Van Hove Bound States in the Continuum: localized subradiant states in finite open lattices

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We show that finite lattices with arbitrary boundaries may support degenerate subspaces, stemming from the underlying translational symmetry of the lattice. When the lattice is coupled to an environment, a potentially large number of these states remains weakly or perfectly uncoupled from the environment, realising a new kind of bound states in the continuum. These states are strongly localized along particular directions of the lattice which, in the limit of strong coupling to the environment, leads to spatially-localized subradiant states.

I. INTRODUCTION

Controlling the spatial and temporal evolution of light, acoustic or matter waves is at the core of a wealth of modern technologies and research. Just as interference between electronic Bloch waves underlies band structure theory in condensed matter, in photonics the interplay between constructive and destructive interference and spatial localisation is the basis of disparate applications such as lasering\textsuperscript{7–9}, slow light\textsuperscript{10}, light focusing\textsuperscript{11,12}, or frequency up-conversion\textsuperscript{13} to name a few. Recent works have also proposed to identify and harness lattice states strongly coupled to their environment based on lattice symmetries for quantum optics\textsuperscript{14–17}, and as structured environments supporting BICs in finite lattices, without specific requirements on lattice symmetry or the existence of flat bands. The key idea is that of \textit{van Hove degeneracies}, which are directly connected with van Hove singularities. A van Hove singularity (VHS) is a divergence in the density of states (DOS), $\rho(E)$, of an infinite lattice\textsuperscript{18–20}. The relation between the dispersion relation of the system, $E(k)$, and its DOS, $\rho(E) = \int dS/|\nabla E(k)|$, where $dS$ is the isofrequency surface element, implies that VHSs are found at the critical points of the Brillouin zone, where $E(k)$ has an extremum. In a \textit{finite} lattice of suitable geometry, the VHS translates into a high-dimensional subspace of degenerate states at the van Hove energy — a van Hove degeneracy (VHD). Further, we show that, when the lattice is coupled to an environment, the states in the VHD split into three subspaces: non-dissipative (‘sub-radiant’) localized states that we name VH BICs, sub-radiant delocalized states, and highly-dissipative localized states, which occur as high-$Q$ resonances for weak coupling. We analyse the impact of these subspaces on the transmission properties of photonic crystals, and discuss their relation to dark states and guided modes. Finally, we discuss the connection of VH BICs with the super-radiance transition in finite lattices.

II. VAN HOVE BICS IN OPEN FINITE LATTICES

We start considering a tight-binding Hamiltonian on a two-dimensional lattice, with $L_x$ columns and $L_y$ rows, with hopping between nearest neighbours. This model can represent a range of material systems including a fiber bundle, where photons hope between single fibers; a set of coupled dielectric resonators placed in a microwave
cavity, among which microwave photons hop; or single electrons hopping in an array of quantum dots. For concreteness, we restrict our calculations to a triangular lattice, as this has no sublattice symmetry, thus avoiding complications due to the interplay between VH and chiral BICs.

In the limit of a large system, $L_x, L_y \gg 1$, the dispersion relation of this system reads

$$E(k) = -2t \left[ \cos k_x a + 2 \cos \frac{k_x a}{2} \cos \frac{\sqrt{3} k_y a}{2} \right],$$

where $a$ is the lattice constant, $t$ is the nearest-neighbor hopping matrix element, and $k = (k_x, k_y)$ is a wavevector in reciprocal space. The critical momenta where $|\nabla E(k)| = 0$ fulfill that either $E(k) = 2t$ or the energy is at the upper or lower edges of the spectrum. We are concerned with the former, which correspond to a saddle point of the spectrum and lead to a divergence in the DOS — a VH singularity (VHS) \[21,22\]. These critical momenta are $k_{VH}^j = (k_x, k_y) = (\pm \pi, \pm \pi/\sqrt{3})$, where $j = 1, \ldots, 4$ indexes the four possible sign combinations.

In a finite lattice, only momenta $k$ compatible with the boundary conditions set by the geometry of the system are possible. When the boundaries allow stationary waves with wave vectors equal to $k_{VH}$, the lattice will support a large number of degenerate states at the VH energy, $E_{VH} = E(k_{VH})$, reflecting the singularity that emerges in the infinite-size limit. We refer to this degenerate space associated with the VHS as a VH degenerate subspace or van Hove degeneracy (VHD).

The exact dimension, $n_{VH}$, of the VH degenerate subspace depends in a sensitive manner on the shape of the system. It can be determined as the number of linearly independent solutions of the Schrödinger equation with eigenenergy $E_{VH}$. This number equals the dimension of the Hilbert space minus the rank of the square matrix $\mathbb{H} - E_{VH} \mathbb{I}$, where $\mathbb{H}$ is the Hamiltonian matrix and $\mathbb{I}$ the $N_{\text{sites}} \times N_{\text{sites}}$ identity matrix, with $N_{\text{sites}}$ the number of lattice sites. The existence of a degenerate eigenvalue of $\mathbb{H}$ implies that the rank of the Hamiltonian is at most the dimension of $\mathbb{H}$ minus two $\[13,23,29\]$. Generally, very symmetric structures, such as a square domain $(L_x = L_y)$, feature large degeneracies, but arbitrary boundaries may also support high-dimensional VHDs, $n_{VH} \gg 1$. The general solution of this problem is highly non-trivial although some results regarding the generalization of Bloch functions to finite lattices are known $\[27,29\]$.

We illustrate this in Fig. 1(a), where we show exact-diagonalization results for the dimension of the VHD at $E = 2t$ for a triangular lattice with rectangular boundaries, as a function of the length of the sides of the rectangle, $(L_x, L_y)$, with $L_i \in [2, 35]$. The strong peaks along the diagonals indicate that generally more symmetric structures (when $L_x/L_y$ is a rational number) support larger degeneracies. We observe a strong even-odd effect [see Fig. 1(c)]: square domains with odd-length sides (i.e., $L_x = L_y$ an odd number) systematically support a large number of degenerate states, $n_{VH} = L_x - 1$, while even-length square domains generally support no VH subspaces, $n_{VH} = 0$.

To illustrate the generality of the mechanism supporting the VHD in finite systems, and the fact it does not require a fine tuning of the lattice geometry, we calculate next $n_{VH}$ for triangular lattices on rectangular domains with a circular hole in the center of the square [Fig. 1(d)]. We consider in particular a hole of radius $1/6$ of the smaller dimension, as this corresponds to a discretized version of a Sinai billiard. This is a well-known chaotic billiard $\[20\]$ — a system that has been studied experimentally with microwave cavities $\[40\]$ and exciton-polaritons in semiconductor microcavities $\[31\]$, among other photonic systems. We find that even this chaotic geometry can support large-dimensional VHDs, see Fig. 1(b). Occasionally, the VHD of Sinai lattices is even larger than that of full $L_x \times L_y$ lattices $\[33\]$.

We consider next the fate of the states in the VHD when the system is coupled to an environment. When we couple a generic finite lattice to an environment, part of the eigenstates in the VHD will acquire a finite width while part of them will remain spatially bound within the lattice and constitute true BICs, similarly to what happens with chiral BICs $\[13,21,22\]$. To prove this, consider the VHD at energy $E_{VH}$, of dimension $n_{VH}$, localized losses at a set of sites $l \in \mathcal{L}$, with loss rate $\gamma_l$, can be described by introducing an effective complex on-site energy, $\gamma_l$, that represents the loss rate at site $l$. Then, the Schrödinger equation for the part of the wavefunction within the lattice, $\Psi$, becomes

$$\mathbb{H} \Psi - E_{VH} \Psi - i \sum_{l \in \mathcal{L}} \gamma_l \Psi_l = 0. \quad (1)$$

Here $\Psi_l$ is the component of $\Psi$ at lattice site $l$. Generally, for each lossy site the rank of the matrix $\mathbb{H} - E_{VH} \mathbb{I} - \gamma_l \mathbb{I}$ is increased by one with respect to the rank of the matrix corresponding to the closed system, $\mathbb{H} - E_{VH} \mathbb{I}$ (there can be exceptions for specific values of $\gamma_l$ where the rank may remain unchanged). This reduction in the rank corresponds to states in the VHD that acquire a finite width; we refer to them as VH resonances. As we will show, these are still strongly localized states, whose spatial profiles display features directly related to the critical moment $k_{VH}$, except perhaps in the limit $\gamma \to \infty$. The other states in the VHD do not acquire a non-zero width but constitute true BICs, which we name van Hove BICs (VH BICs). The number of VH BICs, $n_{\text{BIC}}$, generally satisfies $n_{\text{BIC}} = n_{VH} - |\mathcal{L}|$, where $|\mathcal{L}|$ is the number of lossy sites $\[21,22\]$. Given that $n_{VH} \gg 1$, we have that $n_{\text{BIC}}$ can be very large, depending on the boundary conditions of the finite system. Finally, the spectrum of the open system contains a third subspace of highly-delocalized states coupled weakly to the environment.

We assess the localization of the eigenstates of Eq. (1) by means of the inverse participation ratio (IPR). The
FIG. 1. (a) Number of degenerate states at the VH energy, \( n_{VH} \), for a triangular lattice with \( L_x \) columns and \( L_y \) rows. (b) Same as (a) for a triangular lattice with a central hole of radius 1/6 of the smaller size (Sinai billiard). (c) Even-odd effect in \( n_{VH} \) for \( L_x \times L_y \) lattices without (blue squares) and with (orange circles) a circular hole at the centre. (d) Example \( L_x \times L_y = 20 \times 20 \) lattice with a circular hole of radius \( R = 3.25 \). Each dot is a lattice site, while the dashed line indicates the boundary of the central hole.

IPR of a pure state \( \Psi \) over a basis set \( \{ |i\rangle \} \) is defined as

\[
IPR = \frac{1}{\sum_i |\langle i|\Psi\rangle|^2}.
\]

It quantifies the distribution of \( \Psi \) over that set. Taking \( \{ |i\rangle \} \) as the set of normalised eigenstates with state \( |i\rangle \) localized at site \( i \) of the lattice, a state \( \Psi \) with \( IPR = 1 \) is delocalized throughout the whole lattice, while a state localized on a single site satisfies \( IPR = 1/N_{\text{sites}} \).

We show in Fig. 2(a1) the IPRs of all eigenstates of a 23 × 23 lattice as a function of the imaginary part of their eigenenergy, for a decay rate \( \gamma = 0.102 < t \) (we use \( t = 1 \) as our energy unit throughout). Lossy sites with the same value for the coupling strength \( \gamma \) are placed in the 11 leftmost sites of the bottom row. We observe that the spectrum is divided into three subspaces:

- (A) localized states with \( |\text{Im}(E)| \geq \gamma/4 \);
- (B) localized states with \( |\text{Im}(E)| < \gamma/4 \);
- (C) delocalized states with \( |\text{Im}(E)| < \gamma/4 \).

Figure 2(c1) shows that the states with the largest decay rates occur near \( \text{Re}(E) = E_{VH} \). Finally, Fig. 2(b1) illustrates the absence of delocalized states \( (IPR \approx 1) \) near \( E_{VH} \) for small \( \gamma \). The division into the three subspaces (A,B,C) as well as their main features remain valid as \( \gamma \) is increased. The middle column of Figure 2 shows the same results for \( \gamma \approx t \) while the right column shows results for \( \gamma \gg t \).

Notably, the set (A) of lossy states progressively separates in the \( \text{Im}(E) \) axis such that, for \( \gamma \gg t \), the few states in (A) exhaust the whole set of lossy states and is equal to the number of sites with losses, Figure 2(c3).

In Sec. V we will relate this behavior to the phenomenon of superradiance. Before that, we discuss two types of propagation experiments on finite lattices which enable us to relate the three subspaces to dark states in Sec. III and to guided modes in Sec. IV.

The qualitative evolution of these three subspaces as we increase the coupling \( \gamma \) does not depend on whether \( n_{\text{BIC}} \) is finite or zero. In the case shown in Fig. 2, the number of lossy sites is larger than the dimension of the VHD, but due to the shape of the leaky region, the system supports a small number of lossless states, \( n_{\text{BIC}} = 7 \); however, we have verified that the overall evolution of the spaces (A,B,C) with \( \gamma \) is the same for a variety of shapes and sizes of the leaky region and sizes of the lattice, which supports the generality of this picture. Still, we remark that when \( n_{\text{BIC}} > 0 \), the VH BICs are part of the subspace (B) with \( |\text{Im}(E)| \) strictly equal to zero, irrespective of the actual value of the coupling strength \( \gamma \).

III. VAN HOVE BICS AS DARK STATES IN FINITE LATTICES

We consider first an experiment connecting leads on two opposite borders of a finite lattice. This corresponds, e.g., to pumping radiation into the lattice through waveguides coupled to selected sites on the top edge of a photonic crystal, and collecting the output radiation through waveguides at the bottom edge, see inset of Fig. 3(a).

We show in Fig. 3(a) the DOS for a triangular lattice on a 9 × 9 square domain with 3-site leads centered on the top and bottom edges; and in Fig. 3(b) the transmittance of this system calculated using Landauer-Büttiker formalism. As we have three in-/out-coupling channels, the maximum possible transmittance normalized to the flux incoming through one of the input channels is 3.

Typically the transmittance of such a system is proportional to the DOS, with geometric prefactors depending on the connection to the waveguides. Thus, a peak in the DOS at an energy \( E \) is usually correlated to a peak in the transmission at that energy, although the relative heights of peaks can vary through the spectrum. This correlation holds generally true in Fig. 3 except close to \( E = E_{VH} \), where the presence of BICs leads to a divergence of the DOS which, however, does not translate to the transmission properties. This indicates that large numbers of states at \( E_{VH} \) do not couple to the leads. This situation is reminiscent of the case of chiral BICs, where
the sublattice symmetry leads to an exact zero of the transmittance at zero energy\(^{15}\). However, in the present case the transmittance at \(E_{\text{VH}}\) is not exactly zero due to the tails of other peaks close in energy.

When a state in the VHD becomes coupled to the waveguides, its eigenenergy acquires a finite width and the position of the resonance is shifted away from \(E_{\text{VH}}\). For weak coupling, the width acquired is small, and such a state appears as a narrow, or high-\(Q\), resonances\(^{5,15,17}\). Other states in the VHD do not couple to the waveguides and remain at \(E_{\text{VH}}\); they constitute true BICs (VH BICs), and behave as perfect dark states of the lattice.

Systems with \(n_{\text{VH}} \gg 1\) can support a large number of such dark states. The results on \(n_{\text{VH}}\) as a function of the lattice geometry [Fig. 1] then point to practical guidelines for the design of metasurfaces with a large number of dark states.

### IV. VAN HOVE BICS AS GUIDED MODES

A complementary propagation experiment consists of injecting a wavepacket into the lattice, which is coupled by a number of lossy sites to the environment, and letting it propagate for a long time; this setup models e.g. the propagation of a wavepacket down a fiber bundle with some fibers considerably lossier than others.

We model this situation using a non-Hermitian Hamiltonian\(^{36,37}\),

\[
\hat{H}_{\text{open}} = \hat{H} - i\gamma \hat{\Gamma},
\]

where \(\hat{H}\) is the tight-binding Hamiltonian of the closed lattice, and the coupling to the environment is described by the loss rate \(\gamma\) and the operator

\[
\hat{\Gamma} = \sum_{j=1}^{N_l} \sum_{j'} c_{j'}^\dagger c_j,
\]

identifying a number \(N_l\) of lossy sites in the lattice. The invariance of the trace of \(H_{\text{open}}\) implies a sum rule on the widths of the eigenstates, which here must add to \(-N_l\gamma\).

We show in Fig. 4 the normalised density after a long time evolution simulating one such experiment, with some particular choices of lattice geometry and lossy sites. Expanding the initial wavepacket on the set of eigenstates of Eq. (3), after a long evolution time, the remaining density will be a linear superposition of the eigenstates with smaller \(\text{Im}(E)\), the actual density depending on the overlap of the initial wavepacket each state in that space. Given the division of the eigenstates in the subspaces (A,B,C), we expect only components within (B,C) to survive for long evolution times. Moreover, for a relatively localized initial wavepacket, we expect its overlap with highly delocalized states in (C) to
be small. Hence, in practice only the components on the subspace (B) of VH BICs will be relevant. The wavefunction of a state within the VHD can be written

$$\Psi_{\text{VH}}(r) = \sum_j \sum_{\mathbf{K}} A_j e^{i (k_{\text{VH}}^j \mathbf{r} + \mathbf{K} \mathbf{r})},$$

where $\mathbf{r} = (x, y)$ is a position in the lattice, $k_{\text{VH}}^j$ are the VH wavevectors of that lattice, and the $\mathbf{K}$ sum runs over all reciprocal lattice vectors. For the case of the triangular lattice $k_{\text{VH}}^j = (\pm \pi, \pm \pi/\sqrt{3})$ and $\Psi_{\text{VH}}$ will feature increased density, due to constructive interference, along the diagonals and along zig-zag lines of the lattice, while the destructive interference reduces the density elsewhere. This behavior is transmitted to the VH BICs, and hence to the surviving density profile after a long evolution time, as is apparent in Fig. 4. These local- 

V. VAN HOVE BICS AS LOCALIZED SUBRADIANT STATES

Several authors have considered the superradiant transition in open systems in the language of non-Hermitian Hamiltonians like Eq. (3), see e.g. Refs. [13,14]. As the loss rate $\gamma$ is increased, the nature of the system eigenstates evolves as follows. For small $\gamma$, the eigenstates of $\hat{H}_{\text{open}}$ are well described by the eigenstates of $\hat{H}$ acquiring some width depending on the amplitude of their wave function at the lossy sites. On the other hand, for strong coupling, the eigenstates of $\Gamma$ become good eigen- 

VI. CONCLUSIONS

We have established a very general mechanism sup- 

FIG. 4. Examples of VH lattice scars. The intensity of red color is proportional to the probability density at each lattice site (circles) after a long time evolution of a Gaussian wavepacket, subject to localized losses at the sites marked by blue diamonds. (a) $19 \times 19$ square triangular lattice with losses in the 17 bottom-left sites. (b) $19 \times 19$ Sinai triangular lattice with losses in 4 sites in the upper right corner. The dimensions of the VHD for each closed system are (a) $N_{\text{VH}} = 18$ and (b) 5; only one BIC remains in each system after coupling to the environment. 

porting the existence of bound states in the continuum (BICs) in finite lattices based on van Hove degeneracies, which does not require a distinct symmetry[15,16] or flat band[18,20]. At the energy where the density of states diverges due to a van Hove singularity, there may be a large number of degenerate states depending on the bound- 

aries of the finite lattice. In that case, if the system is coupled to the environment through a finite number of sites, a part of this degenerate subspace generally remains uncoupled from the environment, becoming a set of BICs or localized subradiant states. These VH BICs are spatially localized along specific direction of the lattice, resembling lattice scars[13] and compact localized states found in flat band[18,20]. They do not decay and do not contribute to transport. As such, they could be useful for storing or transmitting information without distor- 

Due to the peculiar spatial structure of VH BICs, they could also be harnessed to engineer exotic models relying on a highly-anisotropic coupling between emitters on a photo- 

On the other hand, states in the VH degenerate space that do couple to the environment are, for weak coupling, spatially-localized high-$Q$ resonances that can find applications in slow light and electromagnetically induced transparency (EIT)[17,18], frequency conversion[19], refractive index sensing (e.g., for biosensing applications[20,21], among others[22,23]). For large coupling, these states exhaust all the losses in the system. Because of this, they can be regarded as superradiant states, while the rest of the spectrum, having negligible widths, describes subra- 

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