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Pairing Obstructions in Topological Superconductors

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The modern understanding of topological insulators is based on Wannier obstructions in position space. Motivated by this insight, we study topological superconductors from a position-space perspective. For a one-dimensional superconductor, we show that the wave function of an individual Cooper pair decays exponentially with separation in the trivial phase and polynomially in the topological phase. For the position-space Majorana representation, we show that the topological phase is characterized by a nonzero Majorana polarization, which captures an irremovable and quantized separation of Majorana Wannier centers from the atomic positions. We apply our results to diagnose second-order topological superconducting phases in two dimensions. Our work establishes a vantage point for the generalization of topological quantum chemistry to superconductivity.

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Topological phases of matter represent one of the main driving forces in condensed matter physics. In their most experimentally relevant realization, topological insulators (TIs) [1–5] have garnered widespread attention owing to their protected surface states. These states can be predicted from the bulk electronic structure alone using topological invariants. All topological invariants discovered so far for translationally invariant, noninteracting systems can be phrased in terms of global momentum-space properties [6–17].

A modern approach to TIs is to characterize them in terms of their position-space structure [18–27]. This point of view is informed by the insight that, if TIs are distinguished from trivial insulators by global properties in momentum space, then Heisenberg's uncertainty principle suggests to study their local properties in position space. Within topological quantum chemistry [21], such a position-space approach has led to a classification and materials prediction program for TIs. In this approach, topology is defined as an obstruction to finding a gauge in which the Fourier transforms of Bloch eigenstates, called Wannier functions, are exponentially localized and preserve all of the symmetries.

Another important class of topological phases of matter are topological superconductors (TSCs), which have a gapped bulk spectrum and exotic edge excitations that are their own antiparticles (so-called Majorana modes) [28–32]. Recently, symmetry indicator invariants have been introduced for a momentum-space-based characterization of TSCs [33–37]. In contrast to TIs, there is, however, as of yet no unifying physical picture of the position-space structure of TSCs.

In this Letter, we present such a position-space picture of TSCs (focusing on class D in the Altland-Zirnbauer classification). The mean-field description of superconductors is formally equivalent to the band theory of noninteracting electrons. However, the ground state of a superconductor involves pairing of electrons and is, therefore, qualitatively different from the ground state of an insulator. This fact leads to striking differences between TSCs and TIs. In particular, we show that topology in superconductors can be phrased in terms of an obstruction to finding a gauge in which electron pairs are tightly (exponentially) bound. Furthermore, expressing the ground state in a basis of Majorana fermions, we find that the total spectral weight on the two Majorana degrees of freedom corresponding to each electron is split evenly, allowing us to introduce the concept of a quantized Majorana polarization. Our results are partially summarized in Fig. 1.

1D p-wave superconductor in particle-hole basis.—We consider a 1D p-wave TSC, which could be realized by a nanowire with a single conduction band that is brought in proximity with an s-wave (trivial) superconductor [38,39]. Within mean-field theory, the nanowire is described by the Hamiltonian $H = \sum_k \Psi_k^\dagger \mathcal{H}_k \Psi_k$, where we have introduced the Nambu spinor $\Psi_k = (c_k, c_{-k}^\dagger)/\sqrt{2}$ and the Bogoliubov–de Gennes (BdG) Hamiltonian

$$\mathcal{H}_k = \begin{pmatrix} \epsilon_k & \Delta_k \\ \bar{\Delta}_k & -\epsilon_{-k} \end{pmatrix}, \quad (1)$$

with μ the chemical potential and $\Delta_k = -\Delta_{-k}$ due to Fermi statistics (the bar denotes complex conjugation). The operator $c_k^\dagger$ creates an electron at momentum $k \in \{1, \ldots, N\} 2\pi/N$, and N is the number of sites (periodic boundary conditions are assumed). For $|\mu| < 2|t|$, H is in the topological phase, which

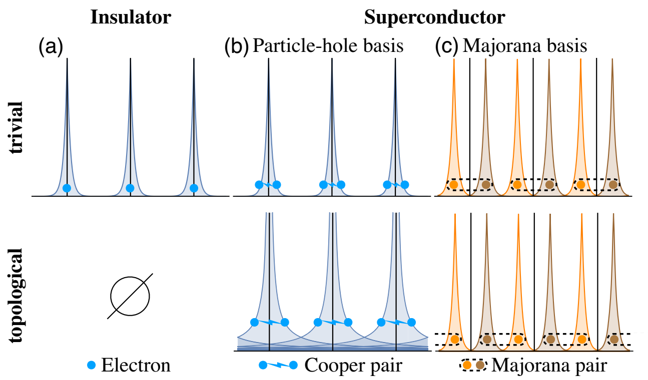

FIG. 1. Position-space picture of insulators and superconductors in 1D, with atomic sites indicated by vertical lines. (a) The ground state of an insulator as a product over Wannier states. All 1D electronic band structures (absent symmetries) can be realized by exponentially localized Wannier functions. In contrast to superconductors, there are therefore no topological insulators in 1D. (b) The fixed-particle number component of the superconducting ground state as a product of Cooper pair states with wave functions decaying exponentially in the trivial phase and polynomially in the topological phase. (c) The ground state as a product over Majorana Wannier functions with quantized *Majorana charge*. In the topological phase, Majoranas from different atomic sites are paired up, leaving behind unpaired Majorana zero modes at the boundaries.

hosts a single Majorana zero mode at each end of the nanowire, while for $|\mu| > 2|t|$ the system is in the trivial phase. We refer to the convention in Eq. (1) as the particle-hole basis. In contrast to insulators, the mean-field description of superconductors allows for the additional freedom of choosing a basis in Nambu space; this freedom is important for our position-space interpretation. We can diagonalize the Hamiltonian by introducing Bogoliubov quasiparticle operators

$$\begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ -\bar{v}_{-k} & \bar{u}_{-k} \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \equiv D_k \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}, \quad (2)$$

where the matrix D_k is unitary, with

$$\begin{aligned} u_k\bar{u}_k + v_k\bar{v}_k &= u_k\bar{u}_k + v_{-k}\bar{v}_{-k} = \mathbb{1}, \\ u_k v_{-k} + v_k u_{-k} &= \bar{u}_k v_k + v_{-k}\bar{u}_{-k} = 0. \end{aligned} \quad (3)$$

For $|\mu| \neq 2|t|$, the spectrum is gapped and H has the ground state

$$\begin{aligned} |\Omega\rangle &= \frac{1}{\mathcal{N}} \exp\left(\sum_k \frac{v_k}{u_k} c_k^\dagger c_{-k}^\dagger\right)|0\rangle \\ &= \frac{1}{\mathcal{N}} \exp\left(\sum_{xy} g_{xy} c_x^\dagger c_y^\dagger\right)|0\rangle, \\ g_{xy} &= \frac{1}{N}\sum_k e^{ik(x-y)}\frac{v_k}{u_k}, \end{aligned} \quad (4)$$

where $|0\rangle$ is the fermionic vacuum, $(-v_{-k}, u_{-k})$ is the negative-energy eigenvector of the BdG Hamiltonian $\mathcal{H}_k$, and $\mathcal{N}$ is a normalization factor. In the second line, we introduced the Fourier-transformed operators

$$c_r^\dagger = \frac{1}{N}\sum_k e^{-ikr} c_k^\dagger, \qquad r = 1\ldots N, \quad (5)$$

that create a particle at site r of the nanowire. We emphasize that the possibility of representing the ground state in the form of Eq. (4), reminiscent of a coherent state of Cooper pairs $c_k^\dagger c_{-k}^\dagger$, singles out the particle-hole basis, since it crucially relies on the anticommutation relations $\{c_p, c_q^\dagger\} = \delta_{pq}, \{c_p, c_q\} = \{c_p^\dagger, c_q^\dagger\} = 0$ of electronic creation and annihilation operators. Furthermore, extracting from Eq. (4) the contribution to the N-particle state $|\Omega_N\rangle$, we obtain the amplitudes

$$\langle r_1 \ldots r_N | \Omega_N \rangle \propto A[g_{r_1 r_2} g_{r_3 r_4} \ldots g_{r_{N-1} r_N}], \quad (6)$$

where $A[\cdot]$ denotes an antisymmetrization over all positions $r_1 \ldots r_N$. Invoking the Paley-Wiener theorem allows one to determine the large-separation dependence of g_{xy} on general grounds. In fact, g_{xy} will fall off exponentially as $|x-y| \to \infty$ if the momentum space function v_k/u_k is analytic [40,41]. On the other hand, if v_k/u_k diverges at some k, g_{xy} will at most fall off polynomially with separation.

We now relate the analytical properties of v_k/u_k to the topological characterization of the superconducting phase. We assume no further symmetries other than particle-hole symmetry (PHS), which in the particle-hole basis reads

$$P\mathcal{H}_k P^\dagger = -\mathcal{H}_{-k}, \qquad P = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} K. \quad (7)$$

PHS quantizes the Berry phase topological invariant

$$\begin{aligned} \gamma &= i\int dk(\bar{u}_k\partial_k u_k + \bar{v}_k\partial_k v_k) \mod 2\pi \\ &= \frac{i}{2}\int dk \mathrm{Tr}[D_k^\dagger \partial_k D_k] \mod 2\pi \\ &= \int_0^\pi dk\partial_k\lambda_k \mod 2\pi \\ &= (\lambda_\pi - \lambda_0) \mod 2\pi, \end{aligned} \quad (8)$$

where we wrote $\det D_k = e^{-i\lambda_k}$ and used that PHS implies $\lambda_{-k} = -\lambda_k \mod 2\pi$ and, hence, $\lambda_0, \lambda_\pi = 0, \pi$. For γ to assume values $0, \pi$, we take the BdG functions u_k and v_k to be periodic functions in momentum space. This property, together with Eq. (5), corresponds to a convention where all atomic orbitals are located at the origin of the unit cell in position space. Our results can be straightforwardly generalized to arbitrary atomic positions [42].

Now, if $\gamma = 0$, we can adiabatically deform the system to one in which only u_k is nonzero and constant. Its inverse is then always well defined, and the ground state in position space, as expressed via g_{xy}, is a coherent superposition of exponentially closely bound Cooper pairs. We next show that, if $\gamma = \pi$, there are necessarily divergences in v_k/u_k, leading to a polynomial decay of g_{xy}. The proof proceeds by contradiction. Without loss of generality, we take $\gamma = \pi$ to be realized by $\lambda_0 = 0, \lambda_\pi = \pi$, implying $\det D_0 = 1$ and $\det D_\pi = -1$. Let us assume that u_k is nonzero throughout momentum space. It therefore has a well-defined inverse, and we may reexpress $\det D_k$ as

$$\begin{aligned}\det D_k &= u_k \bar{u}_{-k}\left(\frac{u_k\bar{u}_{-k} - v_k\bar{v}_{-k}}{u_k\bar{u}_{-k}}\right)\\ &= u_k\bar{u}_{-k}\left(1 - \frac{v_k\bar{v}_{-k}}{u_k\bar{u}_{-k}}\right)\\ &= \frac{u_k}{u_{-k}} = 1 \quad \text{at } k = 0, \pi,\end{aligned} \tag{9}$$

where we used the constraints in Eq. (3). This result is, however, in contradiction to our earlier assertion that $\det D_\pi = -1$. We conclude that either u_0 or u_π are zero in systems with $\gamma = \pi$. This result carries over to an arbitrary number of bands [42].

Thus, the long-distance behavior of the Cooper pair wave function is indicative of the topological character of the phase: In the trivial phase, there is strong pairing and the wave function decays exponentially with separation, while in the topological case, there is weak pairing and the wave function decays only polynomially. This *pairing obstruction* is in close correspondence to the Wannier obstruction of TIs [21,43,53], but, in contrast to insulators [54], the particle-hole symmetry of superconductors allows for topological phases already in 1D.

1D p-wave superconductor in Majorana basis.—We introduce the Majorana modes $a_k = c_k + c_{-k}^\dagger$ and $b_k = (c_k - c_{-k}^\dagger)/i$ and the Majorana BdG functions $v_k^M = (v_k - u_k)/\sqrt{2}$ and $u_k^M = i(v_k + u_k)/\sqrt{2}$. Let a_r and b_r be the Fourier transforms of the Majorana modes [using the same convention as in Eq. (5)]. We can then re-express the ground state in Eq. (4) in terms of Majorana Wannier functions $W_{R\alpha}^M(r)$, $\alpha = a$, b, which we define by

$$\begin{aligned}|\Omega\rangle &= \frac{1}{\mathcal{N}}\prod_R\left(\sum_r W_{Ra}^M(r)a_r + W_{Rb}^M(r)b_r\right)|0\rangle,\\ \begin{pmatrix} W_{Ra}^M(r)\\ W_{Rb}^M(r)\end{pmatrix} &= \frac{1}{N}\sum_k e^{-ik(R-r)}\begin{pmatrix} -v_k^M\\ u_k^M\end{pmatrix},\end{aligned} \tag{10}$$

where R labels the position of the unit cell that the Wannier functions belong to. As for any 1D system [55], the Wannier functions $W_{R\alpha}^M(r)$ can be exponentially localized. In the unit cell, they are centered around the position

$$x_o = \sum_{r,\alpha}\bar{W}_{0\alpha}^M(r)rW_{0\alpha}^M(r) \mod 1. \tag{11}$$

(The subscript o stands for the occupied subspace spanned by the Majorana Wannier functions.) Particle-hole symmetry implies that $x_o = x_e$, where x_e denotes the center of Wannier functions built from the empty Majorana bands. The Wannier centers for all bands (which form a complete basis for the Hilbert space) are always exponentially localized on the lattice sites. We therefore have $x_o + x_e \mod 1 = 0$. We conclude that $x_o = 0, 1/2$ is quantized and provides a topological invariant characterizing the many-body ground state. In fact, we know from the general theory of maximally localized Wannier functions [55] that $x_o = \gamma/2\pi = 0, 1/2$, where γ is defined similar to Eq. (8):

$$\gamma = i\int dk(\bar{u}_k^M\partial_k u_k^M + \bar{v}_k^M\partial_k v_k^M) \mod 2\pi \tag{12}$$

(the two definitions are equivalent). Therefore, the Wannier states in Eq. (10) can be adiabatically continued back to the original delta-localized Majorana basis states at position R, created by the bare operators a_R and b_R, if and only if the Berry phase vanishes: These original basis states have Wannier functions $W_{R\alpha}^M(r) = \delta_{R,r}\delta_{\alpha,1}$ or $W_{R\alpha}^M(r) = \delta_{R,r}\delta_{\alpha,2}$, both of which correspond to $x_o = 0$. This property implies a Majorana pairing obstruction: It is impossible to adiabatically connect the topological superconducting ground state to a collection of physical (i.e., deriving from the atomic positions) electrons or holes. In contrast, in a trivial superconductor it is possible to turn off superconductivity without closing the gap between positive- and negative-energy quasiparticle states.

We next show that the Majorana representation is set apart from other basis decompositions of H in that it allows for a meaningful generalization of polarization to superconductors. Taking the trace of the Majorana version of the constraint in Eq. (3), we find that

$$\begin{aligned}\sum_k \bar{v}_k^M v_k^M &= \frac{N}{2} = \sum_k \bar{u}_{-k}^M u_{-k}^M,\\ \sum_r \bar{W}_{0\alpha}^M(r)W_{0\alpha}^M(r) &= \frac{1}{N}\sum_k\begin{pmatrix}\bar{v}_k^M v_k^M\\ \bar{u}_k^M u_k^M\end{pmatrix}_\alpha = \frac{1}{2}.\end{aligned} \tag{13}$$

This implies that the total spectral weight carried by Majoranas of a or b type is always equal, a property that is not realized in other bases: In the particle-hole basis, for example, the total spectral weight carried by holes is zero in the case of a band insulator. The total Wannier function support within a unit cell splits into equal contributions of Majoranas of a and b type. This result carries over to an arbitrary number of bands [42].

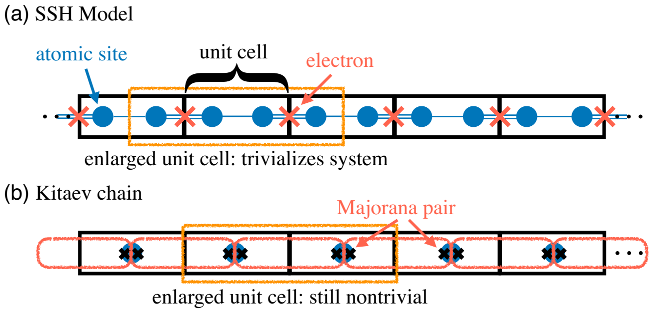

FIG. 2. Comparison of 1D topological insulators and superconductors. (a) In the Su-Schrieffer-Heeger (SSH) model [58], spatial inversion symmetry is required to pin electrons to the unit cell edges, leading to midgap states in an open geometry. However, it is possible to choose an inversion-symmetric enlarged unit cell that has no end states. (b) In the Kitaev chain [59], Majorana modes are paired across unit cells, leaving behind unpaired Majorana zero modes in an open geometry. Since unit cells may not cut through atomic sites, any enlarged unit cell shows the same topological behavior.

We therefore introduce a quantized *Majorana charge*, nominally equal to $1/2$, and a corresponding Majorana polarization [56] that is computed via Eq. (11) or, alternatively, via the Berry phase in Eq. (12). Figure 2 shows how Majorana polarization, unlike electronic polarization, survives translational symmetry breaking. We can now see how the anomalous end states of a 1D superconductor arise in the topological regime, because a Majorana polarization of $1/2$ results in a single Majorana mode localized at the end of an open geometry. Because of particle-hole symmetry, this mode is necessarily a zero-energy state.

2D chiral superconductor and generalization to higher dimensions.—The two-dimensional p-wave superconductor [28,60] can be obtained from a Thouless pump of bulk Majorana fermions. Such a superconductor is characterized by a nonzero Chern number of the occupied BdG eigenstates. We interpret this Chern number as a flow of the Majorana separation from the atomic sites [Eq. (11)] with a transversal momentum coordinate. Consider a two-dimensional BdG Hamiltonian $\mathcal{H}_{\mathbf{k}}$. Particle-hole symmetry implies $P\mathcal{H}_{\mathbf{k}}P^{\dagger} = -\mathcal{H}_{-\mathbf{k}}$, with P defined in Eq. (7). Writing $\mathbf{k} = (k_x, k_y)$, there are two special values of $k_y = 0, \pi$, at which $\mathcal{H}_{(k_x,k_y=0,\pi)} \equiv \mathcal{H}^{0,\pi}_{k_x}$ can be interpreted as the BdG Hamiltonian of a 1D superconductor. In the Majorana basis, we introduce hybrid Wannier functions that are indexed by k_y, affording a k_y-dependent Majorana polarization

$$x_o^{k_y} = \sum_{r,\alpha} \bar{W}^M_{0\alpha}(k_y, r_x) r_x W^M_{0\alpha}(k_y, r_x) \quad \mathrm{mod}\ 1. \tag{14}$$

We note again that we are working in a convention where the atomic positions are all at $\mathbf{r}_i = (0,0)$. Crucially, due to the action of particle-hole symmetry, the related Berry phase is quantized only for $k_y = 0, \pi$, namely, $x_o^{0,\pi} = \gamma^{0,\pi}/2\pi = 0, 1/2$, where γ^{k_y} is evaluated along 1D momentum-space slices of constant k_y. The Berry phase winding as a function of k_y is related to the Chern number

$$C = \frac{1}{2\pi}\int dk_y \partial_{k_y}\gamma^{k_y} = \int dk_y \partial_{k_y} x_o^{k_y}. \tag{15}$$

We conclude that, in a 2D $p_x + ip_y$ superconductor with $C = 1$, the Majorana polarization $x_o^{k_y}$ continuously evolves from 0 to $1 \equiv 0$ as k_y undergoes a noncontractible cycle. Importantly, this implies that it is impossible to exponentially localize the Majorana Wannier functions $W^M_{0\alpha}(k_y, r_x)$ also in the y direction, as they are not smooth functions of k_y.

We therefore find that a topological 2D p-wave superconductor admits neither an exponentially decaying Cooper pair function $g_{\mathbf{xy}}$ nor exponentially decaying Majorana Wannier functions $W^M_{\boldsymbol{R}\alpha}(\boldsymbol{r})$. A natural question is then if there exists a 2D superconductor with a polynomially decaying Cooper pair function but exponentially decaying Majorana Wannier functions. This "Majorana obstructed atomic limit" phase is naturally realized by the recently discovered higher-order TSCs, which feature Majorana zero modes localized at the corners of samples terminated in both the x and y directions [10,13,44,61] (Table I provides an overview). Our results imply that these phases are "stronger" than their insulating counterparts, in that they cannot be trivialized by the introduction of uncharged ancillas [62].

Our methods are, in particular, insightful for topological superconductors that cannot be diagnosed by standard

TABLE I. Overview of topological superconductors without time-reversal symmetry. The 1D chiral TSC hosts zero-dimensional Majorana end states. The 2D chiral TSC can be obtained from it via a Thouless pump, which naturally explains why its Wannier functions cannot be exponentially localized. Another possibility in 2D is the second-order TSC with Majorana corner states. In 3D, the only Wannier obstructed superconductor absent time-reversal symmetry is the second-order TSC with 1D Majorana hinge states similar to the edge states of the 2D chiral TSC.

Dimension	g_{xy} decay	$W^M_{R\alpha}(r)$ decay	Phase label
1D	Exponential	Exponential	Trivial
	Polynomial	Exponential	p-wave TSC
2D	Exponential	Exponential	Trivial
	Polynomial	Polynomial	Chiral TSC
	Polynomial	Exponential	2nd-order TSC
3D	Exponential	Exponential	Trivial
	Polynomial	Polynomial	2nd-order TSC
	Polynomial	Exponential	3rd-order TSC

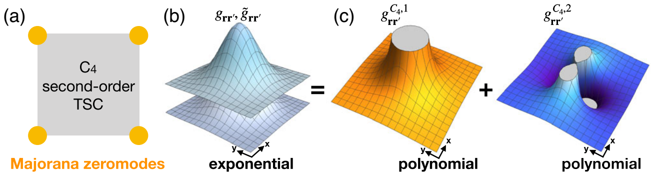

FIG. 3. Real-space structure of a C_4-symmetric second-order topological superconductor. (a) Majorana corner modes in a square-shaped sample geometry. (b) Naively, the two ground state Cooper pair wave functions [generalizations of Eq. (4)] $g_{\mathbf{rr}'}$ and $\tilde{g}_{\mathbf{rr}'}$ decay exponentially with electron separation. (c) When chosen as eigenfunctions of C_4 symmetry, the Cooper pair wave functions of each C_4 subsector, $g_{\mathbf{rr}'}^{C_4,1}$ and $g_{\mathbf{rr}'}^{C_4,2}$, necessarily decay polynomially as a consequence of the nontrivial second-order topology.

topological invariants such as (non-Abelian) Berry phases and symmetry indicators. An example are second-order topological superconductors protected by C_4 rotation symmetry and spinful time reversal [17,45,46]. These host four Kramers pairs of Majorana zero-energy states at the corners of a square-shaped sample and, otherwise, have a gapped bulk and gapped edge spectrum. Generalizing our results to 2D systems with crystalline symmetries, they too can be identified by the decay behavior of their Cooper pair wave functions: We show in the Supplemental Material [42] that the Cooper pairs *in individual C_4 eigenvalue subspaces* are subject to a pairing obstruction. See Fig. 3 for an illustration.

Discussion.—The mean-field BdG description of superconductors is uncannily similar to the Bloch description of noninteracting electrons. This has led to a remarkable amount of concept transfer and cross-fertilization between the descriptions of topological superconductors and insulators. However, it is often not clear what becomes of the physical interpretation of the mathematical quantities involved. An example is the Berry phase, which captures the electric polarization of an insulator, something that is evidently not well defined for superconductors. Employing a position-space picture phrased in terms of Cooper pairs and Majorana excitations, our work gives physical meaning to the Berry phase in the superconducting context via the notion of pairing obstruction and Majorana polarization. A natural next step would be a comprehensive inclusion of symmetries into our framework. Another area of potential future work is to use our formalism to understand the peculiarities of number-conserving models of topological superconductors [63–66].

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