High-degeneracy points protected by site-permutation symmetries

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Space group symmetries dictate the energy degeneracy of quasiparticles (e.g., electronic, photonic) in crystalline structures. For spinless systems, there can only be double or triple degeneracies protected by these symmetries, while other degeneracies are usually taken as accidental. In this Letter we show that it is possible to design higher degeneracies exploiting site permutation symmetries. These design principles are shown to be satisfied in previously studied lattices, and new structures are proposed with three, four and five degeneracy points for spinless systems. The results are general and apply to different quasiparticle models. Here, we focus on a tight-binding approach for the electronic case as a proof of principle. The resulting high-degeneracy points are protected by the site-permutation symmetries, yielding pseudospin-1 and -2 Dirac fermions. The strategy proposed here can be used to design lattices with high-degeneracy points in electronic (e.g. metal-organic frameworks), photonic, phononic, magnonic and cold-atom systems.

Condensed matter systems are not constrained by the Poincaré symmetry. Therefore a rich variety of quasiparticles, without high-energy counterparts, emerge [1]. For instance, higher pseudospin Dirac and Weyl quasiparticles have been studied in Refs. [2–4]. These quasiparticles, arising in high-degeneracy points, present enhanced Klein tunneling [5], and supersonic scattering regimes [6]. Moreover, associated with high-degeneracy (HD) points, hourglass [7–9] and Kane [10, 11] fermions have been proposed and observed in 3D and 2D systems. Focusing in technological applications, beyond the new quasiparticles, a synergy between HD points in the electronic and phononic energy spectra allow for an enhanced thermoelectric performance [12, 13]. However, the space group symmetries, for spinless systems, only constrain the states to have at most twofold (in 2D systems) and threefold (in 3D systems) degeneracy, apart from accidental degeneracies [14, 15]. Finding degeneracy points beyond the space group symmetries constraints is a key to the emergence of new topological and semimetal phases [16–18].

Currently, an extensive case by case search for HD points has been the object of different studies [1, 19, 20]. However, a design principle to achieve such HD points is still missing. Concomitantly, we are facing a great experimental control of lattices formations [21–23], where threefold band degeneracy has been experimentally observed in a photonic [24] and in a cold atoms [25] lattices. Additionally, state-of-the-art organic chemistry allows for a combination of different designed molecules, yielding nontrivial structures [26–28].

In this Letter, we analyze symmetry protected HD occurring in periodic lattices. For a N equivalent sites spinless lattice, we find that (N−1)-degenerated states are protected by a set of (N−1) site-permutation symmetries. This allows us to propose a design principle for these HD points, which we illustrate for a few 2D and 3D lattices. Furthermore, lattices fulfilling the minimum ingredients to the HD points, and robust against long range inter-sites couplings, have been found. The generality of the presented discussion allows for an interpretation in the context of different quasiparticle systems: electronic, photonic, phononic, magnonic, and cold-atoms [29–32]. Here, we focus on electronic spinless tight-binding (TB) models at the Γ point (k = 0) to show that pseudospin-1 and -2 Dirac fermions emerge in the HD points.

Site-permutation symmetries and degeneracy. In 2D spinless systems with azimuthally symmetric inter-site interactions (e.g., s, p_z, d_{2z} orbitals in electronic systems), and in 3D for spherically symmetric interactions (i.e., s orbitals in electronic systems), all point-group (PG) operations at Γ can be decomposed into combinations of the site-permutation operations [33]. More interestingly, beyond the PG symmetries, extra site-permutation symmetries can introduce new degeneracies in the Hamiltonian spectra. These can be understood as a consequence of sublattice equivalences.

Let us start with a simple abstract lattice, where all sites are equivalent. Later we will properly define more general conditions for the lattices. First, let P^{(ij)} be a site-permutation operation that exchanges the i-th and j-th sites, i.e., a pair permutation [34]. Considering a basis localized on the each site, the matrix representation D(P^{(ij)}) of P^{(ij)} has elements D_{kk} (P^{(ij)}) = 1 for k = {i, j}, D_{ij} (P^{(ij)}) = D_{ji} (P^{(ij)}) = 1, and D_{kl} (P^{(ij)}) = 0 otherwise. Therefore, such operators are real and unitary, P^{(ij)} = P^{(ji)} = [P^{(ij)}]^{-1}.

Next, the goal is to find Hamiltonians (H_N) that commute with all these N−1 permutations symmetries.
within the basis set presented above, $H_N$ becomes

$$H_N = t \mathbb{J}_N - (t + m) \mathbb{I}_N = \begin{pmatrix} m & t & \ldots & t \\ t & m & \ldots & t \\ \vdots & \vdots & \ddots & \vdots \\ t & t & \ldots & m \end{pmatrix},$$

where $t$ is a real number, $\mathbb{J}_N$ is the $N \times N$ all-ones matrix and $\mathbb{I}_N$ is the $N \times N$ identity matrix. The role of the $m$ number will be further discussed below. For now, note that $m$ just rigidly shift the eigenvalues of $H_N$. Since the site-permutations symmetries act exchanging lines and columns of the Hamiltonian matrix, the Eq. (2) is the most general form allowed for $H_N$ that is invariant under the permutations, i.e., $P^{(ij)} H_N P^{(ij)} = H_N$. This Hamiltonian has only two sets of eigenvalues ($\lambda_n$) [36], a $N - 1$ degenerated set with $\lambda_1 = \lambda_2 = \cdots \lambda_{N-1} = -t + m$, and a non-degenerated $\lambda_N = (N - 1)t + m$. Therefore, for $N$ site lattices described by these symmetries, a $N - 1$ degeneracy-point emerges.

Lattice constraints. The site permutation operations $P^{(ij)}$ that commutes with $H_N$ are limited to equivalent sites $i \equiv j$. The equivalence here refers to sites with the same local energy, and that couple in the same way with every other site, creating a uniformity in $H_N$. Within a 1st-nearest neighbor (1NN) interaction, this uniformity reflects in the coordination number of the sites $i$ and $j$ being the same. This site coordination number can be cast as $c_1 = n_1(N - 1) + m_1$, where $n_1$ is the number of times a site $i$ couples with each of the remaining $N - 1$ sites $j \neq i$ within the same or neighboring cells, and $m_1$ is the number of times a site $i$ couples with itself on neighboring cells. This condition can be extrapolated for long-range interactions. For each distance defining a $p$-th nearest neighbor (pNN) interaction, a $c_p = n_p(N - 1) + m_p$ coordination condition should be satisfied. Below, lattices fulfilling the conditions for at least 1NN interactions are presented, see Fig. 1. Within these lattices, two Figs. 1(a) and (e) satisfy the long range condition $pNN$ for $p \rightarrow \infty$.

Illustrative systems. Here it is proposed five 2D and three 3D lattices satisfying at least the 1NN constraint. The lattices shown in Fig. 1 have $N = 3, 4, 5$ and 6 equivalent sites within their unit cells, allowing from twofold to fivefold degeneracy. All the proposed lattices have $m_1 = 0$ within the 1NN constraint. The two-dimensional kagome [Fig. 1(a)] and triangular-rectangular lattices [Fig. 1(b)] have $N = 3$ and $n_1 = 2$, i.e. each of the $i = 1, 2$ and 3 sites couples two times with the other two $j \neq i$. For the square-octagonal, pyramidal and snub-hexagonal lattices [Fig. 1(c)-(e)], with $N = 4, 5$ and 6, respectively, the $i$-th site couples only once with each $j \neq i$ neighbor, thus $n_1 = 1$. The three-dimensional tetragonal-crossed, pyrochlore and octrahedral lattices [Fig. 1(f)-(h)], have $N = 4, 4$ and 6, and analogously $n_1 = 2, 2$ and 1, respectively. Interestingly, three of these lattices, the kagome, the square-octagonal and the snub-hexagonal belong to the same class of Archimedean lattices [37]. Additionally, graphene’s $p_z$ orbitals satisfy the Hamiltonian $H_2$ within 1NN with $c_1 = 3$ and $m_1 = 0$, but since $N = 2$, there are only non-degenerated states $(N - 1 = 1$ degeneracy), excluding the spin degeneracy.

These lattices can be designed in photonic [29] and cold-atoms [32] systems. Moreover, these proposed lattices have been experimentally observed or theoretically predicted in crystalline materials. For instance, the
The presence of these HD, with the exception of the kagome lattice, could not be predicted from the space group symmetries of each lattice, since the permutation operations encloses more symmetries than the ones present in the space group. For instance, the space group symmetries predicts at most a (i) non-degeneracy for triangular-rectangular lattice Pmmm space group, while here it was found a twofold degeneracy; (ii) twofold degeneracy for the kagome (P6/mmm), square-octagonal(P4/mmm), pyramidal (P4/mmm), snub-hexagonal (P6/m), crossed-tetrahedral (P4_2/mmc) and cubic-octahedra lattices. The energy scale is $t/n_1$, where the NN hopping strength is $t = -1$, and $n_1$ is the number of equivalent NN

$kagome lattice occurs in MOFs [38, 39] and in Fe$_3$Sn$_2$ [40], while its 3D version, the pyroclore lattice, occurs in many ternary oxide systems [41]. The snub-hexagonal lattice can be grown with MOF surface self-assembly [42, 43], and in a stable boron 2D allotrope [44, 45]. Still within borophene polymorphs, a structure similar to the triangular-rectangular lattices have been experimentally found [46], while a square-octagon lattice has been shown in a carbon 2D allotrope [47].

Tight-binding model. Up until this point no considerations regarding the nature of the $H_N$ was discussed. The analysis above is general for all quasiparticles localized in lattice sites. In order to show the degeneracy points, and its robustness with the site-permutation symmetries, we consider a spinless electronic TB model for each lattice with the on-site energy $\varepsilon_i$ and hopping terms $t_{ij}$ as

$$H_{TB} = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{i \neq j} t_{ij} c_i^\dagger c_j.$$  

(3)

Unless specified, we assume $\varepsilon_i = 0$, and a hopping strength decaying with the distance between the sites as $t_{ij} = t \exp(-\alpha d_{ij})$, with $t = \exp(\alpha d_{1NN}) = -1$ defining the energy scale, and $d_{ij}$ and $d_{1NN}$ as the inter-site distance and 1NN distance, respectively. The $\alpha$ factor controls the range of the inter-site couplings. For $\alpha \gg (d_{1NN})^{-1}$ only 1NN hoppings are significant to $H_{TB}$, while $\alpha \ll (d_{1NN})^{-1}$ a long range interaction emerge with significant contribution from further neighbors.

For the kagome lattice ($N = 3$), the energy dispersion shows a twofold degeneracy between a flat and a parabolic band at $\Gamma$, Fig. 2(a), and the third nondegenerate band completes the set of $N$ states from $H_N$. For the triangular-rectangular lattice, the same degeneracies of the kagome lattice occurs at $\Gamma$, Fig. 2(b). However, in this case a flat band is seen only along the $\Gamma$-$Y$ direction, while asymmetrically, a linear Dirac-like dispersion is observed for the $\Gamma$-$X$ and $\Gamma$-$M$ directions. Triple-degeneracy, forming an isotropic pseudospin-1 Dirac dispersion, is observed in the square-octagonal lattice ($N = 4$), Fig. 2(c). For the $N = 5$ pyramidal lattice of Fig. 2(d), an anisotropic behavior is observed, where the fourfold degeneracy has a Dirac cone with twofold degenerated flat band dispersion along the $\Gamma$-$X$ direction, while two Dirac dispersions with different velocities are present along $\Gamma$-$M$. For the $N = 6$ snub-hexagonal lattice the fivefold degeneracy at $\Gamma$ behave as an isotropic pseudospin-2 Dirac quasiparticle, with the two Dirac cones with velocities distinct by a factor of two, Fig. 2(e), and a nearly flat band in between. In the $N = 4$ crossed-tetrahedral and pyroclore 3D lattices [Fig. 2(f) and (g)] the HD point behave as a pseudospin-1 Dirac quasiparticle at the $k_z = 0$ plane of the BZ, while in the $k_z$ direction the triple point is formed by two flat bands and a quadratic dispersive one. Lastly, in the $N = 6$ cubic-octahedra lattice, the HD point is highly anisotropic, with a Dirac cone and threefold degenerated flat band dispersion for the $\Gamma$-$X$ direction, and doubly degenerated Dirac cones with a non-degenerated flat band for the $\Gamma$-$R$ direction. Furthermore, in its $\Gamma$-$M$ direction a pseudospin-2 Dirac-like quasi-particle emerges.
pyrocore (P6m2) lattices, while it was found from threefold to fivefold degeneracies; and (iii) threefold degeneracy for the cubic-octahedra Pm3m space group, while a fivelfold degeneracy was found.

Long range couplings \( pNN \). Although lattices can be designed to have only local couplings by tuning the distance between the sites, for instance in photonic lattice constructions [21, 22] and designed MOF systems [27, 28], long range interactions may break the site-permutation symmetries. Indeed, for most of the lattices studied here, that is the case, with the exception of the Kagome and the snub-hexagonal lattices. For these two lattices, the \( c_p \) constraint for the \( pNN \) coordination is always fulfilled, leading the form of \( H_N \) being robust. Therefore, the \( \Gamma \) point degeneracies in the kagome lattice and the pseudospin-2 Dirac quasiparticle of the snub-hexagonal lattice are robust against long range isotropic interactions. Particularly, for the snub-hexagonal, the space group predicts a twofold degeneracy, while the site-permutation symmetry shows that a fivefold symmetry is always preserved at \( \Gamma \) [47].

Lattice perturbations. Local perturbations in the lattice, e.g. site substitutions, or bond length distortions, will break the site-permutation symmetry. However, if not all site-permutation symmetries are broken, the Hamiltonian still commutes with a subset of these operations, yielding a smaller degenerate set of eigenvalues.

To illustrate this behavior, we consider the snub-hexagonal lattice. Let us break specific site-permutations symmetries by changing the on-site energy of each site, Fig. 3(f). For instance, if all sites have identical energy, the \( N = 6 \) Hamiltonian commutes with the five site-permutation symmetries \( P^{(1k)} \), with \( k = 2, \ldots, 6 \), leading to the fivefold degeneracy of Fig. 2(e). By changing the on-site energy of site \( k = 2 \), the Hamiltonian cease to commute with \( P^{(1k)} \), but still commutes with the other 4 operations, leading to the fourfold degeneracy of Fig. 3(a). Similarly, by breaking two, three and four of the SP symmetries, a threefold, twofold and non-degenerated points are seen in Fig. 3(b), (c) and (d), respectively.

More generally, this shows that the site-permutation symmetries can generate HD points even in lattices with more than one type of site. The required criteria is that a subset of the site-permutation symmetries is still present. Considering that the sites split into two equivalence sets with \( N_1 \) and \( N_2 \) sites each, the Hamiltonian takes the form

\[
H_{N_1, N_2} = \begin{pmatrix}
H_{N_1} & v_0 V_{12}^\dagger \\
v_0 V_{12} & H_{N_2}
\end{pmatrix},
\]

where \( H_{N_1} \) and \( H_{N_2} \) are given by Eq. (2) for the subset of site-permutation symmetries for each set of equivalent sites, \( V_{12} \) is an all-ones rectangular \( N_1 \times N_2 \) matrix, and \( v_0 \) is the hopping intensity between the subsets. In this form \( H_{N_1, N_2} \) will provide eigenvalues split into four sets: two sets of \( N_1 - 1 \) and \( N_2 - 1 \) degenerate states; and other two non-degenerate states.

For instance, let’s consider splitting the snub-hexagonal lattice into a polar lattice with two non-equivalent sets of three sites, viz. sites 1, 2 and 3 with on-site energy \( \varepsilon_a \) and sites 4, 5 and 6 with \( \varepsilon_b \neq \varepsilon_a \). In this case we can still define two sets of permutation operations that commutes with the Hamiltonian, \( P^{(1k)} \) with \( k = 2, 3 \) and \( P^{(4l)} \) with \( l = 5, 6 \). These two sets allow for two double degenerated eigenvalues at the \( \Gamma \) point, as shown in Fig. 3(e).

Conclusions. In summary, it has been established a design principle for HD eigenvalues in lattice Hamiltonians. Lattices with \( N \) equivalent sites in their unity cell, and azimuthal/spherical inter-site interactions for 2D/3D systems, satisfying the coordination numbers criteria \( c_p \), will present a Hamiltonian with a spectra consisting of two sets of eigenvalues: one non-degenerate state, and \( N - 1 \) degenerate states. These HD points are not predicted by the lattice space groups, rather they are stabilized by a set of site-permutation symmetries. This feature is satisfied in the 2D and 3D lattices shown here. For the case of electronic systems, higher pseudospin Dirac fermions were shown to emerge in these HD points. More importantly, the generality of the discussion allows the interpretation of the results and lattice designs among different quasiparticle systems, e.g. electronic, phononic, photonic, magnonic, cold-atoms.

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