Finite-Temperature Topological Invariant for Interacting Systems

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We generalize the ensemble geometric phase, recently introduced to classify the topology of density matrices, to finite-temperature states of *interacting* systems in one spatial dimension (1D). This includes cases where the gapped ground state has a fractional filling and is degenerate. At zero temperature the corresponding topological invariant agrees with the well-known invariant of Niu, Thouless, and Wu. We show that its value at finite temperatures is identical to that of the ground state below some critical temperature T_c larger than the many-body gap. We illustrate our result with numerical simulations of the 1D extended superlattice Bose-Hubbard model at quarter filling. Here, a cyclic change of parameters in the ground state leads to a topological charge pump with fractional winding $\nu = 1/2$. The particle transport is no longer quantized when the temperature becomes comparable to the many-body gap, yet the winding of the generalized ensemble geometric phase is.

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Introduction.—Starting with the discovery of the quantum Hall effect [1–5] topology has become an important paradigm for the understanding and classification of phases of matter [6–8]. Topology is characterized by integer-valued invariants which describe global properties of the system and are responsible for the robustness of characteristic features like quantized bulk transport, or edge states and edge currents. Invariants such as the winding of the geometric Zak phase or the Chern number of single-particle Bloch functions are defined in terms of the wave function of ground states and are thus restricted to cases where the system is in a pure state.

In recent years several attempts have been made to generalize the concept of topology to finite temperatures and to nonequilibrium steady states of noninteracting fermions [9–18]. For example, it was shown that the generalization of geometric phases to density matrices based on the Uhlmann construction [19] leads to consistent topological invariants in 1D [11,12]. Its application to higher dimensions [13] is, however, faced with difficulties [20]. Other approaches predict an unphysical extensive number of topological phases for arbitrarily small temperatures [16].

Recently, it was shown that the winding of the many-body polarization introduced by Resta [21] is an alternative topological invariant for Gaussian mixed states of fermions in 1D, termed ensemble geometric phase (EGP) [15,17,22], which can also be applied in 2D [23]. It was shown that the EGP of finite-temperature states in noninteracting systems is reduced to the ground-state Zak phase in the thermodynamic limit $L \to \infty$ and thus these states have the same topological classification as the corresponding ground states (following the Altland-Zirnbauer classification [24–26]). Despite being a genuine many-body quantity the EGP can be measured directly [17]. Furthermore, a nontrivial winding of the EGP of a finite-temperature or nonequilibrium steady state upon cyclic parameter variations has direct physical consequences. E.g., it can lead to quantized transport in a weakly coupled auxiliary system initially prepared in a low temperature state [27]. For noninteracting bosons the EGP winding is always zero [28].

In the present Letter, we extend this concept to the case of interactions between particles including the possibility of interaction-induced fractionalization and degeneracy. We show that a generalization of the EGP to systems with a gapped ground state of fractional filling allows us to define a topological invariant for finite-temperature states of one-dimensional systems of *interacting* particles. The winding of the EGP reduces to the well-known Niu-Thouless-Wu (NTW) invariant [29,30] at $T = 0$ and has the same value for all temperatures below a certain critical value. The EGP also provides a theoretical tool to detect topological order present in the ground state in cases where the gap is small or numerical calculations are restricted to nonzero temperatures. We illustrate our results with numerical simulations of the extended superlattice Bose-Hubbard model (Ext-SLBHM) [31] at quarter filling, where the ground state is a doubly degenerate Mott insulator (MI).

Ensemble geometric phase: Integer case.—We consider 1D lattice models with a many-body Hamiltonian $H(\lambda)$ that has a periodic dependence on some variable λ. We assume periodic boundary conditions in space with L unit cells and allow for interactions among the particles. Since single-particle Bloch states $|u_k\rangle$ are no longer a good eigenbasis, topological invariants must be defined in terms of the many-body ground state $|\Phi_0\rangle$. As suggested by Niu, Thouless, and Wu [30], the Zak phase of Bloch wave functions can be generalized by replacing the single-particle crystal momentum k by a twist angle θ of boundary conditions $\Phi(x_1,\ldots,x_j+L,\ldots,x_N)=e^{i\theta}\Phi(x_1,\ldots,x_N)$. Since θ and $\theta+2\pi$ define the same boundary conditions, the parameter space (θ,λ) is a torus T^2. Twisted boundary conditions can be removed and replaced by periodic ones via a canonical transformation to a twisted Hamiltonian, $\bar{H}(\theta)=\hat{U}(\theta)H\hat{U}(\theta)^{-1}$ and $|\Psi_0(\theta)\rangle=\hat{U}(\theta)|\Phi_0(\theta)\rangle$. Here,

$$\hat{U}(\theta)=e^{i\theta\hat{X}},\quad \text{with}\quad \hat{X}=\frac{1}{L}\sum_{j=1}^{L}\sum_{s=1}^{n}(j+r_s)\hat{n}_{js} \tag{1}$$

is the momentum shift operator with $\hat{n}_{js}$ denoting the particle number operator of the sth site $(s\in\{1,2,\ldots,n\})$ in the jth unit cell, and the lattice constant is $a=1$. $0\leq r_s\leq 1$ characterizes the position within the unit cell. In terms of the $|\Psi\rangle$'s the many-body equivalent of the Zak phase then reads $\phi_{\mathrm{MB}}=i\int_0^{2\pi}d\theta\langle\Psi_0(\theta)|\partial_\theta\Psi_0(\theta)\rangle$.

If $|\Psi_0(\theta)\rangle$ is a gapped and *nondegenerate* ground state, a slow (adiabatic) change of the parameter $\lambda=\lambda(t)$ in a closed loop, such that the many-body gap does not close, induces a Thouless pump, described by a current density $\langle\hat{j}\rangle=\partial_\theta E(\theta)/\hbar+i(\langle\partial_t\Psi_0|\partial_\theta\Psi_0\rangle-\langle\partial_\theta\Psi_0|\partial_t\Psi_0\rangle)$. Then, following Niu, Thouless, and Wu, averaging over twisted boundary conditions one finds a strictly integer-quantized particle transport over one time period $\mathcal{T}$. The transported charge Δn is then directly related to the NTW invariant ν

$$\begin{aligned}\Delta n&=\frac{1}{4\pi}\int_0^{\mathcal{T}}dt\int_0^{2\pi}d\theta i[\langle\partial_t\Psi_0|\partial_\theta\Psi_0\rangle-\langle\partial_\theta\Psi_0|\partial_t\Psi_0\rangle]\\&=\frac{1}{2\pi}\int_0^{\mathcal{T}}dt\frac{\partial\phi_{\mathrm{MB}}}{\partial t}=\frac{1}{2\pi}\oint d\lambda\frac{\partial\phi_{\mathrm{MB}}}{\partial\lambda}=\nu,\end{aligned} \tag{2}$$

which is the generalization of the celebrated invariant of Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) for free fermions [2,32] to the case of interactions and disorder. In Ref. [17] the TKNN invariant was generalized to Gaussian mixed states of fermions using the King-Smith–Vanderbildt relation [33] between changes of ϕ_{MB} to those of the many-body polarization $P=(1/2\pi)\mathrm{Im}\log\langle\Psi_0|\hat{U}|\Psi_0\rangle$ introduced by Resta [21], where $\hat{U}\equiv\hat{U}(2\pi)$: $\partial_\lambda\phi_{\mathrm{MB}}=2\pi\partial_\lambda P$. This then allowed to replace the ground-state average by the trace over a density matrix $\phi_{\mathrm{EGP}}=2\pi P=\mathrm{Im}\log\mathrm{Tr}\{\rho\hat{U}\}$ defining the so-called ensemble geometric phase in [17].

Ensemble geometric phase: Fractional case.—In the absence of interactions, gapped ground states (of fermions) occur only at integer fillings per unit cell. This changes with interactions. Here, gapped ground states can exist which have fractional fillings and the Lieb-Schulz-Mattis theorem and its generalizations [34,35] tell us that they attain a "topological order" accompanied by fractionalization and *degeneracy* [36]. In such a case the above arguments do not hold as a parameter loop of λ does not return the initial state to itself (up to a phase), but in general to an orthogonal state in the ground-state manifold. For a d-fold degenerate subspace the NTW invariant (2) must instead be replaced by the gauge-invariant determinant of a Wilson loop [37]

$$\nu_{\mathrm{tot}}=\frac{1}{2\pi}\int_0^{\mathcal{T}}dt\frac{\partial}{\partial t}\mathrm{Im}\log\det\mathsf{W}(t),\qquad \mathsf{W}=\mathcal{P}e^{i\int_0^{2\pi}d\theta\mathsf{A}(\theta)}.$$

Here, $\mathsf{A}_{\mu\nu}(\theta)=i\langle\Psi_0^\mu|\partial_\theta\Psi_0^\nu\rangle$ is a $d\times d$ matrix, and $\mathcal{P}$ denotes path ordering.

We now argue that also ν_{tot} can be related to an expectation value of a unitary operator, which then allows for a generalization to mixed states. To see this, we note that following Niu, Thouless, and Wu [30], ν_{tot} can be expressed as integral of the Berry curvature corresponding to any one of the degenerate ground states $|\Psi_0^\mu\rangle$ over an enlarged torus, extending either the time integration to $\mathcal{T}d$ or the θ integration to $2\pi d$, $(\mu=0,\ldots,d-1)$

$$\nu_{\mathrm{tot}}=\frac{1}{2\pi}\int_0^{\mathcal{T}}dt\int_0^{2\pi d}d\theta\mathrm{Im}\langle\partial_t\Psi_0^\mu|\partial_\theta\Psi_0^\mu\rangle. \tag{3}$$

As a consequence, particle transport is integer quantized only after d cycles of a Thouless pump [32].

As shown by Aligia and Ortiz [38–40], Eq. (3) gives also the winding number of a many-body Berry phase

$$\nu_{\mathrm{tot}}=\oint\frac{d\lambda}{2\pi}\frac{\partial\phi_\mu^{(d)}}{\partial\lambda},\quad\text{with}\quad\phi_\mu^{(d)}=\mathrm{Im}\log\langle\Psi_0^\mu|(\hat{U})^d|\Psi_0^\mu\rangle, \tag{4}$$

which does not depend on the particular ground state. To see this, we note that the lattice Hamiltonian is invariant under spatial translation by one unit cell, described by the unitary lattice shift operator $\hat{T}$. For a d-fold ground-state degeneracy one can construct a basis set of ground states $\{|\Phi_0^\mu\rangle\}$ with $|\Phi_0^\mu\rangle=\hat{T}^\mu|\Phi_0^0\rangle$ and $\mu=0,\ldots,d-1$. Since $\hat{T}^{-1}\hat{U}^d\hat{T}=\hat{U}^d e^{2\pi i dN/L}$ with N being the total number of fermions, and dN/L is an integer for a fractional filling $1/d$, the Berry phases $\phi_\mu^{(d)}$ of all states in this basis have the same value. It should be noted that the finiteness of the absolute value $|\langle\Psi|(\hat{U})^d|\Psi\rangle|$ in the thermodynamic limit is an indicator of a localized, i.e., insulating ground state with filling $1/d$ per unit cell [38,41].

Equation (4) then allows us to define a generalized ensemble geometric phase for mixed states

$$\phi_{\mathrm{EGP}}^{(d)}=\mathrm{Im}\log\mathrm{Tr}\{\rho(\hat{U})^d\} \tag{5}$$

which we now use to construct a topological winding number for mixed states.

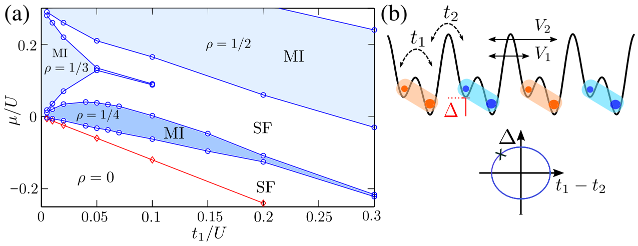

FIG. 1. (a) Phase diagram of Ex-SLBHM for $t_2 = 0.5t_1$, $V_1 = 2V_2 = 0.2U$. Blue and white areas indicate Mott-insulating (MI) and superfluid (SF) phases, respectively. The MI at average filling $\rho = 1/4$ per lattice site is doubly degenerate corresponding to superpositions of two density waves indicated in (b) in blue and orange. (b) Cyclic adiabatic variations of $t_1 - t_2$ and Δ encircling the point $\Delta = t_1 - t_2 = 0$ lead to a fractionally quantized charge pump [42,43].

Extended superlattice Bose-Hubbard model.—Let us discuss a specific example with interaction-induced fractional topological charges and associated fractional winding number [42,43], the one-dimensional extended superlattice Bose Hubbard model (Ext-SLBHM). As shown in Fig. 1(b), bosons at lattice site j, described by annihilation and creation operators $\hat{a}_j$ and $\hat{a}_j^\dagger$, and with on-site interaction strength U move along a 1D lattice with alternating hopping t_1 and t_2 and a staggered potential Δ. In addition, there is a nearest-neighbor and next-nearest neighbor interaction V_1 and V_2, respectively. The Hamiltonian reads in second quantization

$$H = -t_1 \sum_{j,\text{even}} \hat{a}_j^\dagger \hat{a}_{j+1} - t_2 \sum_{j,\text{odd}} \hat{a}_j^\dagger \hat{a}_{j+1} + \text{H.a.} + \frac{\Delta}{2} \sum_j (-1)^j \hat{a}_j^\dagger \hat{a}_j + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1) + \sum_{j,d} V_d \hat{n}_i \hat{n}_{i+d}. \tag{6}$$

Here, $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$. The system has a unit cell of two sites. With periodic boundary conditions and in the absence of interactions one finds two single-particle energy bands with a finite gap, which closes only for $\Delta = t_1 - t_2 = 0$. For sufficiently strong interactions there are further gap openings and Mott insulating (MI) states with fractional fillings emerge. The ground-state phase diagram, obtained from DMRG (density matrix renormalization group) simulations [44] is shown in Fig. 1(a), where MI phases with fractional fillings are indicated.

In the following, we are interested in the phase with average filling of $\rho = 1/4$ per lattice site, or $1/2$ per unit cell. Here, the ground state is doubly degenerate for periodic boundary conditions if the number L of unit cells is even. If one starts in one of the two many-body ground states, say $|\Psi_1\rangle$, and changes $t_1 - t_2$ and Δ in a closed loop in parameter space such that the many-body gap remains open at all points, the ground-state manifold $\{|\Psi_1\rangle, |\Psi_2\rangle\}$ returns to itself up to a $U(2)$ rotation. Then 2 loops in parameter space need to be performed for the initial state to return to itself modulo a phase. Similarly the average current $\langle \hat{j} \rangle$ needs to be integrated over two periods of length $\mathcal{T}$ to lead to an integer-quantized number Δn of pumped particles, which is verified by our numerical simulations in Fig. 2(a). This does no longer hold true, however, for finite temperatures. As expected and shown in the same figure the number of transported particles deviates substantially from unity as soon as the temperature approaches the many-body gap, since higher energy states are occupied.

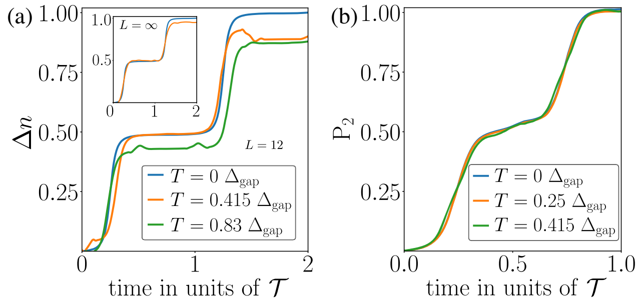

FIG. 2. (a) Integrated particle current in the Ext-SLBHM as function of time for a small system of $L = 12$ unit cells and different temperatures obtained by exact diagonalization in the $\rho = 1/4$ MI phase. Here, $t_{1/2} = 5[1 \pm \cos \lambda(t)]$, and $\Delta = -60 \sin \lambda(t)$, with angle $\lambda(t) = 2\pi t/\mathcal{T} + 3\pi/2$ and $V_1 = 40$, $V_2 = 20$, and U is infinite. The inset shows the same for $L \to \infty$ obtained by LCRG (Light-Cone Renormalization Group, see Supplemental Material [45] for details) [53–55]. (b) Generalized EGP for the twofold degenerate system also obtained by LCRG. One notices that the winding remains strictly quantized even at temperatures where there is a substantial occupation of excited states.

Remarkably, and in sharp contrast, the winding of the generalized EGP $\phi_{\text{EGP}}^{(2)}$ remains strictly unity even at temperatures on the order of the many-body gap as can be seen from Fig. 2(b). (It should be noted that increasing the temperature becomes numerically more demanding.)

It was shown in Ref. [17] for noninteracting fermions, that the winding of the EGP ϕ_{EGP} remains the same for all temperatures $T < \infty$. In the following, we will give some arguments that also for interacting systems the EGP winding of a thermal state is identical to that of the ground state below some critical temperature which is larger than the many-body gap.

Finite-temperature winding.—We first show that there exists a critical temperature T_c different from zero, below which the winding of the EGP coincides with that of the many-body ground state $\Delta\phi_{\text{EGP}}|_{T<T_c} = \Delta\phi_{\text{EGP}}|_{T=0}$. Thus, different, e.g., from the prediction in [16], a temperature-induced topological transition can only occur at a finite, nonzero temperature.

To this end we note that the change of ϕ_{EGP}

$$\Delta\phi_{\text{EGP}} = 2\pi \deg z = \text{Im} \oint \frac{1}{z(\lambda)} \frac{dz(\lambda)}{d\lambda} d\lambda, \tag{7}$$

with $z(\lambda) \neq 0$ for $\lambda \in \delta\mathcal{C}$, is just the winding number or degree of a smooth map $z(\lambda) = \mathrm{Tr}\{\rho(\lambda)(\hat{U})^d\}$ from a closed loop $\delta\mathcal{C}$ in parameter space (λ) into the complex plane $\mathbb{C}$ of the polarization amplitude $z(\lambda)$. It measures the algebraic change of phase of z as the variable λ goes around the loop once. The degree of z is by definition the number of solutions of $z = 0$ inside $\delta\mathcal{C}$ taking into account their algebraic multiplicity (for more details about degree theory, see [56]). Suppose for all temperatures T with $T_1 < T < T_2$, $z \neq 0$ on $\delta\mathcal{C}$, then $\Delta\phi_{\mathrm{EGP}}$ is independent of temperature in the interval (T_1, T_2). These arguments are in parallel with Hopf's homotopy theorem [56]. Now, the condition $z(T, \lambda) \neq 0$ everywhere on $\delta\mathcal{C}$ can always be fulfilled in a finite range of temperatures starting at $T = 0$ until for a critical temperature T_c

$$|z(T_c, \lambda)| = 0, \tag{8}$$

for some λ on $\delta\mathcal{C}$. This defines a temperature-induced topological phase transition.

Critical temperature.—As shown in [17], $T_c = \infty$ for noninteracting fermions. To investigate the possibility of a finite-temperature topological phase transition in an interacting system, we have numerically calculated $|z(T)|$ for the extended SLBHM. The results are shown in Fig. 3 in dependence of T for different system sizes. One recognizes that $|z|$ remains approximately unity below temperatures that are a sizable fraction of the many-body gap Δ_{gap} followed by a falloff, which becomes more pronounced with increasing system size. This behavior is very similar to the noninteracting case, for which one finds a double-exponential scaling (see Supplemental Material [45]) $|z(T)| \sim \exp[-2L\exp(-\beta\Delta_{\mathrm{gap}})]$. Note, that although $z(T) \to 0$ for $L \to \infty$, the temperature T_0, where $|z|$ starts to deviate from unity only scales logarithmically with system size L.

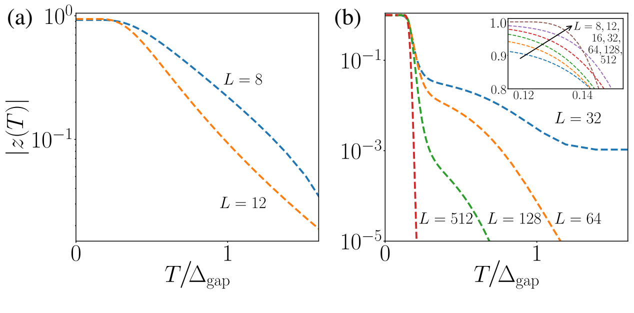

FIG. 3. Temperature scaling of polarization amplitude $|z(T)|$ for the extended SLBHM for the parameters of Fig. 2 and different system sizes (a) for small systems obtained with exact diagonalization, (b) for larger systems obtained with LCRG, which is an infinite size method. Here, $\lambda(t) = 3\pi/4$ but we verified that the results hold for any value of λ. Also a finite length L was cut out and used for the calculation of $|z(T)|$. The inset shows the behavior in the low temperature regime. As shown in [41] $|z(T \to 0)| \to 1$ for increasing system size.

$$T_0 \sim \Delta_{\mathrm{gap}}/\ln L. \tag{9}$$

From our numerical data it remains unclear if $|z(T)|$ has a strict zero, indicating a topological phase transition, or not and it would be interesting to investigate other interacting superlattice models such as [57,58].

In order to show that interactions may lead to a finite value of T_c let us consider the *flattened* Hamiltonian

$$\tilde{H} = E_0 \sum_{\mu=1}^{d} |\Psi_0^\mu\rangle\langle\Psi_0^\mu| + E_1 \sum_{j\neq(0,\mu)} |\Psi_j\rangle\langle\Psi_j|, \tag{10}$$

with $\Delta_{\mathrm{gap}} = E_1 - E_0$. Here, all excited states have the maximum weight compatible with temperature and gap. Since the total Chern number of all excited bands must be opposite to that of the ground state, flattening a many-body Hamiltonian to such a form is expected to lead to the "worst" case. Then for the polarization amplitude $z(T) = \mathrm{Tr}\{\exp(-\beta\tilde{H})(\hat{U})^d\}/Z$ holds $\mathrm{Tr}\{e^{-\beta\tilde{H}}(\hat{U})^d\} = z(0)d(e^{-\beta E_0} - e^{-\beta E_1}) + \mathrm{Tr}\{(\hat{U})^d\}e^{-\beta E_1}$, where $z(0) = (1/d)\sum_\mu\langle\Psi_0^\mu|(\hat{T})^d|\Psi_0^\mu\rangle$ is the zero-temperature polarization amplitude. As shown in [38,41] $|z(0)| \to 1$ in the thermodynamic limit $L \to \infty$ if the ground state is insulating. Since $\mathrm{Tr}\{(\hat{U})^d\}$ does not depend on the Hamiltonian, its phase is fixed and does not change upon parameter variations. Thus, the winding of $\phi_{\mathrm{EGP}}^{(d)}$ for the flattened Hamiltonian $\tilde{H}$ at temperature T remains equal to that in the ground state as long as $e^{-\beta E_0} - e^{-\beta E_1} > |\mathrm{Tr}\{(\hat{U})^d\}|e^{-\beta E_1}/d$. With this we find for the critical temperature T_c, defined through Eq. (8), (with $k_B = 1$)

$$T_c = \frac{\Delta_{\mathrm{gap}}}{\ln[1 + |\mathrm{Tr}\{(\hat{U})^d\}|/d]}. \tag{11}$$

As shown in the Supplemental Material [45] $|\mathrm{Tr}\{(\hat{U})^d\}|$ is intensive and bounded by a value of $\mathcal{O}(d)$.

Summary.—We have introduced a many-body topological invariant for finite-temperature states of interacting many-body systems with fractional filling and ground-state degeneracy. The invariant is based on a generalization of the EGP introduced in [17]. In the limit $T \to 0$ it coincides with the well-known NTW invariant [30]. We showed that there exists a critical temperature T_c, defined by a vanishing polarization amplitude, which generically is larger than the many-body gap. Below T_c the EGP-based topological winding number is identical to the ground-state invariant. The generalized EGP also allows us to detect topological properties from finite-temperature measurements. It can be measured either directly (see [17]) or obtained from the full counting statistics, measurable, e.g., in ultracold atom experiments with a gas microscope. A nontrivial topological winding of the EGP can furthermore induce a quantized transport in a weakly coupled auxiliary system, prepared at a low temperature [23]. We illustrated our results for the Ext-SLBHM model at quarter filling, which has a twofold degenerate ground state and an associated fractional topological charge of $1/2$. The arguments given here can be extended to interacting two-dimensional systems of the Chern class with translational invariance, and thus to systems like fractional Chern insulators with intrinsic topological order. These systems can be mapped to independent one-dimensional systems by transforming to momentum space in one of the spatial directions.

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