superconductivity—notably, the emergence of Majorana flat bands and anomalous BB correspondence uncovered in [28]. For more general BCs, e.g., two open directions, our model-dependent procedure for BB separation and generalized Bloch theorem go through with minor modifications. On the one hand, this prompts the question of whether the concept of a Wannier function may also be generalized for arbitrary BCs. On the other hand, the procedure for incorporating BCs is more involved, calling for separate investigation.

Beyond equilibrium scenarios, our approach should prove advantageous to evaluate in closed form the unitary propagator $\exp(-i\hat{H}t)$ describing free evolution under arbitrary BCs, and to diagonalize the Floquet propagator describing periodically driven fermionic systems [29]. Since our algorithm does not exploit the Hermiticity of the Hamiltonian, a further direction of investigation is the application to open Fermi systems obeying quadratic Lindblad master equations [30], with the potential to shed light onto BB correspondence in engineered topological phases far from equilibrium [31]. Lastly, despite important differences at the single-particle level [18], our algorithm applies to arbitrary BCs in quadratic bosonic systems. This is an intriguing observation, since there is no BB correspondence for bosons, yet a topological classification might be possible in terms of generalized, symplectic Berry phases.

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