Latent Symmetry Induced Degeneracies

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Degeneracies in the energy spectra of physical systems are commonly considered to be either of accidental character or induced by symmetries of the Hamiltonian. We develop an approach to explain degeneracies by tracing them back to symmetries of an isospectral effective Hamiltonian derived by subsystem partitioning. We provide an intuitive interpretation of such latent symmetries by relating them to corresponding local symmetries in the powers of the underlying Hamiltonian matrix. As an application, we relate the degeneracies induced by the rotation symmetry of a real Hamiltonian to a non-Abelian latent symmetry group. It is demonstrated that the rotational symmetries can be broken in a controlled manner while maintaining the underlying more fundamental latent symmetry. This opens up the perspective of investigating accidental degeneracies in terms of latent symmetries.

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Introduction.—Identifying the origin of spectral degeneracies in quantum systems is of fundamental importance for the understanding and control of their structural and dynamical properties. Degenerate states are at the heart of spectacular phenomena like the Jahn-Teller effect [1] and the quantum Hall effect [2,3] as well as the electromagnetic response of, e.g., atoms or molecules [4,5] in general. In lattice systems designed macroscopic degeneracies can realize flat bands within a variety of setups including optical lattices, photonic waveguide arrays, and superconducting networks [6]. Further, degeneracies in the form of conical intersections of molecular potential energy surfaces play a central role for ultrafast dynamical decay processes [7,8] and are responsible, e.g., for molecular self-repair mechanisms in photobiology [9].

When degeneracies occur in the energy spectrum, the first place to seek their origin is commonly the group of geometrical symmetry operations commuting with the underlying Hamiltonian. Prominent examples for such symmetries are the molecular point group in chemistry or the space group in crystallography. If this group is non-Abelian—that is, if at least two symmetry operations do not commute with each other—it induces degeneracies of multiplicities determined by the dimensions of the group's irreducible representations. More challenging is the reverse question of assigning degeneracies to a symmetry group with a physical significance [10,11]. A famous example of a physically significant, yet not obvious, symmetry from the early days of quantum theory is the SO(4) symmetry leading to the conservation of the Runge-Lenz vector in the hydrogen atom [12]. If no such physically meaningful symmetry group can be found, the degeneracy is traditionally called accidental [13]. This often occurs for systems with several or many degrees of freedom where eigenenergies happen to coincide at some location in the corresponding parameter space, intersections of molecular potential energy surfaces being a typical example [14].

In this work, we promote a different viewpoint on assigning degeneracies to symmetries of the system. Instead of performing a symmetry analysis of the Hamiltonian itself, we do this for the effective Hamiltonian obtained from the original one by reducing it onto a subsystem while retaining the energy spectrum. We note that its core property—the preservation of the energy spectrum—clearly distinguishes this approach from those which analyze the symmetries of an effective model obtained by truncation or a mean-field ansatz. Focusing on generic discrete models, we here show how geometrical symmetries of the isospectrally reduced Hamiltonian induce spectral degeneracies for the original system. Such latent symmetries, as introduced recently in graph theory [15], are generally not apparent in the original system at hand. In fact, as we show here, they are directly linked to corresponding local symmetries, though in all powers of the original Hamiltonian. Navigating through the proposed concepts, visualized by minimalistic examples, we (i) show how non-Abelian latent symmetries are necessarily induced by rotation symmetries of a real Hamiltonian, and (ii) demonstrate that these latent symmetries, along with their induced degeneracies, can be preserved even when breaking the original rotational symmetry. Lastly, we link a special case of latent symmetry to what we call here a generalized exchange symmetry of the Hamiltonian.

Degeneracies from latent symmetries.—The concepts and results developed in this work are valid for generic setups described by a finite-dimensional matrix. This matrix can be drawn from a wide range of physical

platforms: It could represent a Bloch Hamiltonian of a tight-binding lattice [16], a molecular Hückel Hamiltonian [17,18], a multiport scattering matrix [19], or very generally the matrix H occurring in (linearized) dynamical problems [20], such as coupled oscillators [21]. To convey the main ideas in a transparent way, we will illustrate it by means of minimalistic prototypical setups.

In order to reveal the latent symmetries of a general complex matrix H, we will rely on a dimensional reduction of H which preserves the eigenvalue spectrum. This *isospectral* reduction is defined as [15,22]

$$\mathcal{R}_S(H,\lambda) = H_{SS} - H_{S\bar{S}}(H_{\bar{S}\bar{S}} - \lambda I)^{-1} H_{\bar{S}S}, \tag{1}$$

whereby S is a set sites and $\bar{S}$ denotes the complement set of all other sites of the given setup. H_{SS} and $H_{\bar{S}\bar{S}}$ denote the respective Hamiltonians of the sub-systems consisting only of the sites in S or $\bar{S}$. $H_{\bar{S}S}$ and $H_{S\bar{S}}$ represent the coupling between the two sub-systems, and I is the identity matrix. The isospectral reduction $\mathcal{R}_S(H,\lambda)$ is equivalent to an effective Hamiltonian gained from a subsystem partitioning of H [23], and its entries are rational functions of the parameter λ.

A Hamiltonian H is *latently symmetric* if there exists an isospectral reduction $\mathcal{R}_S(H,\lambda)$ with a symmetry, that is, which commutes with a group of matrices $\{M\}$ independent of λ. We now demonstrate this concept by means of the simple 6-site Hamiltonian H depicted in fig. 1(a). This Hamiltonian illustrates the minimal prototype of a system with non-trivial latent symmetry. H is parametrized by three real coupling parameters $h_i \neq 0$, $i \in \{1,2,3\}$ and two on-site potentials v_1, v_2. The eigenvalue spectrum of H contains two doubly degenerate eigenvalues for any choice of these parameters. To explain these degeneracies in terms of latent symmetries of H, we reduce it by means of Eq. (1) over $S = \{1,2,3\}$. This yields the symmetric matrix

$$\mathcal{R}_{S=\{1,2,3\}}(H,\lambda) = \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix}, \tag{2}$$

with $a = v_1 + (h_1^2 + h_2^2/\lambda - v_2)$, $b = (h_1 h_2/\lambda - v_2) + h_3$. A graphical representation of Eq. (2) is depicted in Fig. 1(b). The graph is highly symmetric and is invariant under six symmetry operations: three rotations and three reflections. These six operations form the so-called dihedral group D_3, which is non-Abelian.

We now draw a general connection between non-Abelian latent symmetries of a given Hamiltonian H and its eigenvalue spectrum. To this end, we use the fact that *each* of the so-called "nonlinear" eigenvalues belonging to $\mathcal{R}_S(H,\lambda)$ in Eq. (2), defined as the solutions λ_j to the nonlinear eigenvalue problem

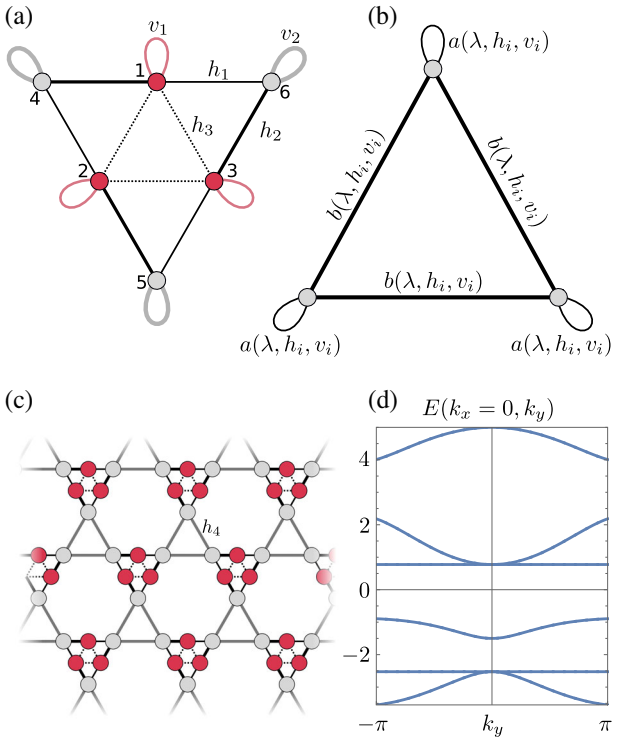

FIG. 1. (a) A six-site Hamiltonian H which features a non-Abelian D_3 permutation symmetry if $h_1 = h_2$, but only an Abelian C_3 permutation symmetry if $h_1 \neq h_2$. A line between two different sites i, j corresponds to a nonvanishing matrix element $H_{i,j}$, taking parametric values h_1, h_2, or h_3 (indicated by different line styles). Loops connecting a site to itself correspond to diagonal matrix elements $H_{i,i}$ with parametric values v_1 or v_2. (b) The result of the isospectral reduction of H over the three red sites $S = \{1,2,3\}$. The reduced Hamiltonian [Eq. (2)] features a D_3 permutation symmetry for any choice of λ, h_i, or v_i. (c) A modified kagome lattice with H as a unit cell. The band structure of this lattice for $k_x = 0$ is plotted in (d) for $h_1 = 4/3$, $h_2 = 5/3$, $h_3 = 0.7$, $h_4 = 3/2$, $v_i = 0$.

$$\mathrm{Det}[\mathcal{R}_S(H,\lambda_j) - \lambda_j I] = 0 \tag{3}$$

is also an eigenvalue of H [22]. Moreover, whenever the eigenvalue spectra of H and of the subsystem $H_{\bar{S}\bar{S}}$ do not intersect, the eigenvalue spectra of $\mathcal{R}_S(H,\lambda)$ and H coincide [22]. This motivates calling $\mathcal{R}_S(H,\lambda)$ an "isospectral reduction." From the above considerations, it is clear that degeneracies in the eigenvalue spectrum of $\mathcal{R}_S(H,\lambda)$ necessarily correspond to degeneracies in the eigenvalue spectrum of H. Moreover, and as we show in Sec. I. of the Supplemental Material [24], non-Abelian symmetries of the isospectral reduction $\mathcal{R}_S(H,\lambda)$ lead to degeneracies in the spectrum of its nonlinear eigenvalues. Thus, non-Abelian latent symmetries of H necessarily induce degeneracies onto the eigenvalue spectrum of H. Specifically, lower bounds on the multiplicity of H's eigenvalues are given by dimensions of the irreducible

representations of the underlying non-Abelian symmetry group of $\mathcal{R}_S(H,\lambda)$.

We emphasize that the above statements are completely general in the sense that they are valid for all kinds of latent symmetries (not just permutations), and for arbitrary (even non-Hermitian) diagonalizable matrices H. Irrespective of this applicability to general symmetries, we concentrate on the special case of permutation symmetries throughout this Letter. After all, permutation symmetries are among the easiest to detect—often by bare eye—and thus provide a convenient workhorse for depicting the main features of latent symmetries.

In the above, we have explained the spectral degeneracies of the prototype example Fig. 1(a) in terms of its latent symmetries. This system has been deliberately designed to be as simple as possible in order to convey the main ideas of latent symmetries. The underlying concept is, however, not limited to such basic examples, but can be applied to larger systems, as we demonstrate now. Figure 1(c) shows a lattice built by taking the prototype Hamiltonian H of Fig. 1(a) as a unit cell. The band structure of this lattice is depicted in Fig. 1(d). At the Γ point, that is, at $\mathbf{k}=0$, the corresponding Bloch-Hamiltonian features the same latent symmetries as H in Fig. 1(a). This explains the two double degeneracies in the band structure [24]. Interestingly, the lattice further hosts two flat bands, which in general can also be designed through latent symmetries [30].

Latent D_n permutation symmetries.—Let us now examine the symmetries of the prototype example of Fig. 1 in more detail. This setup is invariant under permutations which cyclically permute sets of three sites, graphically represented by rotations of multiples of $2\pi/3$. These rotations form the abelian cyclic group of order 3, denoted by C_3. As we have seen above, the setup also featured a latent D_3 permutation symmetry, and this is no coincidence. Indeed, as we show in the Supplemental Material, *every* C_n-permutation symmetric real Hamiltonian H features a latent D_n permutation symmetry [24]. As is well known, the dihedral group D_n is non-Abelian for $n \geq 3$, so that the underlying Hamiltonian automatically features degeneracies. This gives an alternative explanation to those degeneracies, which are classically understood in terms of the combination of the Abelian group $C_{n\geq 3}$ and the real valuedness of H which corresponds to a time-reversal symmetry of H [31].

Latent D_n symmetries without any permutation symmetries.—Above we have stated that a C_n permutation symmetry of a real Hamiltonian is a sufficient condition for a latent D_n permutation symmetry. However, it is not a necessary condition. Indeed, we demonstrate in the following the versatility of latent symmetries by showing that they can even exist when the underlying Hamiltonian H has *no* permutation symmetry at all. Figure 2(a) shows an example of such a Hamiltonian H, which can also be interpreted as

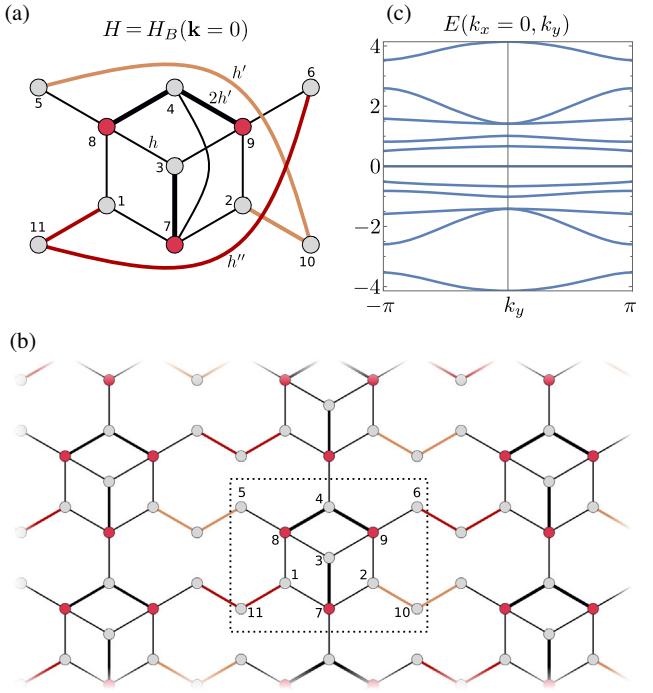

FIG. 2. (a) A Hamiltonian that features no permutation symmetry for $hh'h'' \neq 0$ and $h' \neq h''$. It does, however, feature a latent D_3 permutation symmetry that becomes visible when reducing over $S=\{7,8,9\}$. (b) A lattice whose Bloch-Hamiltonian H_B at $\mathbf{k}=0$ equals H. The dotted box shows the lattice unit cell. (c) The band structure of this lattice for $k_x=0, h=1, h'=1/2, h''=3/4$.

the Bloch Hamiltonian $H_B(\mathbf{k}=0)$ of the lattice in Fig. 2(b) at crystal momentum $\mathbf{k}=0$. A detailed derivation of this lattice is shown in Sec. V of the Supplemental Material [24]. For $hh'h'' \neq 0$ and $h' \neq h''$, H does not feature any permutation symmetry. However, for any choice of those three hopping parameters, it features a latent D_3 symmetry which becomes visible when reducing H over the three red sites $S=\{7,8,9\}$. As a result of this non-Abelian latent symmetry, H has at least one doubly degenerate eigenvalue pair for *any* choice of h' and h''. We can now understand the two double degeneracies in the band structure [depicted in Fig. 2(c)] of the lattice of Fig. 2(b) at $k_x=k_y=0$: At this point, the Bloch-Hamiltonian is given by H, so that it features a latent D_3 symmetry and therefore also degeneracies.

Interestingly, when setting $h'=h''$, H features a C_2 permutation symmetry, graphically corresponding to a reflection about the line connecting the sites 4 and 7. One can thus say that h' and h'' are control parameters for a symmetry breaking, and since H features a latent D_3 permutation symmetry for *any* choice of h,h',h'', this opens the perspective of investigating and understanding symmetry breaking in terms of latent symmetries. In Sec. III. of the Supplemental Material, we show how latent symmetry preserving modifications (which may break permutation symmetries) can be derived [24].

Linking latent to local symmetries.—One might wonder if a latent symmetry leaves some recognizable traces in the original Hamiltonian. This is indeed the case: By expressing $\mathcal{R}_S(H,\lambda)$ as a power series in λ and subsequently analyzing it order by order, one can show [24] that

$$[\mathcal{R}_S(H,\lambda),M]=0 \Leftrightarrow [(H^k)_{SS},M]=0 \quad \forall\ k, \tag{4}$$

where M denotes a symmetry operation. In other words, symmetries of $\mathcal{R}_S(H,\lambda)$ correspond to local symmetries [32,33] of H *in all matrix powers*. In particular, H itself has to be locally symmetric. Indeed, for our introductory example of Fig. 1(a) and $S=\{1,2,3\}$, we see that H_{SS} denotes the inner triangle, which obviously features the same symmetries as the corresponding isospectral reduction $\mathcal{R}_S(H,\lambda)$ depicted in Fig. 1(b).

Equation (4) can be used to facilitate the search for latent permutation symmetries. To this end, let us assume that we are given a (possibly large) Hamiltonian H and want to check if it features a latent permutation symmetry as the one depicted in Fig. 1(b). In other words, we look for a set of three sites $S=\{u,v,w\}$ such that $\mathcal{R}_S(H,\lambda)$ has the form of Eq. (2). Now, instead of computing and checking *all possible* isospectral reductions of H over three sites, we can use Eq. (4) to see that any candidate sites u, v, w necessarily have to fulfill $(H^k)_{u,u}=(H^k)_{v,v}=(H^k)_{w,w}$ for all k. This condition can be augmented by employing the Cayley-Hamilton theorem, which states that any matrix power $H^{k\geq N}$ (N being the dimension of H) is a polynomial in smaller powers. Thus, by computing the matrix powers $H,H^2,\ldots,H^{N-1}$—the cost of which grows polynomially with N—and grouping the sites accordingly, the number of possible candidate sites $\{u,v,w\}$ can be drastically reduced. In particular, if there is any k such that H^k features no three sites with equal on-site potential $(H^k)_{i,i}$, a latent symmetry of the kind Eq. (2) is impossible.

Generalized exchange symmetries.—Having demonstrated the relation of latent symmetries to symmetries of the subsystem H_{SS} and to degeneracies of H, we finally relate a subclass of latent symmetries to symmetries of the original Hamiltonian H. This subclass consists of latent permutation symmetries of real Hamiltonians. Using graph-theoretical tools [34,35], such Hamiltonians can be shown to necessarily feature what we call here a *generalized exchange symmetry* (GES). A GES is an orthogonal symmetric matrix $Q^{(i,j)}$ fulfilling $[Q^{(i,j)},H]=0$ and $(Q^{(i,j)})^2=I$ and which exchanges the two sites i, j while acting on the remaining sites as an orthogonal transformation. In the special case when this transformation is a pure permutation, $Q^{(i,j)}$ becomes a normal exchange symmetry, i.e., it acts *on each* site either as the identity or as an exchange operator. To provide an impression of the GESs, we explicitly computed—by solving the equations derived from its defining properties—$Q^{(1,2)}$ for the Hamiltonian of Fig. 1(a):

$$Q^{(1,2)}=\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{h_1h_2}{d} & 1-\frac{h_1^2}{d} & \frac{h_1(h_1-h_2)}{d} \\ 0 & 0 & 0 & 1-\frac{h_1^2}{d} & \frac{h_1(h_1-h_2)}{d} & \frac{h_1h_2}{d} \\ 0 & 0 & 0 & \frac{h_1(h_1-h_2)}{d} & \frac{h_1h_2}{d} & 1-\frac{h_1^2}{d} \end{pmatrix} \tag{5}$$

with $d=h_1^2-h_2h_1+h_2^2$. Note that for the case of $h_1=h_2$ the GES $Q^{(1,2)}$ becomes the ordinary exchange symmetry which permutes (1,2), (5,6), and leaves 3 and 4 invariant, and therefore describes the reflection about the line that connects sites 3 and 4 in Fig. 1. However, in the case where $h_1\neq h_2$, this pure permutation symmetry is broken, whereas the more abstract GES persists. We note that, while the GESs as an abstract symmetry class persists, the *matrix entries* of $Q^{(1,2)}$ depend on h_1 and h_2. This is an important difference to the latent D_3 permutation symmetry of H, whose matrix representation is independent of the values of h_i.

Finally, let us note that one can use the above insights to prove the existence of degeneracies for real latently $D_{n\geq 3}$ permutation symmetric Hamiltonians in yet another way [24]. Such Hamiltonians feature more than one GES, and by explicitly constructing them it can be shown that at least two of them do not commute with each other. Since the Hamiltonian H commutes with both of these GESs, it directly follows that H has to have at least one degenerate eigenvalue. It remains an open task to classify GESs using group-theoretical tools.

Conclusions.—We have provided a theoretical framework which connects non-Abelian latent symmetries of generic discrete models to their spectral degeneracies. For the important class of latent permutation symmetries, our results may allow for a geometrical explanation of apparently accidental degeneracies. Moreover, by identifying latent symmetries as local symmetries of all powers of the Hamiltonian, our results additionally suggest a convenient method for finding these latent symmetries. We further demonstrate that it is possible to break symmetries of an original Hamiltonian while preserving its latent symmetry. This may inspire techniques to modify—or probe—a given system asymmetrically without affecting its degeneracy.

Our considerations apply quite generally to physical systems possessing a discrete representation in terms of a finite-dimensional matrix. This includes, among others, tight-binding models, molecular Hamiltonians in truncated orbital bases, and multiport scattering setups. We therefore envision the applicability of our results in a broad variety of setups, contributing to the better understanding, design, and control of spectral degeneracies beyond conventional symmetries.

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