Van Hove Singularities and Excited-State Quantum Phase Transitions in Graphene-like Microwave Billiards

Michal Macek$^{1,a)}$ and Barbara Dietz$^2$

$^1$The Czech Academy of Sciences, Institute of Scientific Instruments, Brno, Czech Republic.
$^2$School of Physical Science and Technology, and Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou 730000, China

$^a)$Corresponding author: michal.macek@isibrno.cz

Abstract. We discuss solutions of an algebraic model of the hexagonal lattice vibrations, which point out interesting localization properties of the eigenstates at van Hove singularities (vHs), whose energies correspond to Excited-State Quantum Phase Transitions (ESQPT). We show that these states form stripes oriented parallel to the zig-zag direction of the lattice, similar to the well-known edge states found at the Dirac point, however the vHs-stripes appear in the bulk. We interpret the states as lines of cell-tilting vibrations, and inspect their stability in the large lattice-size limit. The model can be experimentally realized by superconducting 2D microwave resonators containing triangular lattices of metallic cylinders, which simulate finite-sized graphene flakes. Thus we can assume that the effects discussed here could be experimentally observed.

INTRODUCTION: Excited state quantum phase transitions (ESQPTs) [1, 2] are a recent generalization of the quantum phase transitions (QPTs) [3] and correspond to non-analytic behavior in excited spectra of low-dimensional systems. ESQPTs are currently studied in diverse systems including atomic nuclei, molecules, coupled atom-field quantum optics systems, driven quantum oscillators, and also two dimensional lattices, with seminal inputs in most of these fields by Franco Iachello. The interest in ESQPTs stems on one hand from the marked structural changes occurring in the individual systems, on the other hand from possible profound general implications for non-equilibrium thermodynamics, quantum information processing, and transport (for a review see [4]). A general classification of the ESQPTs is based on the dimensionality (number of degrees of freedom) of the system and the types of stationary points of the underlying semi-classical energy manifold, see Refs. [7, 8]. Relation to stationary points may apparently lead to interesting localization effects at the ESQPT energies [9, 10, 14]. In this contribution, we concentrate on the localization of eigenstates in two dimensional lattices, motivated by a recent experimental identification of ESQPTs in artificial graphene simulated by microwave photonic crystals [5]. The experiments performed in Darmstadt [11] used microwave resonators with a set of cylinders in a triangular arrangement, representing nodes of the EM field, see Fig. 1 (a). The ESQPTs were observed in the density of states (DoS) at the energies of van Hove singularities (vHs) in one-phonon bands of the hexagonal lattice. Here, we present numerical solutions of an algebraic model of the system [6]. Complementing Ref. [14], which showed that eigenstates at the ESQPT/vHs energy localize into peculiar stripes oriented parallel to the zig-zag direction of the lattice, we interpret these states structurally as linear sequences of cell-tilting vibrations. Further, we inspect their stability in the large lattice-size limit.

MODEL: We consider the “hopping” limit of the algebraic Hamiltonian introduced by Franco Iachello [6]

$$H = e \sum_{i=1}^{n} b_i^\dagger b_i - \lambda^{(I)} \sum_{(i,j)} (b_i^\dagger b_j + b_j^\dagger b_i) - \lambda^{(II)} \sum_{(i,j)} (b_i^\dagger b_j + b_j^\dagger b_i) + ... \tag{1}$$

where the hopping (Majorana) operator on the hexagonal lattice is expanded into the nearest neighbors (interaction strength coefficient $\lambda^{(I)}$), the next-to-nearest neighbors (coefficient $\lambda^{(II)}$, etc...), terms. The coefficients $\lambda^{(I)}, \lambda^{(II)}, ...$ are symmetry adapted to reflect the hexagonal unit cell.

For an infinite size hexagonal lattice, the energy dispersion relation (EDR) can be written as [6]

$$E(k_x, k_y) = \pm \lambda^{(I)} \sqrt{3 + u(k_x, k_y)} - \lambda^{(II)} u(k_x, k_y)$$
Localization of wave functions:

Selected eigenstates of the hexagonal lattice with NN-hopping interactions ($\lambda$) and the most localized eigenstates at $D_z$ and both $\nu_H$ (at each $\nu_H$ equals half the number of zig-zag rows in the lattice. The eigenstates at both $\nu_H$s have nodal lines parallel to the armchair direction and the number of striped states observed which differs from the edge states along the zig-zag edge, which are of topological origin and relate to the second-neighbor interaction $\lambda'' \neq 0$. The coeﬃcients $\alpha_i$ are not constant throughout the lattice, cf. [14]. Fig. 2(a) shows the evolution of the local-basis participation ratio $P_{\text{loc}}^{\nu_H} = \sum_i 1/|\alpha_i^{(\nu_H)}|^4$ for the ground state (g.s.) and the most localized eigenstates at $D_z$ and both $\nu_H$s ($\nu_H+$ and $\nu_H-$), as a function of $\lambda''/\lambda'$ for a hexagonal lattice with $m \times (2m + 5)$ sites, where $m = 20$. The coefficients $\lambda'$ and $\lambda''$ are affected by noise $\delta \lambda_i^{(\nu_H)}$ uni-
FIGURE 2. Evolution of the local-basis participation ratio $\text{PR}_{\text{loc}}^\nu \equiv \sum_i 1/|\alpha_i^\nu|_4$ for the ground state (g.s.) and the states at the Dirac zero (Dz) and both vHss (vHs$, vHs$+) as a function of the relative strength $\lambda_{II}/\lambda_I$ of first and second-neighbor interaction (panel a) and the size of the lattice with $m \times (2m + 5)$ sites (panel b). The coefficients are affected by noise uniformly distributed in respective intervals $|\delta \lambda_i/\lambda_i| \leq 10^{-3}$ in both panels.

formly distributed in respective intervals $|\delta \lambda_i^{II}/\lambda_i^{II}| \leq 10^{-3}$. The participation ratio $\text{PR}_{\text{loc}}^\nu$ counts, roughly speaking, the sites where $|\alpha_i^\nu| > 0$, thus the lower the $\text{PR}_{\text{loc}}$, the more localized the $\nu$-th eigenstate. We see that at $\lambda_{II}/\lambda_I \approx 0$, the $\text{PR}_{\text{loc}}$-values for both the vHs states are roughly $2 \times$ larger than for the Dirac-point state, while being about $10 \times$ lower than for the ground state. This is consistent with spatial distributions shown in Fig. 1(d-f). As $\lambda_{II}/\lambda_I$ increases, both vHs states gradually delocalize up to $\lambda_{II}/\lambda_I \approx 0.06$, while the edge states at Dz remain essentially unaffected.

Dependencies of $\text{PR}_{\text{loc}}$ on the lattice size $m \times (2m + 5)$ shown in Fig. 2 (b) prove that eigenstates at both vHs and Dz are localized on linear portions of the lattice as $\text{PR}_{\text{loc}}^\nu \propto m^1$, in sharp contrast with the g.s. spread over the whole lattice expressed by the quadratic scaling $\text{PR}_{\text{loc}}^\text{g.s.} \propto m^2$. Thus we have shown that the localization of the eigenstates of the hexagonal lattice into striped states can be robust and we suggest that such effects could be experimentally observed in an apparatus similar as in the detection of the edge states [11].

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