Electron-phonon interaction on bundled structures: Static and transport properties

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We study the small-polaron problem of a single electron interacting with the lattice for the Holstein model in the adiabatic limit on a comb lattice, when the electron-phonon interaction acts only on the base sites. The ground state properties can be easily deduced from the ones of a linear chain with an appropriate rescaling of the coupling constant. On the other hand, the dynamical properties, that involve the complete spectrum of the system, present an "exotic" behavior. In the weak coupling limit the Drude weight (zero-frequency conductivity) is enhanced with respect to its free-case value, contrary to the linear chain case, where for every finite value one has a suppression of the Drude peak. More interestingly, the loss of coherent electron motion and the polaronic localization of the carrier occurs for different coupling values. Thus for intermediate coupling, a different phase appears with large kinetic energy and no coherent motion.

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I. INTRODUCTION

In the past years, a general interest has been growing around the study of physical properties of inhomogeneous discrete structures. The general purpose is to characterize the behavior of systems like amorphous solids, glasses, polymers and biological systems in general, where one can expect the specific geometry to dramatically influence physical properties, ranging from transport and diffusive properties, to the thermal or electrical ones. A very general and powerful formalism has been developed, the so-called random walk problem, where the structure is explored by a classical walker, that randomly jumps to an arbitrary nearest-neighbor site at every time step. This approach can be thought as the discrete version of the classical Boltzmann equation, and the asymptotic behavior of the average distance of the walker from the starting site gives the diffusion law for the considered structure. On translationally invariant graphs, the diffusion law predicts that this distance scales with the time step with a power law depending on the Euclidean dimension of the lattice. On more general graphs, the diffusion law is governed by a new parameter characterizing the structure, generally known as spectral dimension,¹⁻³ that can be different from the Euclidean dimension in which the graph is eventually embedded, giving rise to the so-called anomalous diffusion.⁴⁻⁶ One of the main difficulties of this approach is that the explicit calculation of this important parameter may not be trivial for general structures.

Nevertheless, there exists a wide class of graphs, called bundled structures, where explicit calculations can be performed. The random walk and the oscillation problems have already been studied on these structures,^{6,7} and an anomalous diffusion law for a classical walker moving along the base has been discovered. Furthermore, the nearest-neighbor tight binding model has been explicitly solved for electrons moving on these graphs, by means of an exact resummation of the perturbative expansion in the hopping parameter.⁸ This perturbative approach becomes very complicated, and in a last instance useless, when the electrons experience any kind of interaction, both between them, and with external fields, like, e.g, phonons. This work is devoted to the first extension to the interacting case of the problem of electrons moving on bundled structures. We restrict ourselves to the case of a single electron which interacts with local oscillators only on the base sites of a comb lattice. This is a first step towards the detection of some quantum counterpart of the anomalous diffusion laws.

The subject of electron-phonon (e-ph) interaction on unconventional structures has been already addressed mainly within the framework of the Su-Schrieffer-Heeger⁹ model, originally introduced to describe the properties of poliacetylene chains.¹⁰ We will attack the problem of *e*-ph interaction on unconventional structures from another point of view. Rather than a realistic description of actual compounds, we aim to provide a general picture of the mutual effect of e-ph coupling and geometric complexity. We will therefore focus on the Holstein model,¹¹ which despite its simplicity, is expected to capture all the main physical properties of more general interactions. In Sec. II we sketch the basic formalism for bundled structures, and show how the problem can be mapped onto a base-only one. In Sec. III the small-polaron problem on the comb lattice is discussed, with particular emphasis on the dynamical properties. Section IV is devoted to conclusions and future perspectives.

II. GENERAL FORMALISM

A bundled structure can be built joining each point of a base graph \mathcal{B} with a copy of a fibre graph \mathcal{F} in such a way that there is only one common site between \mathcal{B} and \mathcal{F} . As previously explained, we shall limit our study to the simplified case in which the particles experience interaction only on the base sites. Within this hypothesis, the generic Hamiltonian for a single electron on a bundled structure assumes a block form:

$$\begin{pmatrix} H_B & H_{BF} \\ H_{FB} & H_F \end{pmatrix}.$$
 (1)

 H_B and H_F act on the base and the fibers sites, respectively, while $H_{BF} = H_{FB}^T$ are rectangular matrices containing the hopping terms joining the fibers to the base. Consequently, a generic state can be written as

$$|\phi\rangle = \begin{pmatrix} |\psi\rangle\\|\eta\rangle \end{pmatrix},\tag{2}$$

with $|\psi\rangle$ belonging to the base and $|\eta\rangle$ to the fibers. Since this separation of degrees of freedom is completely formal, we must ensure that it does not introduce unphysical states in the Hilbert space. So we impose a normalization constraint: $\langle \psi | \psi \rangle + \langle \eta | \eta \rangle = \langle \phi | \phi \rangle = 1$. Let us write the eigenvalues equation for this structure:

$$H_{B}|\psi_{\epsilon}\rangle + H_{BF}|\eta_{\epsilon}\rangle = \epsilon|\psi_{\epsilon}\rangle,$$

$$H_{F}|\eta_{\epsilon}\rangle + H_{FB}|\psi_{\epsilon}\rangle = \epsilon|\psi_{\epsilon}\rangle.$$
 (3)

Because H_F does not contain any interaction term, one can get rid of $|\eta_{\epsilon}\rangle$ from Eq. (3), reducing to a "base-only" problem:

$$(\boldsymbol{\epsilon} - \boldsymbol{H}_{B} - \boldsymbol{H}_{BF}(\boldsymbol{\epsilon} - \boldsymbol{H}_{F})^{-1}\boldsymbol{H}_{FB})|\psi_{\boldsymbol{\epsilon}}\rangle = 0,$$

$$\langle\psi_{\boldsymbol{\epsilon}}|[1 - \boldsymbol{H}_{BF}(\boldsymbol{\epsilon} - \boldsymbol{H}_{F})^{-2}\boldsymbol{H}_{FB}]|\psi_{\boldsymbol{\epsilon}}\rangle = 1.$$
(4)

Explicitly using the simple form of the rectangular matrix H_{BF} (reflecting the peculiar geometry of the bundled structure), it can be shown that the composite operators in Eq. (4) have only diagonal terms simply expressed in term of the fiber-only Green's functions:

$$[H_{BF}(\boldsymbol{\epsilon}-H_F)^{-1}H_{FB}]_{ij} = \delta_{ij}n_f t^2 F_{00}(\boldsymbol{\epsilon}), \qquad (5)$$

$$[H_{BF}(\epsilon - H_F)^{-2}H_{FB}]_{ij} = \delta_{ij}n_f t^2 \sum_m F_{0m}(\epsilon)F_{m0}(\epsilon).$$
(6)

Here n_f is the number of independent fibers joined to a single site of the base; *t* is the hopping constant relative to the link joining the fiber and the base; $F_{lm}(\epsilon) = [\epsilon - H_F]_{lm}^{-1}$ is the fiber Green's function, and *i*=0 indicates the first site of the fiber when coming from the base. So we have reduced ourselves to an effective problem for the only base sites:

$$\left(\boldsymbol{\epsilon} - \boldsymbol{H}_B - \boldsymbol{n}_f t^2 \boldsymbol{F}_{00}(\boldsymbol{\epsilon})\right) |\psi_{\boldsymbol{\epsilon}}\rangle = 0, \tag{7}$$

$$\langle \psi_{\epsilon} | \psi_{\epsilon} \rangle = \frac{1}{1 + n_f t^2 \sum_{m} F_{0m}(\epsilon) F_{m0}(\epsilon)} \equiv n(\epsilon).$$
(8)

We can rewrite Eq. (7) as

$$(f(\epsilon) - H_B) |\psi_{\epsilon}\rangle = 0, \qquad (9)$$

defining $f(\epsilon) = \epsilon - n_f t^2 F_{00}(\epsilon)$. Two effects keep track of the presence of the fibers. A time-dependent potential $V(\tau) = n_f t^2 \int d\tau' \psi^*(\tau) F_{00}(\tau - \tau') \psi(\tau')$, of purely geometrical origin, acts on the base, accounting for the possibility for the particle to explore the fibers when moving on the base. On the other hand, the normalization of the eigenvectors $n(\epsilon)$ depends self-consistently on the corresponding eigenvalue. This fact will have a dramatic consequence in presence of interaction, and the Schrödinger equation contains a nonlinear term. Both these aspects will be analyzed in the subsequent section.

Let us note that the decomposition (1) and (2) holds under the very general hypothesis that the fibers and the base are connected only by an hopping term. If H_F contains instead an interaction term, we generally do not know the explicit form of the Green's functions $F_{ij}(\epsilon)$ and consequently the expressions (5) and (6) cannot be computed exactly.

III. ELECTRON-PHONON INTERACTION: THE COMB LATTICE CASE

In this section we turn to the problem of electron-phonon interaction on bundled structures. We will consider the simplest model for *e*-ph interaction, namely the Holstein molecular crystal model:¹¹

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + \tilde{g} \sum_{i} n_{i} (a_{i} + a_{i}^{\dagger}) + \omega_{0} \sum_{i} a_{i}^{\dagger} a_{i}.$$
(10)

In this model tight-binding electrons interact with local dispersionless oscillators of frequency ω_0 , \tilde{g} is an *e*-ph coupling between the displacement $a_i + a_i^{\dagger}$ of the oscillator and the local electronic density $n_i = \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}$. On really general grounds, the model is expected to display a polaronic behavior for large e-ph coupling. A polaron is a bound state of electrons and phonons in which the electron moves carrying with itself a phonon cloud that strongly diminishes its mobility, eventually giving rise to localization.^{11,12} Since, at least for $\tilde{g} = 0$, the electron motion is completely free, some kind of transition or crossover from a weak-coupling freecarrier state, and a strong-coupling polaronic state must occur at some coupling. Despite the simplicity of the model, even the case of a single particle interacting with the set of oscillators is a nontrivial many-body problem that can be solved only in particular limits. We mention the solution obtained in Ref. 13 within the dynamical mean field, which is exact in the limit of infinite spatial dimensions, and the theorem by Gerlach and Löwen that claims that no phase transition occurs for finite ω_0 .¹⁴ In general cases one has to resort to approximate techniques or numerical studies.^{15–17}

The nature of the transition between a free carrier (for $\tilde{g} = 0$) and a polaron depends on the value of ω_0/t and spatial dimensionality.¹⁶ In fact, even for a single particle we have two independent parameters in the Hamiltonian (10), which determine different physical regimes. In particular, while \tilde{g} is

a measure of the strength of the *e*-ph interaction, $\gamma = \omega_0/t$ is a measure of the adiabaticity of the system, i.e., it controls the relative value of the typical phononic and electronic energy scales. It has been shown that in the adiabatic regime $\gamma \ll 1$, the condition that rules the polaronic crossover is $\lambda = \tilde{g}^2/(2\omega_0 td) > 1$, where *d* is the dimensionality. This condition is simply understood as an energy convenience condition as soon as we notice that the polaronic energy is $E_{\text{pol}} = -\tilde{g}^2/\omega_0$, and the free carrier energy is $E_{\text{free}} = -2td$. Notice that E_{free} contains the total kinetic energy.^{15,16}

We will restrict ourselves to the extreme adiabatic limit $\omega_0/t=0$, in which the lattice degrees of freedom become classical. In this limit, the Hamiltonian can be recast in the form

$$H = -t \sum_{\langle i,j \rangle,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.} \right) + g \sum_{i} n_{i} x_{i} + \frac{1}{2} k \sum_{i} x_{i}^{2}.$$
(11)

Here $g = \sqrt{2k/\omega_0 \tilde{g}}$, k is the elastic constant, and x_i are the classical variables associated to the local displacements of the oscillators. It can be shown that the relevant adimensional coupling the adiabatic limit is $\lambda = g^2/4kt$.

Kabanov and Mashtakov¹⁸ have solved the model for a single particle for 1-2-3 dimensional systems showing that in the one-dimensional case the system has a localized bound state for arbitrarily small e-ph coupling, evidencing only a crossover between a weak-coupling large polaron extended on many lattice sites, and a strong-coupling small polaron localized on a single site. In two and three spatial dimensions a first-order transition (level crossing) occurs between a delocalized state and a small polaron one. We will generalize the approach of Ref. 18 to the case of a comb lattice, a specific bundled structure, in which the base is a linear chain, and two semi-infinite chains are linked to each site of the chain (fibers). We will also consider only the case in which the *e*-ph interaction is limited to the base. This lattice can be viewed as a good model for describing the geometry of many branched polymers,¹⁹ and, on the other side, it is simple enough to obtain explicit results.

In order to reduce ourselves to a base-only problem, we can follow the procedure outlined in the previous section. Attention must be paid to the fact that ϵ indicates only the contribution of the electronic degrees of freedom to the full eigenvalue and the energy is given by $\epsilon + \frac{1}{2}k\Sigma_i x_i^2$. The Schrödinger equation for the base degrees of freedom can be obtained from the one in Ref. 18 in two steps. First of all, the electron eigenvalue ϵ must be substituted with $f(\epsilon)$, defined in Eq. (9), a quantity that keeps track of the effects of the fibers on the electron dynamics. The second step amounts to renormalize the wave function according to Eq. (8), i.e., $\psi_i \rightarrow \psi_i' / \sqrt{n(\epsilon)}$.²⁰ We then obtain, following Kabanov and Mashtakov,¹⁸

$$(f(\boldsymbol{\epsilon}) + 2\lambda tn(\boldsymbol{\epsilon})|\psi_i'|^2)\psi_i' = t\sum_l \psi_{i+l}'.$$
 (12)

It is now clear that the condition (8) introduces an effective rescaling of the coupling constant $\lambda = g^2/4kt$. For $n(\epsilon) \le 1$,

the interaction term is less effective with respect to the baseonly problem. Furthermore, every energy level can be mapped onto one of the base-only problem, with a coupling changing self-consistently with the energy value.

As a consequence, the physical quantities involving expectation values on a single eigenfunction will have similar behaviors for the bundled structure and the base-only cases. On the other hand, we expect different properties for quantities which involve matrix elements between different eigenfunctions, like, e.g., spectral properties.

In what follows, we choose the explicit case of the comb lattice, comparing our results with the ones of the onedimensional case. The fiber is a semi-infinite linear chain and the expressions (5) and (6) take the explicit form

$$F_{00}(\epsilon) = \frac{1}{2t^2} (\epsilon - \operatorname{sgn}(\epsilon) \sqrt{\epsilon^2 - 4t^2}), \quad (13)$$

$$n(\epsilon) = \frac{\sqrt{\epsilon^2 - 4t^2}}{|\epsilon|}.$$
 (14)

Looking at Eq. (12), we expect that, due to the effective reduction of the coupling constant, the crossover from a large to a small polaron, typical of the one dimensional case, will occur for a larger value of λ . Moreover, the ground state properties of the one-dimensional case can be recovered from the ones of the comb lattice through a redefinition of the coupling and a rescaling of the wave function:

$$\lambda \to \lambda n(\epsilon_{\lambda}),$$

$$\psi_{i} \to \psi_{i} / \sqrt{n(\epsilon_{\lambda})},$$
(15)

$$x_{i} \to x_{i} / \sqrt{n(\epsilon_{\lambda})}.$$

Here we emphasize the dependence on λ of the eigen values ϵ_{λ} .

We have also investigated if the rescaling of the eigenvalue equation could induce a level crossing in the ground state at some value of the coupling, thus modifying the nature of the crossover with respect to the 1*d* case. The first derivative of $\epsilon(\lambda)$ turns out to be proportional to the same quantity of the base-only case, through a continuous function of ϵ , built up by $F_{00}(\epsilon)$ and its derivative. In this way we conclude that the properties of the ground state for a comb lattice, or generally for a bundled structure whose fibers are semi-infinite linear chains, are the same of the ones of the base-only case.

We performed a numerical solution of the problem for finite, but quite large lattices, up to 20×20 sites. Henceforth, energies will be expressed in units of the hopping amplitude *t*, and lengths in units of the lattice constant *a*. Our numerical data perfectly confirm the previous considerations. In Fig. 1 we plot the ground state energy as a function of the coupling constant λ . It presents a continuous crossover between a large polaron state whose energy is only slightly modified with respect to the free value $\epsilon_0 = -2\sqrt{2t}$ to a strong cou-



FIG. 1. Ground state energy for a 20×20 comb lattice (in units of *t*), as a function of the coupling constant λ .

pling small polaron state, in which $\epsilon_0 = -2t\sqrt{2}\lambda$. This behavior is completely analogous to the one-dimensional system.¹⁸

In order to estimate the crossover value λ_c , we plot the density-displacement correlation functions $\langle |\psi_0|^2 x_i \rangle$ for i = 0, 1, 2 (Fig. 2), where i=0 indicates the site where the electron localizes.¹⁵ This quantity is a direct probe of the polaronic behavior, measuring the degree of correlation between the electron and the lattice deformations.



FIG. 2. Density-displacement correlation functions for a 20 \times 20 comb lattice for different distances of the sites from the density peak. The change of the slope of the local correlation function (bottom panel) is the signal of the polaronic crossover, and permits us to extract the critical value $\lambda_c = 0.925$.



FIG. 3. The local density displacement correlation function for the linear chain is derived from the data by the comb lattice case with the scaling explained in the text [see Eq. (15)].

All the nonlocal correlation functions decay rather sharply above a given value of λ . Roughly at the same coupling value, the local correlation function abruptly changes the slope, signaling a crossover from a weak-coupling to a strong-coupling regime. This value can be associated to the crossover from a large polaron extended on several lattice sites to a single-site small polaron. We can therefore estimate the crossover coupling λ_c with the value where the first derivative of the local correlation function is maximum, or equivalently with the value for which the nearest-neighbors correlation function starts to decrease. Using the first criterion we obtain an estimate $\lambda_c = 0.925$, which has to be compared with the one-dimensional value $\lambda_c = 0.75$.

Notice that our comb lattice can be viewed as a first step beyond one-dimensionality. The crossover coupling for d = 2 is $\lambda \approx 1$. One should anyway keep in mind that we are not considering *e*-ph interaction on the fibers.

In Fig. 3 we show how the 1D quantities can be recovered with the scaling relations (15): Once the local densitydisplacement correlation function $\langle |\psi_0|^2 x_0 \rangle$ and λ are scaled, respectively, by $n^{3/2}(\epsilon_{\lambda})$ and $n(\epsilon_{\lambda})$, the curve lies on top of the one for the linear chain.

As expected no qualitative difference with respect to the one-dimensional case has been found for the ground state properties.

A. Transport properties

The study of the transport properties in the polaronic problem has been widely studied,^{15,12} since it directly characterizes the onset of localization.

One of the most striking features of bundled structures is an anomalous diffusion for a classical walker moving along the base.⁶ We expect quantum counterpart for this property, namely some peculiar behavior for the conductivity. Note that this expectation is not in contradiction with the general properties of the eigenstates described in the previous section, since the optical response is expressed in terms of matrix elements between *different* eigenstates. In fact, the map-



FIG. 4. Contributions to the conductivity along the backbone, compared with the 1D case. In both cases we show the Drude weight D, the total sum rule for the optical conductivity (17), and the finite frequency optical weight.

ping (15) involves different normalizations, and therefore different effective coupling constants, for every energy level.

The optical conductivity is given by

$$\sigma(\omega) = D\,\delta(\omega) + \sum_{n\neq 0} \frac{|\langle \psi_n | J_x | \psi_0 \rangle|^2}{\epsilon_n - \epsilon_0}, \qquad (16)$$

where the coefficient of the zero-frequency delta function contribution is the so called Drude weight, which explicitly characterizes the transport properties: a vanishing D is the signature of an insulating state,²² whereas a metal has a finite value of such a quantity. The Drude peak can be evaluated by means of the so-called f sum rule,²³

$$\int_{0}^{\infty} \sigma(\omega) d\omega = -\frac{\pi e^2}{2} \langle H_{kin} \rangle \tag{17}$$

and involves the calculation of the kinetic energy and of the integral over all finite frequencies of the optical conductivity. Quite naturally we only consider the conductivity along the backbone, in which anomalous behavior can be expected. We compute the Drude weight given by Eq. (16), the total weight of the optical excitations, related to the kinetic energy by Eq. (17), and the integral over finite (nonzero) frequencies. Both the kinetic energy and the finite frequency optical conductivity show an anomalous behavior with respect to the one dimensional case as it is transparent from a comparison between the data in Fig. 4 and the ones for the one-dimensional case reported in the inset.

For small values of the coupling constant the absolute value of the kinetic energy presents a small but visible enhancement with respect to its free value. This is confirmed by a perturbative calculation for $\lambda \ll 1$. In this limit, we can introduce a continuous approximation of Eq. (12):^{18,21}

$$(\alpha + 2t + 2\lambda t |\psi(x)|^2) = -a^2 t \frac{d^2 \psi(x)}{d x^2},$$
 (18)

which has an exact solution of the form

$$\psi(x) = \sqrt{\frac{\lambda}{2a}} \frac{n(\epsilon_{\lambda})}{\cosh(\lambda n(\epsilon_{\lambda})x/a)}.$$
 (19)

In the one-dimensional case $n(\epsilon_{\lambda}) = 1$ and α just represents the electronic contribution to the ground state energy, while for the comb lattice they are given by Eqs. (13) and (14). Thus the averaged kinetic energy is $E_{KIN} = -2t(1)$ $-\lambda^2 t/6a^2$) for the 1D case, while $E_{KIN} \simeq -\sqrt{2}t(1)$ $+\lambda^2 t/8a^2 - \lambda^4/128a^4$) on the comb lattice. This result can be easily understood by inspection of the particular geometry of the lattice. In the free case, the ground state wave function has a constant value on the backbone sites with exponentially decreasing tails on the teeth. Switching on the interaction, the backbone sites become energetically favorable and the particle is therefore recalled on the backbone, increasing the charge density on the substructure. and consequently of the kinetic energy. Further increasing λ the localization tendency which leads to small polaron formation becomes effective. In this regime the usual behavior is recovered, the kinetic energy decreases its absolute value, while the e-ph interaction energy is substantially decreased.

For small values of λ the finite frequency contribution remains zero up to a given value of λ , and continuously acquires a finite value at some value of λ for both the structures. This can be attributed to finite size effects: a finite number of sites cuts off the available states with proper symmetry in Eq. (16).

A striking feature emerges from Fig. 4. The coupling value for which the Drude weight vanishes ($\bar{\lambda} \approx 0.72$) is sizeably smaller than the crossover coupling extracted from the correlation functions ($\lambda_c \approx 0.925$), which in turn coincides with the kink in the kinetic energy curve. This is never the case in usual one-dimensional and two-dimensional lattices, where the loss of coherence and the small polaron formation essentially coincide, as can be seen in the inset, and as it is valid also for finite phonon frequencies.

However, our results are not in contradiction with general criteria for small polaron formation¹⁵ but they confirm a crucial physical point. In fact the condition $\lambda > 1$ implies that the electronic energy to be overcome by the *e*-ph interaction energy for small polaron formation is not the coherent one but the total kinetic energy. These quantities coincide for a single particle on a conventional lattice, but they may differ for interacting systems or unordered structures.

For $\bar{\lambda} < \lambda < \lambda_c$ the system is in a state in which the coherent transport is strongly suppressed while the kinetic energy is still large, substantially equal to its noninteracting value. We attribute this contribution to local incoherent electron hopping between the teeth sites.

This system represents, to our knowledge, the first one in which coherent motion is strongly inhibited, but there is a sizeable range of parameters in which no polaronic effects are found. This phenomenon represents the quantum heir of anomalous diffusion. It should be noted that, as the e-ph coupling is extended to the whole lattice this effect is expected to be emphasized.

IV. CONCLUSIONS AND PERSPECTIVES

The static and dynamical properties of an electron interacting with local classical oscillators on a comb lattice have been extensively analyzed. Even though our work represents only the first attempt to tackle the problem of interacting fermions on unconventional structures, interesting and peculiar features have been discovered. On really general grounds, we have shown that the static properties (averages on a single state) of a general bundled structure can be easily obtained from the ones of the base-only problem by means of a rescaling of the parameters. As an example, we have studied the small polaron crossover on a comb lattice, comparing it with the one-dimensional case, explicitly confirming this property. Nevertheless, dynamical properties cannot be so simply recovered. A numerical study of the optical response on the comb lattice has highlighted two anomalous properties. Contrarily to the one-dimensional case, for small *e*-ph couplings, the DC conductivity (measured by the Drude weight) is increased with respect to the bare noninteracting

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value. By increasing the coupling a rather surprising feature has been found, namely the coherent motion is strongly suppressed while a sizeable incoherent kinetic energy is still present. The loss of coherence is therefore not due to the self-trapping associated with the polaron crossover (that occurs for larger e-ph coupling, when also the incoherent kinetic energy is suppressed), but to the drastic effects of a unconventional geometry on the electronic properties. The occurrence of such an effect in classical systems has been demonstrated and widely discussed⁶ within the framework of the random walk. We note that our approach is not completely the analogous of the random walk problem: the absence of *e*-ph interaction on the teeth sites implies that, in the classical analogous, the motion of the walker on these sites could be deterministic. The quantum counterpart of anomalous diffusion driven by the geometry would be achieved only if the e-ph interaction was extended to the whole lattice.

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