Robust conductance zeros in graphene quantum dots and other bipartite systems

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Within the Landauer transport formalism we demonstrate that conductance zeros are possible in bipartite systems at half-filling when leads are contacted to different sublattice sites. In particular, we investigate the application of this theory to graphene quantum dots with leads in the armchair configuration. The obtained conductance cancellation is robust in the presence of any single-site impurity.

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I. INTRODUCTION

The cancellation of the electronic conductance on account of destructive quantum interference (DQI), independent of the coupling strength to the leads, is a quantum mechanical effect without correspondence in classical circuits. Finding systems where such property occurs is of both fundamental and practical interest, as in designing of on/off switches, for example. The existence of the DQI phenomena has been investigated previously in various quantum dots or molecular systems [1–9]. More recently, this topic received renewed attention in connection with the transmission phase lapse of π at the conductance zeros between the resonances of a quantum dot, arguably one of the longest standing puzzles in mesoscopic physics, whose elucidation spanned 30 years [10,11].

In this paper we demonstrate the presence of a robust zero transmission in graphene quantum dots (QD) at half-filling (i.e., *zero* Fermi energy), starting from an analysis of quantum transport in bipartite lattices. Such systems, known to provide an appropriate description for graphene, are composed of two sublattices A and B with hopping only between A and B sites and no hopping in the same sublattice (see Fig. 1). In the Landauer formalism, where the conductance between two points $\mathbf{G}_{ij}$ is proportional to the transmittance $\mathbf{T}_{ij}$, it was previously found that zeros are obtained in graphene QDs when both leads are connected to the same sublattice, $\mathbf{T}_{AA}$ or $\mathbf{T}_{BB}$ [12,13]. Moreover, it was shown that this type of zeros occurs with a π phase lapse of the transmission amplitude, a property characteristic to Fano zeros. Here we focus on the origin of the transmission zeros and their characteristic properties in a setup that involves DQI when the transport leads are connected to both sublattices, $\mathbf{T}_{AB}$.

To this end we first prove the conductance cancellations in a *multiterminal* bipartite conductor whose transport leads are contacted to A points. In some specific circumstances, $\mathbf{T}_{AA} = 0$ between *any* pair of A leads, a result that is left invariant by the presence of a perturbation at *any* A sites. Later, this property is used as a building block in constructing new connected systems, also bipartite, in which the existence of $\mathbf{T}_{AB}$ zeros is studied. Our theory is then applied to a graphene quantum dot at half-filling, when the two leads are connected to armchair edges. The robustness of such conductance zeros is studied in the presence of lattice defects.

II. THE LANDAUER FORMALISM

The general Hamiltonian of a bipartite lattice considers all the hopping terms between sublattice A and B points,

$$H = \sum_{i_A, j_B} t_{i_A, j_B} |i_A\rangle\langle j_B| \,, \tag{1}$$

as shown in Figs. 1 and 2.

This is a known appropriate representation of nanosized graphene sheets (also called graphene quantum dots) [12,14], artificial molecules composed of connected quantum dots [15–17], or alternant chemical molecules described by the Hückel Hamiltonian [1,18,19].

In the following considerations we are interested in the general multiterminal case of a QD connected to a number of N_l one-channel transport leads, indexed by α or $\beta = 1, \ldots, N_l$. The leads are described by a one-dimensional tight-binding or discrete chain Hamiltonian [19–21] and the contact points between them, and the QD are individual sites denoted by i_α and i_β.

Within the Landauer formalism, the transmission amplitude between leads α and $\bar{\alpha}$ at energy E [20,22],

$$\mathbf{t}_{\alpha,\bar{\alpha}}(E) = -\delta_{\alpha,\bar{\alpha}} + 2i\frac{\tau_\alpha \tau_{\bar{\alpha}}}{\tau_l} \sin k \, G^{\text{eff}}_{i_\alpha, i_{\bar{\alpha}}}(E), \tag{2}$$

determines the conductance between the same leads,

$$\mathbf{G}_{\alpha,\bar{\alpha}}(E) = \frac{e^2}{h}\mathbf{T}_{\alpha,\bar{\alpha}}(E) = \frac{e^2}{h}|\mathbf{t}_{\alpha,\bar{\alpha}}(E)|^2, \tag{3}$$

with $\mathbf{T}_{\alpha,\bar{\alpha}}$ the transmittance. The argument of the transmission amplitude is denoted by $\arg t(E) = \phi(E)$. Note that in Eq. (2) the effective Green's function,

$$G^{\text{eff}}(E) = \frac{1}{E - H^{\text{eff}}} \,, \tag{4}$$

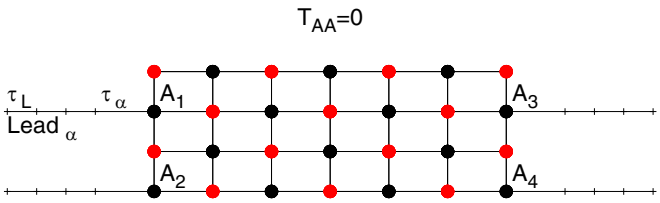

FIG. 1. A zero-transport bipartite conductor with all terminals connected at A sites. The system exhibits zero transmission at $E = 0$: $\mathbf{t}_{\alpha,\bar{\alpha}}(0) = 0$ for any pair of leads $\alpha \neq \bar{\alpha}$. This is realized when the bipartite Hamiltonian is nonsingular such that it has no zero-energy eigenstate. The $\mathbf{T}_{AA}$ zeros are invariant under any A-site perturbation, but they can be modified by B-site impurities, as discussed in the text.

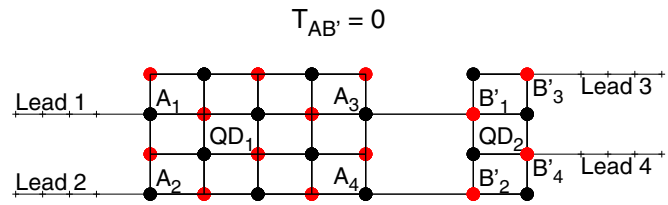

FIG. 2. A quantum conductor with $\mathbf{T}_{AB}$ zeros: $\mathbf{T}_{13}$, $\mathbf{T}_{14}$, $\mathbf{T}_{23}$, and $\mathbf{T}_{24}$. The system is composed from two serially connected quantum dots, QD_1 and QD_2, each of them having zero conductances between any pair of leads, as explained in Fig. 1. The $\mathbf{T}_{AB}$ zero is invariant under any perturbation applied to A or B' sites. Particularly, it can be modified by a selected pair of B and A' site perturbations.

depends on the energy $E = 2\tau_l \cos k$, with k the wave number. τ_l is the lead hopping energy and τ_α the constriction parameter or the hopping energy between QD and lead α. For simplicity, we assume throughout the paper that $\tau_\alpha = \tau_{\bar{\alpha}} = \tau_c$.

The effective Hamiltonian that determines Eq. (4) incorporates, in addition to the bipartite Hamiltonian, Eq. (1), the potential at the contacts V such that $H^{\text{eff}} = H + V$, where

$$V = \frac{\tau_\alpha^2}{\tau_l} e^{-ik} \sum_{\alpha=1}^{N_l} |i_\alpha\rangle\langle i_\alpha| \, . \tag{5}$$

Although the effective Hamiltonian is non-Hermitian, since V is complex, it has proven to be a useful tool in describing the transport properties of open mesoscopic systems [23,24].

III. THE $\mathbf{T}_{AA}$ ZEROS

We apply the formalism described above to the case of a multilead quantum conductor, as depicted in Fig. 1. All the external leads are connected to the same sublattice of the bipartite system, A. External perturbations may be present at A sites, $\epsilon_i \neq 0$ with $i \in A$.

In this case, we show that the transmission amplitude $\mathbf{t}_{\alpha,\bar{\alpha}}$ with $\alpha \neq \bar{\alpha}$ satisfies

$$\mathbf{t}_{\alpha,\bar{\alpha}}(0) = 0 \text{ with } i_\alpha, i_{\bar{\alpha}} \in A, \tag{6}$$

regardless of how many other leads are connected to the same sublattice points A. This result is derived by using the Dyson expansion for the effective Green's function $G^{\text{eff}}(E)$ in Eq. (4). For the matrix blocks that contain matrix elements between A sites, $G^{\text{eff}}_{AA}(E)$ and $G_{AA}(E)$, we write

$$G^{\text{eff}}_{AA}(E) = G_{AA}(E) + G_{AA}(E) V_A G^{\text{eff}}_{AA}(E), \tag{7}$$

where the potential matrix V_A contains only the A-site terms from Eq. (5) and the A-site impurities, as we have considered. We note that on account of the chiral symmetry of the Hamiltonian, the matrix elements of the *bare* Green's function $G(E) = 1/(E - H)$ between points of the same sublattice at *zero* energy cancel, as previously discussed in Refs. [13,16,25]. Therefore,

$$G_{i,i'}(0) = 0 \text{ for } i, i' \in A \text{ or } i, i' \in B \, . \tag{8}$$

With $G_{AA}(0) = 0$ in Eq. (7) and from Eq. (2) one obtains the cancellation from Eq. (6).

We note that the validity of this result is conditioned by the absence of the eigenvalue $E = 0$ from the bipartite lattice spectrum [1,13], which assures that the perfect conductance cancellation at $E = 0$ occurs *between* resonances. Such a "perfect" *zero* is independent of the coupling strength with the leads, since it is decided by the zeros of the *bare* Green's function. In this respect it is different from the usual low conductance between resonances, which is never a perfect *zero* and is, in general, coupling dependent.

The invariance of $\mathbf{T}_{AA}$ zeros in Fig. 1 to any A-site perturbations underlies the destructive interference in the "off" states for naphthalene or perylene when the contact points of Büttiker probes and source and drain electrodes belong to the same sublattice [19]. In general, the invariance of the $\mathbf{T}_{AA}$ zeros is removed only by at least one B-site perturbation. The multiterminal conductor with $\mathbf{T}_{AA} = 0$ in Fig. 1 can be used to explain the occurrence of conductance zeros in bigger systems that incorporate it as a building block, as shown in the next section.

IV. THE $\mathbf{T}_{AB}$ ZEROS

To prove the existence of the transmission zeros that appear when the leads are connected to different sublattices, one at an A site and the other at a B site, we consider a quantum conductor composed of a sequence of two serially connected quantum dots QD_1 and QD_2, described in Fig. 2. Each quantum dot is a bipartite lattice, described by Hamiltonians $H_1(A, B)$ and $H_2(A', B')$, respectively, with no zero-energy eigenvalue and with all leads connected to the same sublattice points as in Fig. 1. The coupling potential between the two dots is realized only between A points of the first dot with B' points of the second, as depicted Fig. 2, leading to an additional interaction term of the form $V_{12}(A, B') = |A_3\rangle\langle B'_1| + |A_4\rangle\langle B'_2| + \text{H.c.}$

The resulting Hamiltonian of the composed system $H_1 + H_2 + V_{12}$ is bipartite too, with $A + A'$ and $B + B'$ designating the two sublattices.

In the composed bipartite system the tunneling amplitude is zero between points in the A and B' sublattices,

$$\mathbf{t}_{\alpha,\beta}(0) = 0 \text{ with } i_\alpha \in A \text{ and } i_\beta \in B'. \tag{9}$$

This is the main result of this section and will be proven below.

The effective Hamiltonian H^{eff} that determines the transmission amplitude in the composed system, in agreement with Eq. (5), is written as

$$H^{\text{eff}} = H_1(A, B) + H_2(A', B') + V_{12}(A, B') + V_1(A) + V_2(B'), \tag{10}$$

where H_1, H_2 describe the two independent QDs, while V_{12} describes the coupling between them. $V_1(A)$ and $V_2(B')$ are the non-Hermitian terms from (5) associated with the coupling to the leads.

The matrix elements $G^{\rm eff}_{i_\alpha,i_\beta}(0)$ of $G^{\rm eff}_{AB'}(E)$ for two lattice points $i_\alpha \in A$ and $i_\beta \in B'$ are calculated from the Dyson equation written for the total interaction potential in Eq. (10),

$$G^{\rm eff}(E) = G(E) + G(E)[V_{12}(A,B') + V_1(A) + V_2(B')]G^{\rm eff}(E)\,. \tag{11}$$

Since the initial system H in (10) is decoupled, its Green's function matrices $G_{AB'}$ and $G_{AA'}$ are equal to zero in the expansion of the Dyson equation, leading to

$$G^{\rm eff}_{AB'}(E) = G_{AA}V^1_{AA}G^{\rm eff}_{AB'} + G_{AA}V^{12}_{AB'}G^{\rm eff}_{B'B'}. \tag{12}$$

V^1_{AA} and $V^{12}_{AB'}$ are the matrices of the operators $V_1(A)$ and $V_{12}(A,B')$ in (10). Since QD_1 as a bipartite system does not have an $E=0$ eigenstate and $G_{AA}(0)=0$ in Eq. (8), $G^{\rm eff}_{AB'}(0)=0$. Then, with input from (2) the cancellation (9) follows.

A slightly less general result is obtained by considering a single incoming and a single outgoing lead. One lead is on an A-site coupling to the point i_α, and the other lead is at a B'-site coupling to the point $i_\beta \in B'$. For this two-terminal conductor one can prove that the transmission zero $\mathbf{t}_{\alpha,\beta}(0)$ has no π phase lapse. In the formula (12) of $G^{\rm eff}_{AB'}(E)$ we introduce the Dyson expansion for $G^{\rm eff}_{B'B'}(E)$ and retain only the lowest order term in the limit of $E \to 0_\pm$ when the bare functions $G_{AA} \to 0$ and $G_{B'B'} \to 0$. We then obtain

$$G^{\rm eff}_{AB'}(0_\pm) \simeq G_{AA}(0_\pm)V^{12}_{AB'}G_{B'B'}(0_\pm). \tag{13}$$

The transmission $\mathbf{t}_{\alpha,\beta}(0_\pm)$ in Eq. (2) becomes a summation of products $G_{i_A,j_A}G_{i_{B'},j_{B'}}$ with $i_A,\ j_A \in A$ and $i_{B'},\ j_{B'} \in B'$. Since every product term G_{i_A,j_A} or $G_{i_{B'},j_{B'}}$ describes a π phase lapse process [13], an overall 2π phase is obtained and consequently, no observable phase variation occurs. From these considerations one obtains

$$\Delta \arg \mathbf{t}_{\alpha\beta}(0) = 0. \tag{14}$$

The stability of the $\mathbf{T}_{AB}$ zero obtained in (9) is now investigated in the presence of a disorder potential represented by impurity energies located at various sites of the lattice. The effective total Hamiltonian becomes

$$H'^{\rm eff} = H^{\rm eff} + \sum_i \epsilon_i |i\rangle\langle i|\,. \tag{15}$$

From the Dyson expansion for $G'^{\rm eff}_{AB'}$, straightforward calculations lead to

$$G'^{\rm eff}_{AB'}(0) = G^{\rm eff}_{AB}(0)\epsilon_B G'^{\rm eff}_{BA'}(0)\epsilon_{A'}G^{\rm eff}_{A'B'}(0)\,, \tag{16}$$

where ϵ_B and $\epsilon_{A'}$ are the matrices of B and A' located impurities. Equation (2) generates the lowest order terms of the tunneling amplitude between contact points $i_\alpha = A_1, A_2$ and $i_\beta = B'_3, B'_4$,

$$\mathbf{t}_{\alpha,\beta}(0) = \epsilon_B C_{BA'}\epsilon_{A'} + \mathcal{O}(\epsilon^3). \tag{17}$$

$C_{BA'}$ is a matrix containing Green's function products derived by the perturbative method. For instance, for the output lead connected at $i_\alpha = A_1$ and the input one with $i_\beta = B'_3$ it is written $C_{BA'} = G_{A_1B}G_{BA}V^{12}_{AB'}G_{B'A'}G_{A'B'_3}$, with all Green functions at $E=0$ calculated for H_1+H_2 from Eq. (10).

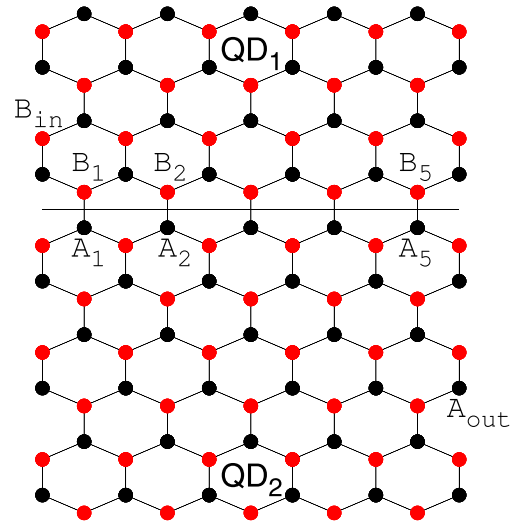

FIG. 3. Zero transmission in graphene: $\mathbf{t}_{A_{\rm out},B_{\rm in}}(0)=0$ for all $B_{\rm in} \in QD_1$ and $A_{\rm out} \in QD_2$ for any constriction τ_c.

This result shows a significant difference between the $\mathbf{T}_{AB}$ and $\mathbf{T}_{AA}$ zeros. The cancellation $\mathbf{T}_{AB'}=0$ in Fig. 2 is invariant in the presence of any single-site impurity and could be modified only by at least a selected pair of A', B located impurities. In contrast, the existence of a same sublattice zero, $\mathbf{T}_{AA}=0$ in Fig. 1, is invariant in the presence of any A-site-located impurities but can be modified by one B-located impurity.

To predict the general features of the DQI processes we consider here only noninteracting electron systems [1,6,22]. As discussed in other works, the presence of interaction terms (onsite or long range) may lead to energy shifts, small decreases, or splitting of the DQI dips [6,26–28]. One can therefore expect that the obtained DQI processes remain robust even in the presence of interaction, as long as the adiabatic turning on of the interaction terms does not induce new energy levels (or a density peak) between adjacent QI resonance energies. This is discussed on the basis of the Friedel sum rule in Ref. [29]. Moreover, the electron-hole symmetry (specific to bipartite lattices) survives interaction models such as Hubbard or extended Hubbard (the PPP model [30,31]). Remarkably, electron-hole symmetry was also proven experimentally in a carbon nanotube [32].

V. THE ARMCHAIR ZEROS IN GRAPHENE

In this section we study the existence of the $\mathbf{T}_{AB}$ zeros for a two-terminal graphene QD at $E=0$. In Fig. 3 the graphene sheet has the incoming lead connected at the site $i_1 = B_{\rm in}$, which belongs to the B sublattice on the left armchair boundary while the contact point of the outgoing lead $i_2 = A_{\rm out}$ belongs to the A sublattice on the right armchair boundary. In order to apply the above-discussed formalism, the graphene is formally separated into two smaller dots QD_1 and QD_2 that are serially connected through N_{zz} lines B_1A_1,..., B_5A_5 that play the role of connection leads between them. Each

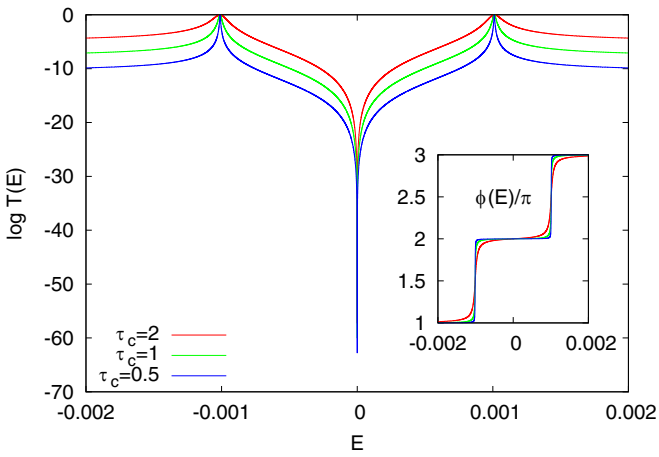

FIG. 4. Zero transmission and no phase lapse in a graphene quantum dot at $E = 0$. $\mathbf{T}(0)$=0 for any τ_c is proven in the text. The lattice picture and the contact points are in Fig. 3. $\tau_l = 2$. The lead-dot constriction parameters τ_c are written on the figure. E, τ_l, and τ_c are in units of t. In the inset the transmission phase is in π units.

smaller dot behaves like a zero-conductance device described in Fig. 1. QD_1 has leads connected to the B sublattice and QD_2 to the A sublattice. Both of them have no zero-energy eigenstate [33]. In this instance, Eq. (9) applies and the conductance cancels at $E = 0$.

From Ref. [33] the rectangular graphene lattice has pairs of zigzag edge states Ψ_{zz+} and Ψ_{zz-} with the wave numbers $\xi_j = \pi j/(N_{zz} + 1)$ and δ_j that satisfy the characteristic equation

$$\sinh \delta_j N_{ac} = 2 \cos(\xi_j/2) \sinh \delta_j (N_{ac} + 1/2). \tag{18}$$

N_{zz} counts the zigzag points, and N_{ac} is the number of hexagonal cells in the armchair direction. The two zigzag state energies are

$$E_{zz\pm} = \pm \frac{\sinh(\delta_j/2)}{\sinh \delta_j (N_{ac} + 1/2)}. \tag{19}$$

For graphene in Fig. 3 we have $N_{zz} = 5$ and $N_{ac} = 5$. From Eq. (18) we obtain only one pair of zigzag edge states having wave numbers $\xi_5 = 5\pi/6$ and $\delta_5 = 1.317$. Their zigzag energies calculated with Eq. (19) are $E_{zz\pm} = \pm 0.001t$. t is the nearest-neighbor hopping, equal to 2.7 eV for nanographene [28].

In Fig. 4 we show numerical results of transmittance $\mathbf{T}(E)$ and the transmission phase $\phi(E)$ when two transport leads are contacted to points A_{out} and B_{in}, as explained in Fig. 3.

The maxima with $\mathbf{T}(E) = 1$ for tunneling energies is obtained at the two resonance energies equal to the zigzag eigenstates calculated above, $E \simeq E_{zz+}$ and $E \simeq E_{zz-}$. Between the two resonances the system shows a zero transmittance at $E = 0$ with no phase lapse of the transmission phase between them. At resonances the phase $\phi(E)$ increases with π as expected.

The $\mathbf{T}_{AB}$ zeros have an increased robustness. Two different impurities, such as ϵ_B located in QD_1 and ϵ_A located in QD_2, do not modify the $\mathbf{T}_{AB}(0) = 0$ of Fig. 3. In order to lift the conductance zero, one needs at least one ϵ_A impurity in QD_1 and one ϵ_B impurity in QD_2. This results from Eq. (17) and can be applied to design an AND logical gate by using the graphene QD. In this case the two control parameters ϵ_A and ϵ_B can be simulated by external perturbations applied on the two selected sites as in the case of Büttiker probes [19].

Furthermore, the transmission cancellation proven in this paper explains the DQI in molecular systems that contain a series of subsystems. If, for instance, the building block is a metabenzene, we can obtain the zero conductance in biphenyl [7], and if we use a T shape as a building block, we obtain the 2–3 hard zero in butadiene [34]. One can also start with a multiterminal lattice as pictured in Fig. 1. As an example, a three-terminal naphthalene, with all $\mathbf{T}_{AA} = 0$, determines the DQI in perylene-type lattices obtained in Refs. [35] and [36]. Finally, we note that the second dot in Fig. 2 can be chosen arbitrarily, allowing for the prediction of DQIs in more complex systems.

VI. CONCLUSIONS

This paper discusses a particular transmission cancellation property characteristic to bipartite lattices and molecules that is potentially useful to nanoelectronics. We demonstrate the existence of *zero* transmission at half-filling in bipartite systems, such as graphene quantum dots, when the two transport leads are contacted to certain sites from the A and B different sublattices. This *perfect* transmission cancellation, independent of the coupling strength to the leads, is different from the usual low conductance between resonances, and the property can be used for on/off nanoswitches or logical gates. The algorithm described in this paper is appropriate for bipartite systems that can be separated in two subsystems, each of them bipartite and lacking midspectrum (zero) energy. Then if the two leads are connected to any A site of the first subsystem and, respectively, to any B site of the second subsystem, the transmission exhibits a cancellation.

A high robustness is proven for the $\mathbf{T}_{AB}$ conductance zeros which survive to any single-site perturbation, and at least two impurities (located in different sublattices) are necessary to remove them. This is unlike the $\mathbf{T}_{AA}$ zeros, which are invariant to any A-site perturbations and can be lifted by a single B-site impurity. In addition to the conductance cancellation, no π lapse of the transmission phase occurs if the leads are connected to different sublattices, contrary to the case when the leads are connected to the same sublattice.

Our results can be used to predict the existence of DQIs and to understand their robustness in various physical systems—such as finite tight-binding lattices or molecules—that are composed from various building blocks with certain bipartite characteristics.

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