Insights into low-energy physics from crystalline symmetry

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These are notes for a pedagogical lecture given at the Les Houches school on *New Developments in Topological Condensed Matter*, September 2019. The focus of these notes is to explain how crystal symmetries can be used to gain insight into what types of low-energy behaviour are possible in a condensed matter system. Specifically, they focus on the use of theorems of the "Lieb-Schulz-Mattis" type to constrain the low-energy phase structure of the theory, with particular attention paid to new developments around the use of non-symmorphic crystal symmetry. The text and figures both borrow liberally from published work both by myself and others.

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I. INTRODUCTION

In this lecture, we will be interested in the properties of insulators in *clean*, i.e. non-disordered systems. In contrast to other types of insulators — e.g. Anderson or many-body localized insulators — such insulating states of matter can only arise in time-reversal invariant systems when there is 'commensuration' between the density of particles in a system and a crystalline lattice. Commensuration means that the number of particles in the system is a rational multiple of the number of crystalline unit cells in the system. If time-reversal symmetry is broken, insulating states can also arise if the density is commensurate with the magnetic field, i.e. when the filling of a Landau level is a rational number (the integer/fractional quantum Hall effects). These lectures aim to both explain the role of commensuration in systems with time-reversal symmetry, and also to place a finer classification on the possible insulating states and their patterns of entanglement.

The systems of interest to us will be models of spinless fermions, bosons, electrons, or spins, characterized by (at least) the following symmetries:

(i) $U(1)$ charge conservation, required to 'count' the particles in the system;

(ii) crystalline space-group symmetry; and

(iii) time-reversal symmetry.

Note that in some examples when discussing electronic systems we will assume the absence of spin-orbit coupling, in which case we can work with Hamiltonians that also enjoy a $U(1)_s$ spin-rotation invariance (and, in these cases, time-reversal will be less important).

We say that a system is an insulator when it preserves the $U(1)$ charge conservation symmetry and has a gap between its ground state(s) and excited states. There are **two broad classes of insulators** that we shall discuss:

(i) **short-range entangled (SRE) insulators**: this first class is exemplified by the familiar **band insulator** which can emerge absent electron-electron interactions. Recall that a band insulator — whether trivial or any of a myriad of topological band insulators — has a unique ground state irrespective of boundary conditions, and preserves both time reversal and all the microscopic lattice symmetries (in addition to the aforementioned $U(1)$). The ground state of a band insulator is also translationally invariant. However, a band insulator is not the only state with such properties: for instance, a **bosonic Mott insulator** with a single boson per site on any lattice also satisfies all these criteria, as do **quantum paramagnets** that remain disordered down to $T = 0$ but do not show fractionalization, and **fragile Mott insulators** whose ground states preserve lattice symmetries but transform in a nontrivial representation of those symmetries. Here, the term 'short-range entangled' reflects the fact that these systems can be continuously transformed into product states by a finite-depth, local unitary circuit (adiabatic transformation of the Hamiltonian). Aficionados will note that this definition automatically includes all **symmetry-protected topological phases**, where the only obstruction to such a mapping is that such a unitary mapping is either discontinuous or breaks a symmetry[1].

(ii) **fractionalized insulators with long-range entanglement (LRE)**: insulators in this second class have a number of exotic properties. First, they typically exhibit the fractionalization of quantum numbers of any global symmetries present, i.e. the low-energy quasiparticle excitations carry quantum numbers that are non-integer multiples of the microscopic charge quantum defined in the UV. A standard example is the fractional charge in the fractional quantum Hall effect, or spin-1/2 spinons in a fractionalized Mott insulator. Second, their ground-state degeneracy is sensitive to boundary conditions, and scales exponentially with the genus of the surface on which they are defined. A specific consequence of this is that they always have a ground state degeneracy on the [hyper]torus implicit in the definition of periodic boundary conditions[2] (Note that the second fact can be shown to follow from the first). Local operators cannot distinguish between these degenerate ground states, i.e. there is no local order parameter or broken symmetry that can diagnose which ground state one is in. Third, even when

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[1] In fact so-called 'invertible intrinsic topological orders' such as the integer quantum Hall state are also fall into this class for the purposes of these lectures.

[2] On finite systems, the degeneracy is replace by an exponentially small near-degeneracy — more on this later.

the symmetries are broken, the ground state wavefunctions of such insulators cannot be transformed by a local unitary into trivial product states. Such gapped fractionalized states of matter are said to have (non-invertible) intrinsic topological order. Since it does not require any symmetry, the physical manifestation of topological order is really the fractionalization of *statistics* — the emergence of anyons in $d = 2$, and e.g. the emergence of low-energy fermions from a purely bosonic model in $d > 2$.

Note that we have adopted a somewhat strong definition of an insulator as a *gapped* phase. Strictly speaking, measuring insulating electrical response cannot probe the spectral gap, but only the gap to charge excitations; it is possible that the spin excitations remain gapless, but absent symmetry breaking (where such excitations would be Goldstone modes) the coexistence of a charge gap with gapless spin excitations is itself a form of fractionalization. For instance, in 1D, where topological order is absent, strong correlations can lead to a Mott insulating phase with a charge gap but with spin excitations described in terms of a gapless Luttinger liquid. (Indeed, the original Lieb-Schulz-Mattis arguments concerned the Heisenberg chain, which may be viewed as the strongly correlated limit of the 1D Hubbard model.)

In general, deciding which of these possibilities emerges in a given system is a complicated question seemingly of the sort that can seemingly only be settled by resorting to numerics or worse, experiments. However, there are simple criteria based on the filling and the lattice symmetries that can rule out the possibility of a short-range entangled state. In such cases, the observation of a gap and the absence of broken symmetry becomes sufficient to deduce the presence of fractionalization. For example, the absence of ordering seen in neutron scattering experiments on the electrically insulating kagome lattice antiferromagnet herbertsmithite leads us to believe that its ground state is "exotic". Note that, since the material is an electrical insulator, it has a charge gap. The absence of order in the ground state can be explained by one of two possibilities: the system could either have a spin gap and topological order; or the system could host a 'Fermi surface' of neutral spin-1/2 fermion excitations, i.e. it exhibits spin-charge separation, and hence the spectrum could remain gapless. Experiments, and numerical simulations — such as DMRG and variational Monte Carlo — remain divided as to which of these two scenarios is actually at play in the real material. However, due to the insights afforded by crystal symmetry, we can be reasonably confident that a trivial quantum paramagnetic state is impossible. In this sense, placing tighter and tighter bounds on symmetry-breaking from experimental measurements can increase confidence in the expectation of an exotic phase. In contrast, similar measurements on a honeycomb lattice material with the same symmetries would *not* carry such an implication. The distinction between these two examples can be simply phrased in terms of the fact that the kagome (honeycomb) lattice has an odd (even) number of spins-1/2 per unit cell, and linked to old lore on Mott insulators. However, as we will see below, there are (especially in three dimensions) many cases where although a system has an even number of spins-1/2 per unit cell, it is nevertheless unable to form an SRE insulator without triggering symmetry breaking. It seems that the old lore is less than complete. It is important to develop methods to deduce which lattices might host interesting insulating phases and at which fillings such phases might emerge: in short, to systematize the lore.

In these lectures, we will attempt to explain the above facts, and to give a precise definition of when an insulator must be "exotic", as discussed above. We will first give a modern perspective — due to Hastings, Oshikawa, and Lieb-Schulz-Mattis (HOLSM; in reverse chronological order) — on the old canard that "Mott insulators require odd filling". We will see that the odd/even dichotomy originates if one considers just the subgroup of the crystal symmetry group generated by lattice translations. We are thus naturally led to explore the consequences of assuming the full set of space group symmetries, and we thus find that stronger results are possible for systems with **nonsymmorphic** symmetries. For the approach taken in these sections to be useful for systems of spinful electrons, we will require that spin-orbit coupling is absent. We therefore adopt a different technique that can also address systems with spin-orbit coupling. We then discuss various generalizations and other perspectives on these results.

II. FRACTIONAL FILLING AND TRANSLATIONAL SYMMETRY

As a first task, we would like to put some flesh on the bones of the observation that odd/even filling are somehow distinct in electronic systems. Let us first specify the setting in which the HOLSM commensurability theorems may be applied. We study lattice systems with a specified space group $\mathcal{G}$, described by a local Hamiltonian $\hat{H}$ that preserves all the symmetries of $\mathcal{G}$. In addition, we assume that the system has (at least) one global charge $\hat{\mathcal{Q}}$ conserved by $\hat{H}$, *i.e.* $[H, \hat{\mathcal{Q}}] = 0$ (we may thus replace $\hat{\mathcal{Q}}$ by its c-number expectation value $\mathcal{Q}$ throughout). We make no assumptions as to the origins of the conserved charge, so for instance the systems we consider could be built out of

(i) spinless fermions or bosons, where $\mathcal{Q}$ is just the conserved particle number;

(ii) spinful fermions with SU(2) spin symmetry, in which case $\mathcal{Q}$ is one-half the total fermion number (since the two spin components may be treated independently); or

(iii) lattice spins with (at least) U(1) spin rotational invariance, in which case we may take the charge on lattice site $\mathbf{r}$ to be $S + \hat{S}^z_{\mathbf{r}}$ where $S, \hat{S}^z_{\mathbf{r}}$ are its total spin and magnetization, and define $\mathcal{Q}$ accordingly.

This is as good a place as any to note that when considering spinless fermions, integer spins, or bosons, due to the lack of spin degeneracy the distinction between odd and even filling becomes one between fractional and integer filling. In much of the following, we will adopt the latter nomenclature. (When discussing the role of non-symmorphic symmetries, for half-integer spins or spinful electrons the distinction is between any even filling and special fillings that are multiples of $4, 6, 8$, or 12, and in the boson/spinless fermion/integer spin case it is between arbitrary integer fillings and those that are multiples of $2, 3, 4$ or 6. The reason these fillings are special are because any crystallographic point group has order $1, 2, 3, 4$, or 6, which follows from the crystallographic restriction theorem.)

Considering a finite system with $\mathcal{N}_c = L_x \times L_y \times L_z$ unit cells, we may then define the *filling* to be the charge per unit cell, *i.e.* $\nu = \mathcal{Q}/\mathcal{N}_c$, which will be held fixed in the thermodynamic limit. We impose periodic boundary conditions that identify $\mathbf{r}$ and $\mathbf{r} + L_i\mathbf{a}_i$. Note that in the case when ν is a fraction, we choose N_c so to ensure that $\mathcal{Q} = \nu\mathcal{N}_c$ is an integer, in accord with the quantization of charge. We work in units where $\hbar = e = 1$, so that the quantum of flux is $\Phi_0 = 2\pi$.

The original HOLSM theorem states that at fractional ν, it is impossible for the system to have a unique, translationally-invariant, gapped ground state. To recap the discussion in the introduction, this leaves open the following three logical possibilities for an *electrically* insulating ground state:

(i) **The system remains gapless.** Since it is an electrical insulator, the gapless excitations must then carry spin but not charge.

(ii) **The system is gapped, and breaks translational symmetry**, thereby enlarging the unit cell. The effective filling in the new unit cell is then an integer.

(iii) **The system is gapped, and preserves translational symmetries, but has a non-unique ground state in the thermodynamic limit.** In this case, we have a ground state degeneracy that cannot be associated with a broken symmetry. One route to this is for the low-energy excitations to be fractionalized, so that the emergent low-energy description is the deconfined phase of a lattice gauge theory[1,2]; the degenerate ground states may then be associated with processes that create a quasiparticle-hole pairs from the vacuum, and thread them around a noncontractible loop (here we assume periodic boundary conditions) before fusing them back into the vacuum. The resulting states are topologically distinct from the original ground state, but no local observable can tell them apart.

Evidently, cases (i) and (iii) are exotic. We will focus mainly on case (iii).

We now sketch the argument that leads to these conclusions; we give an intuitive proof, and refer the reader to Refs. 3–8 for a more formal treatment. The strategy is to begin with a ground state $|\Psi\rangle$, and adiabatically (actually, this should be quasi-adiabatic – see below) insert a flux quantum through a periodic direction. us to the original Hamiltonian. This procedure produces an eigenstate $|\tilde{\Psi}\rangle$. Earlier work has argued that for an insulator, $|\tilde{\Psi}\rangle$ must be a 'low energy' state, *i.e.* its energy approaches that of the ground state in the thermodynamic limit.[5,6,9,10] However, this could just be a 'boring' adiabatic that just jiggles around a unique ground state, so that $|\tilde{\Psi}\rangle$ is identical to $|\Psi\rangle$. The key step is to show that $|\tilde{\Psi}\rangle$ is distinct from $|\Psi\rangle$, which would then establish ground state degeneracy. In the case of fractional filling, these states differ in crystal momentum[5,6,9,10], as we now demonstrate.

For specificity[3], let us take the example of a d-dimensional hypercubic lattice with lattice spacing a.

First, let's give a simple heuristic computation of the momentum change: simply apply basic electrodynamics. Recall that the induced emf is given by the changing flux; since the emf acts around a circle of ciircumference L_x the

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[3] We can generalize the results to any lattice, as will be evident when we discuss the non-symmorphic case below.

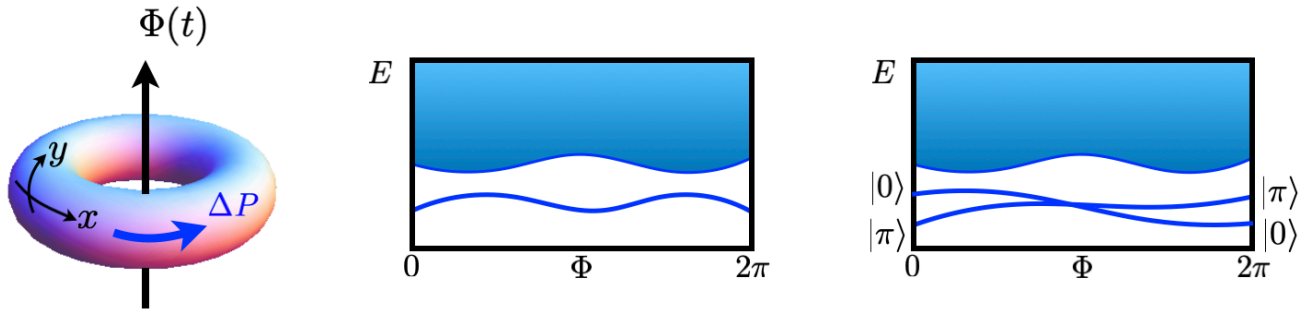

FIG. 1: Flux insertion. A time-dependent flux is threaded through a non-contractible loop on the torus and changed from 0 to $\Phi_0 = 2\pi$. If there is a unique ground state it returns to itself (center), but degenerate ground states on odd×even lattices can exchange in the cycle leading to a change in ground state momentum.

force acting on each charge is just $F_x = \frac{1}{L_x}\frac{d\Phi}{dt}$. Summing this over all the charges in the system and integrating over time gives the change in momentum $\Delta P_x = 2\pi\mathcal{Q}/L_x = 2\pi\nu L_y L_z$.

More formally, it is useful to think of the the adiabatic cycle in two steps:

(Step 1) Imagine adiabatically threading 2π flux through a handle of the torus (recall that our system is defined with periodic boundary conditions), say the one enclosed by a noncontractible loop parallel to the x-axis. The particles are assumed to couple minimally to this gauge flux, with unit charge. Suppose we began with a ground state $|\Psi\rangle$; as translation in the x-direction is a symmetry, we may assume that this is a state of fixed momentum: in other words, we have

$$\hat{T}_x|\Psi\rangle = e^{iP_0}|\Psi\rangle \tag{1}$$

for some crystal momentum P_0. Now, the flux insertion can be implemented via a spatially uniform uniform time-dependent vector potential $\boldsymbol{A}(t) = \frac{2\pi}{L_x a} f(t)\hat{\mathbf{x}}$, with $f(0) = 0$, and $f(1) = 1$, and f is chosen to preserve (quasi) adiabaticity. Since the system is in an insulator, it is possible to argue that we can inserting 2π flux while remaining close to the ground state (We state this without proof, but note that this is a key technical hurdle addressed by Hastings in Refs. 5,6). The insertion of flux produces a new state $|\Psi'\rangle$; however, it is clear that our choice of $\boldsymbol{A}(t)$ preserves $\hat{T}_x$ as a symmetry. Thus, we may conclude that

$$\hat{T}_x|\Psi'\rangle = e^{iP_0}|\Psi'\rangle, \tag{2}$$

i.e. the crystal momentum is unchanged during the adiabatic process. However, as we insert the flux, the Hamiltonian also changes from $\hat{H}(0)$ at $t = 0$ to $\hat{H}(2\pi)$ at $t = 1$ — it now describes a system with an inserted flux. Therefore, we need another step to be able to compare the Hamiltonians before and after flux insertion.

(Step 2) We complete the adiabatic cycle by performing a large gauge transformation, implemented by the operator

$$\hat{U} = \exp\left\{ i\frac{2\pi}{L_x}\int d^d r\, \hat{\mathbf{x}}\cdot\mathbf{r}\hat{\rho}(\mathbf{r})\right\} \tag{3}$$

where we have employed second-quantized notation and $\hat{\rho}(\mathbf{r})$ is the density operator corresponding to the conserved charge $\hat{\mathcal{Q}}$. It is straightforward to show that

$$\hat{T}_x\hat{U}\hat{T}_x^{-1}\hat{U}^{-1} = e^{i\frac{2\pi}{L_x}\int\hat{\rho}(\mathbf{r})} = e^{i2\pi\mathcal{Q}/L_x} = e^{i2\pi\nu L_y L_z}. \tag{4}$$

Using (4), we see that the final result of the adiabatic cycle is to produce a state $|\tilde{\Psi}\rangle = \hat{U}|\Psi'\rangle$, whose crystal momentum P_1 is given by

$$e^{iP_1}|\tilde{\Psi}\rangle \equiv \hat{T}_x|\tilde{\Psi}\rangle \;=\; \hat{T}_x\hat{U}|\Psi'\rangle = e^{i2\pi\nu L_y}\hat{U}\hat{T}_x|\Psi'\rangle = e^{i(P_0+2\pi\nu L_y L_z)}|\tilde{\Psi}\rangle. \tag{5}$$

Clearly, if L_y is chosen relatively prime to q (note that we may still choose L_x so that $\nu L_x L_y$ is an integer, so there is no inconsistency) then $|\Psi\rangle$, $|\tilde{\Psi}\rangle$ differ in their crystal momentum, *i.e.* the ground state after flux insertion is distinct from the one we began with[4]. Given that $|\tilde{\Psi}\rangle$ is a low-energy state degenerate with the ground state in the thermodynamic limit, we have a ground-state degeneracy, and therefore the system must fall into one of the three categories discussed above.

Caveats. Actually, this argument, originally given by Oshikawa, is a little bit too slick — as noted by Hastings[6]. It has two problems. The first can be motivated by thinking about topological order: the ground states that become topologically degenerate in the thermodynamic limit are actually split by an exponentially-small-in-system size gap in the finite systems that are necessary to consider in the proof. So any adiabatic flux insertion does not actually toggle between the putatively topologically degenerate states, but we require this in order for the proof to work. Second, it turns out that the energy bounds that follow from the system being insulating used by Oshikawa are too weak to give a useful answer in $d = 3$. Hastings[6] fixed these by (i) introducing the notion of "quasiadiabatic" flux insertion where the flux is inserted fast enough to 'jump the level crossing' between the different quasi-degenerate states, but slow enough that it does not produce excitations above the gap; and (ii) by leveraging gauge invariance to give a tighter bound on the energy. To do all this rigorously requires some fairly technical steps (see, e.g. Ref. 5, although Hastings himself was eventually able to constrict a signficantly simpler argument[6]. Here, we will use more intuitive arguments with the understanding that they are 'rigorizable' using the same methods as those depoloyed by Hastings.

Examples: Fermions: $d = 1$ spinless fermions at half filling; Hubbard at half filling in $d = 2, 3$ – give a bilayer example. Bosons: Bose-Hubbard model at integer filling; Spins: spin-1/2 chain versus $S = 1$ AKLT state.

III. INTEGER FILLING AND NON-SYMMORPHIC CRYSTALS

We see that if we attempt to apply the above arguments at integer filling ($\nu \in Z$), it is clear that the change in momentum upon flux insertion is always a reciprocal lattice vector: in other words, we cannot use crystal momentum to differentiate between $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$. Thus, *using translational symmetries alone* there is no further HOLSM theorem possible: the only dichotomy is between fractional/integer (odd/even) filling. Intuitively this is because translational symmetry only allows us to count the filling of the energy bands of a crystal — but *not* to diagnose whether energy bands are forced to touch in the Brillouin zone. A moment's thought about the free fermion case will convince you that it is exactly such a constraint that would be implied if a HOLSM theorem were to exist at integer ν.

To see how to go further, it is useful to think a little bit more about the meaning of the reciprocal lattice. Recall that the reciprocal lattice defines the set of Bragg peaks that emerge upon diffraction from a crystal. It is a fact that the set of vectors in the reciprocal lattice is *always* a Bravais lattice. However, there are 230 possible space groups in $d = 3$, and the relationship between a the symmetries of a space group (viewed in real space) and the symmetry properties of its Bragg pattern (in reciprocal/Fourier space) is one-to-one. Since there are only 14 Bravais lattices, there is a disconnect between the counting: how are distinctions between the different space groups that share the same reciprocal lattice encoded in Fourier space? It turns out that the answer to this question can be viewed as an alternative (and, in my opinion, more transparent) formulation of crystallography (see the appendix and references for a discussion).

The basic picture is that there can be additional 'extinctions' in the Bragg pattern caused by destructive interference between n different sublattices (See Fig. 3 for an example). Some thought about Bragg scattering will convince you that such perfect destructive interference can only happen if the sites of scattering are identical and somehow arranged so that waves that scattered from each of the n sites are precisely an integer multiple of $2\pi/n$ out of phase so they precisely cancel. Evidently, such effects can only occur crystals with a high degree of point group symmetry, and can *never* occur unless the unit cell contains more than one site. Such extinctions exist in 155 of the 230 space groups, and these are termed [non-exceptional] 'non-symmorphic' crystals — because the symmetries that force Bragg peaks to vanish are quite special.

At this point, it is useful to be a little bit more precise. A non-symmorphic symmetry $G = \{g|\boldsymbol{\tau}\}$ involves a point-group transformation g followed by a translation through a fraction of a lattice vector $\boldsymbol{\tau}$ in a direction left invariant

[4] To quote the late author Terry Pratchett, we have discovered that "Coming back to where you started is not the same as never leaving."

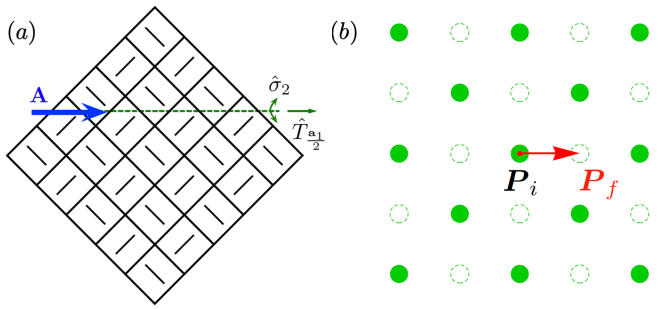

FIG. 2:

FIG. 3: (a) The Shastry-Sutherland lattice ($p4g$ wallpaper group) has a glide plane. (b) This leads to systematic extinctions (missing Bragg peaks). Flux insertions that lead to a change in momentum corresponding to a missing peak can be used to extend HOLSM arguments to integer filling.

by g: in other words, we have

$$G : \mathbf{r} \to g\mathbf{r} + \boldsymbol{\tau}, \quad \text{with} \quad g\boldsymbol{\tau} = \boldsymbol{\tau}. \tag{6}$$

There are two types of non-symmorphic operations:

(i) g is a mirror reflection, in which case τ is always one-half a lattice vector, and G is termed a *glide reflection*. This is the only possible non-symmorphic symmetry in $d = 2$. Note that a glide mirror always squares to a translation.

(ii) g is an n-fold rotation, in which case τ is always $1/n$ of a lattice vector, and G is termed a *screw rotation*.

Such operations are sketched in Figs. 3, 4, 4.

Now, it is important to be a little bit careful with these definitions. After all, when discussing point group symmetry, there is a sort of 'gauge freedom' in deciding where to choose the origin of space when defining the point-group. A non-judicious choice of origin can 'fake' you into believing a symmetry operation is non-symmorphic: for instance, it can seem as though the honeycomb lattice has a glide plane, if we choose the origin at one of the lattice sites. However, by choosing the origin at the center of the hexagons, it is evident that this 'glide' is really the product of a lattice translation and an ordinary mirror reflection: it is a **removable** glide. This is to be contrasted with an **essential** screw or glide, which is one that cannot by reduced to the product of an ordinary reflection and translation by any change of origin[11]. A simple diagnostic[11] distinguishes these cases: a glide or a mirror $\{g|\boldsymbol{\tau}\}$ is removable iff the fractional translation $\boldsymbol{\tau}$ is the projection of a lattice vector onto the invariant subspace of g (i.e. the plane of the reflection or the axis of a rotation).

The formal definition of a **non-symmorphic crystal** is that it is one where no point is left invariant, up to translations by lattice vectors, by all the symmetries. There are two ways in which a crystal can be non-symmorphic. The first and most intuitive way is for the crystal to have one or more essential glide or screw symmetries, and this is true of the 155 non-exceptional space groups. The second way is more subtle: in precisely two 3D space groups (nos. 24 and 199 in the International Tables of Crystallography) any *individual* glide or screw is removable, but cannot all be removed simultaneously — in other words, they are removable about different origins. Some thought will convince you that also in this case it is impossible that the crystal has a point left invariant by the point-group. Mathematically, a symmorphic space group is a semidirect product of translations and point group operations; this is not the case for a non-symmorphic space group. From the numbers, we see that non-symmorphicity is by no means an exotic space-group property: over two-thirds (157) of the 230 three-dimensional space groups have $\mathcal{S} > 1$, including such mineralogically ubiquitous ones as the diamond ($Fd\bar{3}m$) and hexagonal close-packed ($P6_3/mmc$) structures.

Returning to the task at hand, namely demonstrating HOLSM constraints, recall that at integer filling we could not use the crystal momentum to distinguish states. Our intuitive argument above suggests that, on non-symmorphic lattices, one can still distinguish these states using the quantum numbers of the non-symmorphic operations[12]. Let us now see how this argument proceeds. For simplicity, since we are working at integer ν, we may take $L_i = L$. As

before, we begin with a ground state $|\Psi\rangle$, and assume it is an eigenstate of G, *i.e.*

$$\hat{G}|\Psi\rangle = e^{i\theta}|\Psi\rangle \tag{7}$$

We assume that the crystal has an essential non-symmorphic symmetry $G = \{g|\boldsymbol{\tau}\}$ as above. We consider the smallest reciprocal lattice vector $\mathbf{k}$ left invariant by g, so that $g\mathbf{k} = \mathbf{k}$ and $\mathbf{k}$ generates the invariant sublattice along $\hat{\mathbf{k}}$. We now thread flux by introducing a vector potential $\boldsymbol{A} = \frac{\mathbf{k}}{L} f(t)$ with $f(t)$ as in the preceding section. (Note that as $\mathbf{k}$ is in the reciprocal lattice, $\mathbf{k}\cdot\mathbf{a}_i$ is always an integer multiple of 2π, so this is always a pure gauge flux; the example using translation in the previous section is simply a specific instance of this.) As before, upon flux insertion $|\Psi\rangle$ evolves to a state $|\Psi'\rangle$ that is degenerate with it. Once again, to compare $|\Psi'\rangle$ to $|\Psi\rangle$, we must return to the original gauge, which can be accomplished by the unitary transformation $|\Psi'\rangle \to \hat{U}_{\mathbf{k}}|\Psi'\rangle \equiv |\tilde{\Psi}\rangle$, where

$$\hat{U}_{\mathbf{k}} = \exp\left\{\frac{i}{L}\int d^d r\, \mathbf{k}\cdot\mathbf{r}\hat{\rho}(\mathbf{r})\right\} \tag{8}$$

removes the inserted flux. Since $\boldsymbol{A}$ is left invariant by G, threading flux does not alter $\hat{G}$ eigenvalues, so $|\Psi\rangle$ and $|\Psi'\rangle$ have the same quantum number under $\hat{G}$; however, on acting with $\hat{U}_{\mathbf{k}}$, the eigenvalue changes, as can be computed from the equation:

$$\hat{G}\hat{U}_{\mathbf{k}}\hat{G}^{-1} = \hat{U}_{\mathbf{k}} e^{2\pi i \Phi_g(\mathbf{k})\mathcal{Q}/L} \tag{9}$$

where we have defined the phase factor $\Phi_g(\mathbf{k}) = \boldsymbol{\tau}\cdot\mathbf{k}/2\pi$, and $\mathcal{Q} = \nu L^d$ is the total charge on the d- torus. It may be readily verified that since $g\mathbf{k} = \mathbf{k}$, $\Phi_g(\mathbf{k})$ is unchanged by a shift in real-space origin. For a non-symmorphic symmetry operation G, this phase $\Phi_g(\mathbf{k})$ must be a fraction. This follows since $\boldsymbol{\tau}$ is a fractional translation. (Recall that if a lattice translation had the same projection onto $\mathbf{k}$ as $\boldsymbol{\tau}$, this would yield an integer phase factor[13] However, this would render the screw/glide removable *i.e.* reduced to point group element×translation by change of origin and hence not truly non-symmorphic.) Thus, for $\hat{G}$ non-symmorphic, $\Phi_g(\mathbf{k}) = p/\mathcal{S}_G$, with $p, \mathcal{S}_G$ relatively prime. From (9) we conclude that $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ have distinct $\hat{G}$ eigenvalues whenever $\Phi_g(\mathbf{k})\mathcal{Q}/L = pL^{d-1}\nu/\mathcal{S}_G$ is a fraction. Since we may always choose L relatively prime to the $\mathcal{S}_G$, the result of flux insertion is a state distinguished from the original state by its $\hat{G}$ eigenvalue, unless the filling is a multiple of $\mathcal{S}_G$.

What is $\mathcal{S}_G$? For a glide, $\mathcal{S}_G = 2$, but for a screw it is more subtle. Naively, we need to act with an n-fold screw n times to reduce it to a translation, so it seems as though $\mathcal{S}_G = 1/n$. However, it may be possible that a smaller power of the screw is actually removable; this occurs, for instance in both the diamond and hcp lattices. Accordingly we define the 'rank' $\mathcal{S}_G$ of G to be the smallest power of G that is removable, i.e. $\mathcal{S}_G = \min\{q|\mathcal{S}_G^q = \text{translation} \times \text{P.G.}\}$.

Defining the rank of a space group is a bit more subtle – we need to consider all different non-symmorphic operations and choose the lcm of the different $\mathcal{S}_G$s, though there are subtleties (that we will not go into here). But for any non-symmorphic space group we may define a rank $\mathcal{S}_\mathcal{G} > 1$, and trivial insulators are only allowed is the filling is a multiple of $\mathcal{S}_\mathcal{G}$ ($2\mathcal{S}_\mathcal{G}$ for electrons or half-integer spins).

From this argument, we see that in any crystal with an essential screw or a glide, we can extend the applicability of the HOLSM theorem to *odd integer* fillings, by considering ground states that are invariant under the glide symmetry (in addition to translations). A modified approach can be constructed for two 'exceptional' 3D space groups where this approach fails is provided in the appendix.

Examples: hcp and diamond lattices, even though there are two sites per unit cell cannot host a trivial insulator— in particular they cannot host a band insulator. This makes the non-symmorphic constraint a nice way to 'discover' semimetals — at an even integer filling of electrons, the Fermi volume must vanish but gaplesness implies semimetallic behaviour[14]. This is true for instance of the famous Fu-Kane-Mele model on the diamond lattice[15] (see Fig. 4). The Shastry-Sutherland lattice is a good example of 2D non-symmorphic lattice (Fig. 3, and we can consider simple tight-binding models on these. In band theory, bands come in 'sets' of $\mathcal{S}_\mathcal{G}$ — linked to the elementary band representations discussed by various people including e.g. Jenn Cano's talk at this school.

IV. SYSTEMS WITH SPIN-ORBIT COUPLING: A MATRIX PRODUCT STATE APPROACH

As we have seen above, results for spinful electrons rely on the presence of $U(1)_s$ spin rotation symmetry. This is because we can then address up and down spins separately: the 'effective filling' is then halved, and we may simply

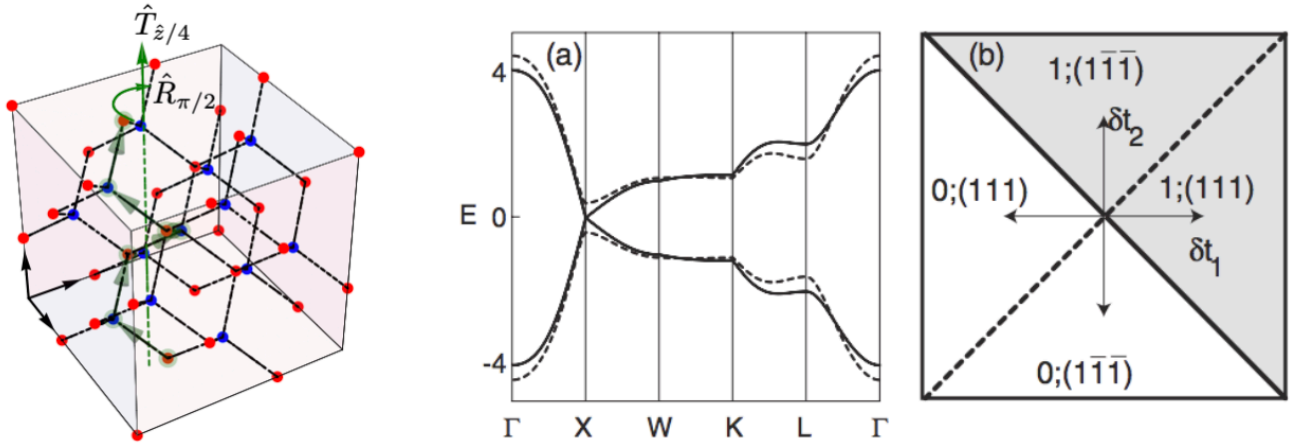

FIG. 4: The diamond lattice has both a glide plane and a four-fold screw axis, shown here, that squares to the product of a translation and ordinary rotation. Its non-symmorphic rank is 2: as long as either glide/screw are preserved, pairs of bands stick at points/planes in the Brillouin zone, as in the Fu-Kane-Mele model (center, solid). A lattice distortion can open either a trivial or topological band insulating gap (right, and center dashed lines).

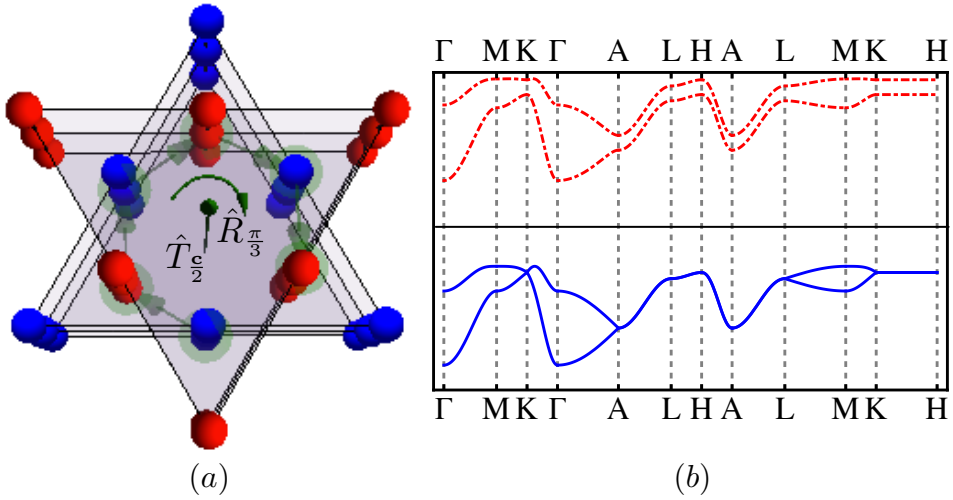

FIG. 5:

FIG. 6: (a) The hexagonal close-packed lattice has both a glide plane and a two-fold screw axis, shown here. Its non-symmorphic rank is 2. (b) As long as either glide/screw are preserved, pairs of bands stick at points/planes in the Brillouin zone, but such sticking is absent when they are broken.

port over the results for spinless fermions or bosons. This approach fails when there is spin-orbit coupling, since there is no spin rotation symmetry.

It turns out there is a distinct approach using MPS techniques that is more appropriate to this setting[16]. For simplicity we will focus on the case of translational symmetry although the generalization to non-symmorphic groups is straightforward.

The argument below is quoted more or less verbatim from Ref. 16. Let us assume the system has a symmetric short-ranged ground state $|\Psi\rangle$ that satisfies the area law for entanglement. Let $\hat{T}_x$ be the translation $x \mapsto x+1$. Each unit cell may contain many sites and orbitals. We take $\hat{\mathcal{T}}$ to represent the time-reversal operator.

We choose a bond $\bar{x} \in (x_0 - 1, x_0)$ and Schmidt decompose $|\Psi\rangle$ across the bond:

$$|\Psi\rangle = \sum_{\alpha} s_{\bar{x}\alpha} |\alpha\rangle_{\bar{x}L} |\alpha\rangle_{\bar{x}R}. \tag{10}$$

Crucially, since we have assumed $|\Psi\rangle$ obeys an area law, the Schmidt spectrum $s_{\bar{x}\alpha}$ is discrete – and hence so is the label α. Now, each Schmidt state is an eigenstate of the 'left' number operator $\sum_{x<\bar{x}} \hat{N}_x$ that measures the total charge to the left of the cut. However, the eigenvalues are subtle because they become ill-defined in the $L \to \infty$ limit; instead, we need to work with the well-defined quantity, which is the charge relative to the mean filling $\hat{Q}_x = \hat{N}_x - \nu$:

$$\sum_{x<\bar{x}} \hat{Q}_x |\alpha\rangle_{\bar{x}L} = Q_\alpha |\alpha\rangle_{\bar{x}L}, \quad Q_\alpha = \sum_{x<\bar{x}} \langle\alpha|\hat{Q}_x|\alpha\rangle_{\bar{x}L}. \tag{11}$$

This behaves well since the expectation value on the RHS vanishes as $x \to \infty$, which is a consequence of the area law: the Schmidt states differ from the ground state only in the vicinity of the cut.

We now use translational invariance. Since $\hat{T}_x|\Psi\rangle = |\Psi\rangle$ it follows that the Schmidt decompositions across different bonds are related:

$$s_{\bar{x}\alpha} = s_{\bar{x}+1\,\alpha}, \quad \hat{T}_x|\alpha\rangle_{\bar{x}\,L/R} = |\alpha\rangle_{\bar{x}+1L/R}, \quad \langle\alpha|\hat{Q}_x|\alpha\rangle_{\bar{x}\,L/R} = \langle\alpha|\hat{Q}_x|\alpha\rangle_{\bar{x}+1\,L/R}. \tag{12}$$

Now, the Schmidt states at the two cuts are related by adding a 'row' of sites:

$$|\alpha\rangle_{\bar{x}+1\,L} = \sum_{p,\beta} B^p_{\alpha\beta} |p\rangle_{x_0} |\beta\rangle_{\bar{x}L}. \tag{13}$$

We now define a charge eigenbasis for the added sites, $\hat{Q}_{x_0}|p\rangle_{x_0} = Q_p|p\rangle_{x_0}$, with $Q_p \in \mathbb{Z} - \nu$. Charge conservation implies that whenever $B^p_{\alpha\beta} \neq 0$, $Q_\alpha = Q_\beta + Q_p$, but as long as $|\Psi\rangle$ is SRE, $Q_\alpha - Q_\beta \in \mathbb{Z}$ because any two Schmidt states only differ by adding/rearranging particles near the cut[5]. This is a contradiction unless $\nu \in \mathbb{Z}$ — which is nothing other than the HOLSM theorem.

We now discuss how to incorporate time-reversal symmetry (TRS). Under TRS, each Schmidt state is part of either a Kramers singlet or a doublet:

$$\hat{\mathcal{T}}^2|\alpha\rangle_{\bar{x}\,L} = (\mathcal{T})^2_\alpha |\alpha\rangle_{\bar{x}\,L}, \quad (\mathcal{T})^2_\alpha = \pm 1. \tag{14}$$

Now $(\mathcal{T})^2_\alpha$ is related to $(-1)^{Q_\alpha}$, but really depends on the total filling, ,e, $(\mathcal{T})^2_\alpha = (-1)^{\hat{N}_x}$. Since the total charge diverges, there is an ambiguous but (as long as $|\Psi\rangle$ is SRE) α-independent phase, $\mathcal{T})^2_\alpha = e^{i\Phi}(-1)^{Q_\alpha}$. Again, because of translational invariance, both Q_α and the TR 'character' $\mathcal{T})^2_\alpha$ are independent of $\bar{x}$.

We now use this to determine the action of time-reversal squared $\hat{\mathcal{T}}^2$ on the Schmidt decomposition of the translated state:

$$\begin{aligned}
(\hat{\mathcal{T}})^2|\alpha\rangle_{\bar{x}+1\,L} &= \sum_{p,\beta} B^p_{\alpha\beta} \left(\hat{\mathcal{T}}^2|p\rangle_{x_0}\right) \left(\hat{\mathcal{T}}^2|\beta\rangle_{\bar{x}L}\right) \\
&= e^{i\Phi} \sum_{p,\beta} B^p_{\alpha\beta} (-1)^{Q_p+\nu+Q_\beta} |p\rangle_{x_0} |\beta\rangle_{\bar{x}L} \\
&= (-1)^\nu e^{i|phi} (-1)^{Q_\alpha} |\alpha\rangle_{\bar{x}+1\,L}
\end{aligned} \tag{15}$$

where we used the fact that $Q_\alpha = Q_\beta + Q_p$. Note that there is a relative factor of $(-1)^\nu$ when compared to the action on $|\alpha\rangle_{\bar{x}\,L}$. Translational invariance demands that $(-1)^\nu = 1$, for otherwise the TR character would be $\bar{x}$-dependent — and so, $\nu \in 2\mathbb{Z}$.

Therefore if $\nu \notin 2\mathbb{Z}$ one of our assumptions must be violated: the phase is either gapless, breaks a symmetry, or is symmetric but LRE. [e.g. In a gapless system, the entanglement spectrum is also gapless, and as $s_\alpha \to 0$ the Schmidt

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[5] This is not true e.g. for a cat state of two charge-density wave orders which is symmetric but not SRE. $Q_\alpha - Q_\beta$ no longer needs to be an integer and the argument does not apply.

states form a continuum and we cannot sharply define their symmetry properties, whereas in a broken-symmetry state the ambiguous phase $e^{i\Phi}$ becomes spatially dependent.]

Finally, we comment that there is another approach involving defining the system on a complicated manifold that is especially helpful in the exceptional space groups and in obtaining tight filling constraints[16].

V. SUMMARY

We have discussed how thinking about the interplay of crystal symmetry and charge conservation can provide insight into the phase structure of many-body systems. This lecture has attempted to give only a taste of the applications of the LSM theorem. There are many directions to extend these ideas and we can only give a very incomplete list of these. One is the link to quantum anomalies and to the surface states of symmetry-protected topological phases[17]. Another is to explore implications for competing orders and deconfined criticality[18]. Yet another to derive similar constraints for gapless systems[4], where we can view the 'counting' of momentum as measuring properties of the Fermi surface, such as its enclosed volume, and linking them to topological invariants[19]. Similar approaches can be used to study Kondo lattices[20]. We direct the reader to the references for further reading.

Acknowledgements

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Appendices

These appendices are excerted from the Supplement to Ref. 12 and provide alternative perspectives and a self-contained introduction to Fourier-space crystallography.

Appendix A: Fourier-Space Crystallography

In this appendix, we rederive our results (and extend them to the two exceptional cases) in a different language, that of Fourier-space crystallography. This is a reformulation of crystallography and space-group classification originally due to Bienenstock and Ewald and developed more fully by Mermin and collaborators,[11,13,21] that is especially well-suited to a many-body formulation. As this approach will be unfamiliar to most of our readers, we will summarize the basic ideas before discussing the many-body generalization.

A key idea of the Fourier-space approach to crystallography is to permit all operations that preserve the *correlation functions* of the crystal (*i.e.*, its diffraction pattern) rather than its real-space positions — as a consequence, a translation that merely shifts the origin of the crystal is equivalent to the identity. Building on this, the basic tenets of the Fourier-space approach are:

(i) the action of a group operation on a given Fourier-space density (Bragg peak amplitude) is to multiply it by a phase factor:

$$g : n_{\mathbf{k}} \to e^{2\pi i \Phi_g(\mathbf{k})} n_{g\mathbf{k}} \tag{A1}$$

where $\Phi_g(\mathbf{k})$ is a linear function of $\mathbf{k}$ and the 2π is introduced so that $\Phi_g(\mathbf{k})$ can be chosen rational.

(ii) a shift of real-space origin acts as a gauge transformation on the phase factors:

$$\chi : \Phi_g(\mathbf{k}) \to \Phi'_g(\mathbf{k}) = \Phi_g(\mathbf{k}) + \chi(g\mathbf{k} - \mathbf{k}), \tag{A2}$$

where χ is also a linear function. (Note that this is not to be confused with gauge transformations corresponding to the conserved U(1) charge.)

(iii) requiring that the group multiplication rule is faithfully represented yields a group compatibility condition on the phase factors:

$$\Phi_{gh}(\mathbf{k}) = \Phi_g(h\mathbf{k}) + \Phi_h(\mathbf{k}) \tag{A3}$$

Note that in order to maintain consistency of notation with the original formulation of the Fourier-space approach, we define symmetry transformations passively,[11,13,21] in contrast to the main text where the transformations are active. The classification of different space groups then reduces to the classification of all the possible sets of phase factors, up to gauge equivalence in the sense above, given a Bravais lattice and a compatible point group. Owing to the primacy given to the diffraction pattern rather than the real-space structure, this formulation of crystallography naturally extends to quasicrystals. As an aside, we note that in Fourier space crystallography, it is conventional to speak of 'the' symmetry g without worrying about the associated translation, since this emerges as the corresponding phase factor $\Phi_g(\mathbf{k})$; really, then, the set $\hat{G} \sim \{g|\boldsymbol{\tau}\}$ in real space is replaced by $\hat{G} \sim \{g|\Phi_g\}$ in Fourier space, with the caveat that Φ_g is to be understood in a gauge-fixed sense — this is equivalent to the statement that writing $\hat{G} \sim \{g|\boldsymbol{\tau}\}$ requires a choice of origin.

A phase factor $\Phi_g(\mathbf{k})$ for the action of a group operation g on a given Fourier component $n_{\mathbf{k}}$ of of the density is gauge invariant if and only if the reciprocal lattice vector $\mathbf{k}$ is left invariant by g *i.e.* if $g\mathbf{k} = \mathbf{k}$. An essential screw or glide has $\Phi_g(\mathbf{k}) \not\equiv 0$ (throughout this section, we use '$\equiv$' to mean 'modulo integers', since only the fractional part of the phase function matters), and manifests itself through the vanishing of the Fourier component $n_{\mathbf{k}}$ — thus, of the 157 space groups, 155 are characterized by systematic extinctions in their Bragg patterns. The remaining two exceptional cases do not have any gauge invariant phase factors; rather, they are characterized by gauge invariant phase *differences*. It is evident that such phase differences correspond to an obstruction, not in fixing a gauge to render any *given* screw or glide simple (free of an associated fractional translation) but in finding a gauge about which *all* screws/glides are simultaneously simple. Since 'choosing a gauge' is Fourier-space language for 'choosing a real-space origin', the result follows. Applying symmetry to the Bloch theory of energy bands, it was shown by König and Mermin that the existence of gauge invariant phase differences in space groups nos. 24 and 199 leads to a required touching of bands in the Brillouin zone, which suggests that this should be true in the interacting case as well, and which we confirm below.

Appendix B: Many-body polarization

The central result of this appendix — and in some ways the most elegant formulation of our results — is that the Fourier space approach has a natural interpretation as 'many-body' crystallography if we consider the action induced by the symmetry generators on the twist operators. We shall show that in this language the phase factors appear in an analogous fashion to the single particle case, but multiplied by the operator $\hat{\mathcal{Q}}/N$, accounting for the many-body structure; the same notion of gauge equivalence and the group compatibility condition will hold. With the usual caveats about the choice of N and ν, the properties for the ground states demonstrated in the main text follow immediately. In addition, the exceptional cases appear quite straightforward in this language. This is by its nature a rather telegraphic account; we defer a detailed discussion to future work.

We begin by introducing a full set of *flux-insertion operators.* These are defined by first adiabatically turning on a gauge field $\boldsymbol{A} = \boldsymbol{k}/N$ with an integer number of flux quanta through each non-contractible loop on the torus; we call this operation $\hat{F}_{\mathbf{k}}$. Since an integer number of quanta is not observable, the final Hamiltonian is equivalent to the initial one, after applying a gauge transformation. The necessary transformation is

$$\hat{U}_{\mathbf{k}} = \exp\left\{-\frac{i}{N}\int d^d r\,(\mathbf{k}\cdot\mathbf{r})\hat{\rho}(\mathbf{r})\right\}. \tag{B1}$$

The product of the two transformations $\hat{T}_{\mathbf{k}} = \hat{U}_{\mathbf{k}}\hat{F}_{\mathbf{k}}$, which we will colloquially term a *twist operator*, returns the Hamiltonian to itself. Furthermore, since the system is assumed to be an insulator, the energy cannot change more

than an exponentially small amount. Thus the twist operators $\{\hat{T}_{\mathbf{k}}\}$ for reciprocal lattice vectors $\mathbf{k}$ are operators on the space of ground states. Crucially, if the ground state is unique, it must be a simultaneous eigenstate of all of them. This will contradict the transformation properties of the $\{\hat{T}_{\mathbf{k}}\}$ in a non-symmorphic lattice if the filling is not a multiple of the non-symmorphic rank $\mathcal{S}$.

Let us consider a symmetry operator $\hat{G} \sim \{g|\boldsymbol{\tau}\}$ as before. It acts on the gauge transformation operator $\hat{U}_{\mathbf{k}}$ via conjugation: a straightforward calculation yields

$$\begin{aligned} \hat{G}^{-1}\hat{U}_{\mathbf{k}}\hat{G} &= \exp\left\{\frac{i}{N}\int d^d r\,(g\mathbf{k})\cdot\mathbf{r}\hat{\rho}(\mathbf{r})\right\} e^{-i\mathbf{k}\cdot g^{-1}\boldsymbol{\tau}\hat{\mathcal{Q}}/N} \\ &\equiv \hat{U}_{g\mathbf{k}}\, e^{2\pi i\Phi_g(\mathbf{k})\hat{\mathcal{Q}}/N} \end{aligned} \tag{B2}$$

where we have used the fact that $\mathbf{k}\cdot(g^{-1}\mathbf{r}) = g\mathbf{k}\cdot\mathbf{r}$, and identified the phase function

$$\Phi_g(\mathbf{k}) = \frac{1}{2\pi}\left(g^{-1}\boldsymbol{\tau}\right)\cdot\mathbf{k} = \frac{1}{2\pi}\boldsymbol{\tau}\cdot(g\mathbf{k}) \tag{B3}$$

which is manifestly a linear function of $\mathbf{k}$. (Note that when $g\mathbf{k} = \mathbf{k}$ these reduce to the definitions in the main text.)

The adiabatic turning on of the flux $\hat{F}_{\mathbf{k}}$ transforms as $\hat{G}^{-1}\hat{F}_{\mathbf{k}}\hat{G} = \hat{F}_{g\mathbf{k}}$, and so the full flux-threading operator transforms as

$$\hat{G}^{-1}\hat{T}_{\mathbf{k}}\hat{G} = \hat{T}_{g\mathbf{k}}\, e^{2\pi i\Phi_g(\mathbf{k})\hat{\mathcal{Q}}/N} \tag{B4}$$

Furthermore, we have the relations

$$\hat{T}_{\mathbf{k}_1}\hat{T}_{\mathbf{k}_2} = \hat{T}_{\mathbf{k}_1+\mathbf{k}_2}. \tag{B5}$$

In order to understand the gauge transformation induced by a change of origin, consider the transformation $\mathbf{r} \to \mathbf{r}+\mathbf{a}$ which accomplishes such a change. We then have

$$\hat{U}_{\mathbf{k}} \to \hat{U}_{\mathbf{k}}\, e^{2\pi i\chi(\mathbf{k})\hat{\mathcal{Q}}/N} \tag{B6}$$

where $\chi(\mathbf{k}) = \mathbf{a}\cdot\mathbf{k}$ is again a linear function of $\mathbf{k}$. From this, it follows that under a gauge transformation we must have $\Phi_g(\mathbf{k}) \to \Phi'_g(\mathbf{k})$, where

$$\Phi'_g(\mathbf{k}) = \Phi_g(\mathbf{k}) + \chi(g\mathbf{k}) - \chi(\mathbf{k}) \tag{B7}$$

which we obtain by undoing the gauge transformation to return to the original gauge, performing the symmetry operation, and then redoing the gauge transformation to return to the new gauge. Note that (B6) has the same form as (A1), except that the phase factor is multiplied by the number operator. In addition, the phase factor transforms identically under gauge transformations — as is evident from comparing (B7) and (A2). Going further, we can verify that the group compatibility condition (A3) is obeyed for a pair of transformations $\{g|\boldsymbol{\tau}\}, \{h|\boldsymbol{\tau}'\}$.

Thus, the 'many-body' definition of the phase function that can be inferred from the action of the symmetry generators on the set of twist operators is consistent with that obtained from considering the 'classical' action of symmetry on the reciprocal space amplitude of the particle density. Since the phase function, the space on which it acts (*i.e.*, the reciprocal lattice), the group compatibility condition and the gauge transformation all agree, the results of the Fourier-space classification of space groups corresponds with a classification of the algebra of twist operators, with the caveat that the phase factors are multiplied by an additional factor reflecting the many-body physics. By replacing $\hat{\mathcal{Q}}$ by its eigenvalue $N^3\nu$ (valid since particle number is a good quantum number), it is evident that many-body phase factors differ from the phase factors for single-particle Fourier-space crystallography by a factor $N^2\nu$. For $\nu = 1$ and for an appropriate choice of N^2 that is indivisible by any of the denominators of the nonzero (*i.e.*, up to addition by integers) phase factors, the fact that a phase factor or phase difference is nonzero in the single-particle case, which flags a non-symmorphic space group, retains the property that it is nonzero in the many-body sense. In this sense, the non-symmorphicity of the space group, and attendant consequences for the phase factors and the symmetry structure, carry through to the many-body case. We will demonstrate below a few consequences of this correspondence.

1. Alternative Proof of Ground-State Degeneracy for Non-Exceptional Non-Symmorphic Space groups

We now reproduce the degeneracy of the 155 non-exceptional non-symmorphic space groups, discussed in the main text, which is straightforward in the Fourier-space language. Consider the expectation value $\langle\Psi|\hat{T}_{\mathbf{k}}|\Psi\rangle$. Here, $\mathbf{k}$ is chosen along along the invariant plane/axis of an essential glide/screw g, which satisfies $g^q = \mathbf{1}$ (as always, $q = 1, 2, 3, 4$ or 6). Then, $\Phi_g(\mathbf{k}) \not\equiv 0$ by definition, and since we have $g\mathbf{k} = \mathbf{k}$ the phase is gauge invariant. From this combined with the fact that $g^q = \mathbf{1}$ and the group compatibility condition, we must have $q\Phi_g(\mathbf{k}) \equiv 0$; thus, the denominator of the phase factor must be a divisor of q. A further constraint is placed on the phase factor if some power $\tilde{q} < q$ of the phase factor is removable, for in this case in some gauge we must have $\tilde{q}\Phi_g(\mathbf{k}) \equiv 0$, for otherwise $g^{\tilde{q}}$ would be essential. If we choose $\tilde{q}$ to be the smallest power for which $g^{\tilde{q}}$ is removable we must have $\tilde{q}$ be a divisor of q (this can be verified by explicit computation). Thus, the denominator of $\Phi_g(\mathbf{k})$ must be $\tilde{q}$ and the numerator must be relatively prime to this for if not, a smaller factor than $\tilde{q}$ would render $\Phi_g(\mathbf{k}) \equiv 0$. From our definition of the non-symmorphic rank of a space group operation as the smallest power to which it can be raised to make it removable, it is evident that $\mathcal{S}_g = \tilde{q}$, and from the above discussion we see that the phase factor is of the form $\Phi_g(\mathbf{k}) = p/\mathcal{S}_g$ with $p, \mathcal{S}_g$ relatively prime. From this, we see that if the ground state preserves the symmetry we have (replacing $\hat{\mathcal{Q}}$ by $N^3\nu$)

$$\begin{aligned}\langle\Psi|\hat{T}_{\mathbf{k}}|\Psi\rangle &= \langle\Psi|\hat{G}^{-1}\hat{T}_{\mathbf{k}}\hat{G}|\Psi\rangle \\ &= \langle\Psi|\hat{T}_{g\mathbf{k}}|\Psi\rangle\, e^{i2\pi\Phi_g(\mathbf{k})N^2\nu}\end{aligned} \tag{B8}$$

Since $g\mathbf{k} = \mathbf{k}$ and the gauge-invariant phase factor is given by $\Phi_g(\mathbf{k}) = p/\mathcal{S}_g$, we find that

$$\langle\Psi|\hat{T}_{\mathbf{k}}|\Psi\rangle = \langle\Psi|\hat{T}_{\mathbf{k}}|\Psi\rangle\, e^{i2\pi N^2\nu p/\mathcal{S}_g} \tag{B9}$$

Now if the ground state $|\Psi\rangle$ is unique, then it is an eigenvector of $\hat{T}_{\mathbf{k}}$, since this operator transforms ground states into other ground states. It then follows that the filling must be a multiple of $\mathcal{S}_g$ (by taking N to be a large number that is relatively prime to $\mathcal{S}_g$). In other words, if the symmetries are preserved, then any sufficiently large system whose size N is relatively prime to $\mathcal{S}_g$ must have degenerate ground states. To make the connection to the proof quoted in the main text apparent, observe that since $\hat{T}_{\mathbf{k}} = \hat{U}_{\mathbf{k}}\hat{F}_{\mathbf{k}}$, and $\hat{F}_{\mathbf{k}}$, $\hat{U}_{\mathbf{k}}$ correspond to inserting a flux and performing a gauge transformation, it is clear that $\langle\Psi|\hat{T}_{\mathbf{k}}|\Psi\rangle = \langle\Psi|\hat{U}_{\mathbf{k}}|\Psi'\rangle = \langle\Psi|\tilde{\Psi}\rangle$, and thus the two approaches are equivalent (modulo changes due to the active versus passive definition used in this appendix.)

Appendix C: Proof of Degeneracy for Exceptional Cases and Definition of Non-Symmorphic Rank

This approach using twist operators can also be used to define the non-symmorphic rank arising from the interplay of all the symmetries in the group, a particular application of which is to rule out a featureless phase for the two exceptional space groups not covered by our preceding discussion. To do so, we first need to introduce the idea of many-body polarization. A sharp characterization of the insulating phase is given by the electronic polarization,[22,23] a quantity that is nonzero in the insulator but ill-defined in the metallic phase. Specifically, in this paper we consider a definition of the polarization[24–26] appropriate to the specific periodic system size N. Recall that if the ground state is unique then it must be an eigenstate of all the $\hat{T}_{\mathbf{k}}$. Eq. (B5) implies that the phase of the eigenvalues have a linear dependence on $\mathbf{k}$

$$\hat{T}_{\mathbf{k}}|\Psi\rangle = e^{-2\pi i\mathbf{k}\cdot\boldsymbol{\mathcal{P}}^{(N)}}|\Psi\rangle \tag{C1}$$

where we use the superscript to remind us that this definition is for a finite system. (We write (C1) in units where $e = 1$; in general units, $\boldsymbol{\mathcal{P}}$ should be replaced by $\boldsymbol{\mathcal{P}}/e$ throughout.) The behavior of the finite-system polarization $\boldsymbol{\mathcal{P}}^{(N)}$ in the thermodynamic limit can be used to define the many-body polarization of the ground state when a Chern number is not present. Even in the latter case, although polarization is no longer well-defined, $\boldsymbol{\mathcal{P}}^{(N)}$ on a system of a fixed size still makes sense; note that as it is a vector, the group operations transform $\boldsymbol{\mathcal{P}}^{(N)}$. Now, replacing the expectation values in Eq. (B8) by the exponential of the polarization, and using Eq. (B3), we find that the combination

$$\begin{aligned}w^{(N)} &= -\nu N^2\boldsymbol{\tau}\cdot g\mathbf{k} + \boldsymbol{\mathcal{P}}^{(N)}\cdot(g\mathbf{k} - \mathbf{k}) \\ &= \left(-\nu N^2 g^{-1}\boldsymbol{\tau} + g^{-1}\boldsymbol{\mathcal{P}}^{(N)} - \boldsymbol{\mathcal{P}}^{(N)}\right)\cdot\mathbf{k}\end{aligned} \tag{C2}$$

is an integer. Since this is true for every reciprocal lattice vector $\mathbf{k}$,

$$g\boldsymbol{\mathcal{P}}^{(N)} + \nu N^2 \boldsymbol{\tau} \equiv \boldsymbol{\mathcal{P}}^{(N)} \tag{C3}$$

where the equivalence is modulo a Bravais lattice vector. Now we take (C3) for systems of size N and $N+1$, multiply them by $2N+3$ and $2N-1$ respectively and subtract. This cancels off the factor of N^2, leaving

$$g\boldsymbol{\mathcal{P}} + \nu\boldsymbol{\tau} \equiv \boldsymbol{\mathcal{P}} \tag{C4}$$

where $\boldsymbol{\mathcal{P}} = (2N+3)\boldsymbol{\mathcal{P}}^{(N)} - (2N-1)\boldsymbol{\mathcal{P}}^{(N+1)}$. From this, it is clear that

$$g\left(\frac{\boldsymbol{\mathcal{P}}}{\nu}\right) + \boldsymbol{\tau} = \frac{\boldsymbol{\mathcal{P}}}{\nu} + \frac{1}{\nu}\,\mathbf{a}_G \tag{C5}$$

for some Bravais lattice vector $\mathbf{a}_G$. Thus, if we define the coordinate $\mathbf{r}_0 = \boldsymbol{\mathcal{P}}/\nu$ we find that

$$\hat{G} : \mathbf{r}_0 \to g\mathbf{r}_0 + \boldsymbol{\tau} = \boldsymbol{r}_0 + \frac{\boldsymbol{a}_G}{\nu} \tag{C6}$$

for some Bravais lattice vector $\boldsymbol{a}_G$, *i.e.*, $\boldsymbol{r}_0$ is invariant under the symmetries up to $1/\nu^{\text{th}}$ of a Bravais lattice vector. If $\nu = 1$, then $\boldsymbol{r}_0$ can be used as a center for all group operations, and hence the lattice must be symmorphic. For a non-symmorphic lattice, the minimum value of ν for which such a point $\boldsymbol{r}_0$ exists can be defined as the non-symmorphic rank $\mathcal{S}$; this is the minimum filling where trivial insulators have a chance to exist.

Intuitively, $\boldsymbol{\mathcal{P}}$ is the polarization of a unit cell (relative to the origin appearing in the definition of $\hat{U}_{\mathbf{k}}$), so $\mathbf{r}_0 = \boldsymbol{\mathcal{P}}/\nu$ is the center of charge of the ν electrons in the cell. If there is a single electron per unit cell, this center of charge is well-defined (within each unit cell). If the group is non-symmorphic, applying the right symmetry will change the charge-center, and thus the new wave function is different from the original one. When there are more electrons in a unit cell, the center of charge becomes less well defined, with ν^3 locations in a grid in each unit cell (on account of dividing the polarization, defined only modulo a lattice vector, by ν). Thus, for a large enough value of ν, it becomes easy to ensure that these charge centers are mapped among themselves.

This argument applies to the two exceptional groups. For any one element of these groups, there is a symmetric location for the charge center. But the group elements do not have a common point of symmetry. We find in fact that $\mathcal{S} = 2$ for these groups.

As the remaining 155 non-symmorphic space groups were covered by our previous arguments, this concludes the proof that all non-symmorphic space groups have $\mathcal{S} > 1$. We observe that the phase-space approach motivates two possible lines of further inquiry: (i) it extends naturally to higher dimensions, and to quasicrystals;[27] (ii) it has a natural formulation in the language of cohomology,[28] and suggests that the existence of gapped featureless phases with space-group symmetries may be understood within this language. Similar technology has been brought to bear, with fruitful consequences, for situations with local symmetries.[29]

Appendix D: Some Examples

a. Shastry-Sutherland Lattice

The SSL is generated by the primitive vectors $\mathbf{a}_1 = (b+c)\hat{\mathbf{x}}, \mathbf{a}_2 = (b+c)\hat{\mathbf{y}}$ and the four-site basis $\left\{\frac{b}{2}(\hat{\mathbf{x}}-\hat{\mathbf{y}}), \frac{b}{2}(-\hat{\mathbf{x}}+\hat{\mathbf{y}}), \frac{c}{2}(\hat{\mathbf{x}}+\hat{\mathbf{y}}), -\frac{c}{2}(\hat{\mathbf{x}}-\hat{\mathbf{y}})\right\}$ with $b \neq c$, and corresponds to 2D space group $p4g$. The non-symmorphic operation is a glide comprised of a reflection about a plane parallel to $\mathbf{a}_1$ and passing through the origin in the specified coordinate system, followed by a translation by $\mathbf{a}_1/2$. Since the two primitive vectors are orthogonal, it follows that this cannot be the projection of a lattice vector on the glide plane and therefore the glide is essential, leading to $\mathcal{S} = 2$ (in two dimensions, this is the only nontrivial value of $\mathcal{S}$). Since there are four sites per unit cell, a spin-$\frac{1}{2}$ model will have saturation magnetization of 2 per unit cell; half this value corresponds to a filling of $\nu = 1$, and thus the half-magnetization plateau must either break symmetry or exhibit topological order.

b. Hexagonal Close-Packing

The hcp lattice is generated by the primitive vectors $\mathbf{a}_1 = a\hat{\mathbf{x}}, \mathbf{a}_2 = a\left(-\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right), \mathbf{a}_3 = c\hat{\mathbf{z}}$ and two-site basis $\left\{\mathbf{0}, \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3\right\}$ and corresponds to space group $P6_3/mmc$ (no. 194). The crystal possesses a screw axis involving a sixfold rotation about $\mathbf{a}_3$ centered at the point $(2\mathbf{a}_1 + \mathbf{a}_2)/3$, followed by a translation by $\frac{1}{2}\mathbf{a}_3$. Applying this twice yields the product of a pure translation (by $\mathbf{a}_3$) and a three-fold rotation, and so the non-symmorphic rank of this operation is 2. The only other non-symmorphic element is a glide reflection, also of rank 2, from which we conclude that the rank of the group is $\mathcal{S} = 2$. Our result then shows that in the absence of broken lattice symmetries, a noninteracting band insulator (of spinful electrons) must be metallic unless the filling is a multiple of 4. Furthermore, if interactions are included and open a gap, except at such fillings the resulting insulating ground state cannot be featureless, and so must break symmetry or exhibit topological order.

c. Diamond

The diamond lattice is characterized by the non-symmorphic space group $Fd\bar{3}m$. In coordinates in which the fcc Bravais lattice primitive vectors are $\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}})$ and the two-site basis is $\left\{\mathbf{0}, \frac{a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})\right\}$, the crystal has a 4_1 screw axis consisting of a fourfold rotation about the $\hat{\mathbf{z}}$ axis centered at $\hat{\mathbf{x}}/4$, followed by a translation through $\hat{\mathbf{z}}/4$. Applying this twice yields a two-fold screw that is removable, as can be readily diagnosed by the fact that lattice vectors $\mathbf{a}_1, \mathbf{a}_2$ have projections of $\hat{\mathbf{z}}/2$ onto the axis. As all the remaining non-symmorphic operations are glides which also have rank 2, $\mathcal{S} = 2$. Now, take a model of local spin-$\frac{1}{2}$ moments on the diamond lattice, described by a Hamiltonian with U(1) spin symmetry and hence conserved magnetization along some axis, which we label $\hat{S}^z$. Following our prescription, we identify the charge at position $\mathbf{r}$ as $\hat{\mathcal{Q}}_{\mathbf{r}} = \hat{S}^z_{\mathbf{r}} + \frac{1}{2}$. From this, we find that the total charge is $\hat{\mathcal{Q}} = \sum_{\mathbf{r}} \hat{\mathcal{Q}}_{\mathbf{r}} = \hat{S}^z_{\text{tot}} + N^3$, where $\hat{S}^z_{\text{tot}} = \sum_{\mathbf{r}} \hat{S}^z_{\mathbf{r}}$ and we have used the fact that there are two spins in each unit cell. This corresponds to a filling of $\nu = s^z + 1$ where s^z is the magnetization per unit cell. A gapped, featureless, and topologically trivial paramagnetic ground state (the spin analog of a featureless insulator) is ruled out unless ν is a multiple of 2. In particular, if in addition to the U(1) symmetry the $\mathbb{Z}_2$ symmetry $\hat{S}^z_{\mathbf{r}} \to -\hat{S}^z_{\mathbf{r}}$ is preserved (which includes the fully SU(2)-symmetric limit) the total magnetization must vanish and so $\nu = 1$. In this case, any gapped ground state must either break lattice symmetry, or form a topologically ordered spin liquid. This suggests a route to a three-dimensional quantum spin liquid on the diamond lattice by frustrating the tendency of spins to magnetically order. We also observe that the pyrochlore lattice has the same space group as diamond, but *four* sites in each unit cell; for a spin-$\frac{1}{2}$ model on this lattice with vanishing total magnetization, we find $\nu = 2$ and therefore a gapped, featureless quantum paramagnet is an allowed ground state.

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