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Bose Polaron in a One-Dimensional Lattice with Power-Law Hopping

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Abstract: Polarons, quasiparticles resulting from the interaction between an impurity and the collective excitations of a medium, play a fundamental role in physics, mainly because they represent an essential building block for understanding more complex many-body phenomena. In this manuscript, we study the spectral properties of a single impurity mixed with identical bosons in a one-dimensional lattice with power-law hopping. In particular, based on the so-called T-matrix approximation, we show the existence of well-defined quasiparticle branches for several tunneling ranges and for both, repulsive and attractive impurity-boson interactions. Furthermore, we demonstrate the persistence of the attractive polaron branch when the impurity-boson bound state is absorbed into the two-body continuum and that the attractive polaron becomes more robust as the range of the hopping increases. The results discussed here are of relevance for the understanding of the equilibrium properties of quantum systems with power-law interactions.

Keywords: Impurity physics, optical lattices, power-law hopping

1. Introduction

The study of a single impurity immersed in a many-body quantum system is one of the central topics in condensed matter physics that continuously reveals new intriguing phenomena. The polaron concept, originally proposed by Landau and Pekar [1,2] to describe the screening of electrons in a crystal, provides a useful approach to understanding nontrivial many-body properties. In the last years, the polaron idea has not only been used to describe electrons in solids but also impurities dressed by spin fluctuations [3,4], bound electron-hole pairs in semiconductors [5,6], hybrid impurities of light-matter nature [7,8], and to describe highly imbalanced mixtures in ultracold quantum gases [9–12], among others. Furthermore, the vast relevance of the polaron concept has recently encouraged the development of studies that explore the physics of impurities in more exotic scenarios. For instance, bipolarons (bound states between two polarons) [13–17], dipolar polarons [18–21], and charge polarons [22–25].

The introduction of optical lattices and optical tweezers on various experimental platforms has motivated the study of the physics of impurities beyond the homogeneous space scenario. In particular, the transport of impurities in one-dimensional lattices has been addressed within the weak and strong coupling regime [26–32] and variational schemes have been employed to describe polarons and bipolarons in one-dimensional lattices [33]. More recently, the effects of the superfluid to Mott-insulator transition of two-dimensional bosons on the polaron physics have been analyzed for weak boson-impurity interactions [34], and a non-self-consistent T-matrix approximation has been employed to describe single impurities and the formation of bipolarons in square lattices [17].

Most of the current studies on lattice polarons consider short-range couplings, either contact interactions or nearest-neighbor hoppings, overlooking the effects of longer-range couplings. An interesting question is to study the physics of lattice polarons when the nearest-neighbor tunneling is replaced with a hopping whose amplitude follows a power law. This modification is of particular interest since power-law interactions arise in several quantum simulation platforms, such as trapped ions [35,36], polar molecules [37,38], Rydberg atoms [39], nuclear spins in solid-state systems [40], and atoms in photonic crystal waveguides [41]. Recently, the physics of quantum systems with

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long-range interactions has attracted plenty of attention [42]. In particular, it has been shown that power-law couplings lead to new Lieb-Robinson bounds for quantum information dynamics [43], exotic spin dynamics [44–46], multifractality and intriguing localization properties in the presence of a quasiperiodic potential [47–50], and modifications in both, the superfluid to Mott-insulator transition and the Bose-Einstein condensation [51–54].

In this manuscript, we study the spectral properties of a single impurity mixed with identical bosons in a one-dimensional lattice with power-law hopping. To this end, we first examine the scattering problem of a single impurity and a single boson, based on the so-called $T-$matrix formalism, we show the effects of the range of the hopping on the two-body bound state. In particular, we illustrate the dependence of the energy of the dimer on the power of the hopping and the stability of the repulsively and attractively bound states. Afterwards, we modify the two-body $T-$matrix to include the effects of a BEC and study the emergence of well-defined quasiparticle branches for different hopping ranges. Furthermore, we analyze the spectral properties of the polarons and their dependence on the power of the hopping. The results here discussed go beyond previous findings, in the sense that they explore the consequences of the range of the hopping on the spectral properties of one-dimensional polarons.

2. Model

We consider a mobile impurity mixed with identical bosons in a one-dimensional lattice of length L and with inter-site couplings decaying as a power law with power α. In the second quantization formalism, the Hamiltonian that describes the above system is given as follows

$$\begin{aligned}\hat{H} = &-t_B \sum_{i,j\neq i} \frac{1}{|i-j|^\alpha} \hat{b}_i^\dagger \hat{b}_j + \frac{U_B}{2} \sum_i \hat{b}_i^\dagger \hat{b}_i^\dagger \hat{b}_i \hat{b}_i - \mu_B \sum_i \hat{b}_i^\dagger \hat{b}_i \\ &- t_I \sum_{i,j\neq i} \frac{1}{|i-j|^\alpha} \hat{c}_i^\dagger \hat{c}_j + U_{BI} \sum_i \hat{b}_i^\dagger \hat{c}_i^\dagger \hat{c}_i \hat{b}_i,\end{aligned} \tag{1}$$

where $\hat{b}_i$ ($\hat{b}_i^\dagger$) and $\hat{c}_i$ ($\hat{c}_i^\dagger$) annihilates (creates) a boson and an impurity at site i, the tunneling amplitude between nearest neighbors is t_B for the bosons and t_I for the impurities, $U_B > 0$ is the on-site boson-boson repulsion, μ_B is the chemical potential of the bosons, and U_{BI} is the on-site interaction between the bosons and the impurity. For simplicity, we set $\hbar$ and the lattice constant a to unity, and consider the case of equal nearest-neighbor tunneling amplitudes, that is $t_B = t_I = t$. It is important to mention here that from a thermodynamic point of view [42], $1/|i-j|^\alpha$ hops in one-dimensional lattices are considered long-range when $\alpha < 1$ whereas short-range when $\alpha > 1$. Through the manuscript, we consider $\alpha > 1$, only.

3. Single-particle Physics

Before entering into the study of an impurity immersed in a BEC, it is convenient to briefly summarize the main characteristics of a single particle moving in a lattice with power-law hopping. The single-particle Hamiltonian is given as follows

$$\hat{H} = -t \sum_{i\neq j} \frac{1}{|i-j|^\alpha} \hat{b}_i^\dagger \hat{b}_j. \tag{2}$$

The above Hamiltonian can be easily diagonalized using the Fourier transform operators

$$\begin{aligned}\hat{b}_k &= \frac{1}{\sqrt{L}} \sum_j e^{-ikj} \hat{b}_j \\ \hat{b}_k^\dagger &= \frac{1}{\sqrt{L}} \sum_j e^{ikj} \hat{b}_j^\dagger,\end{aligned} \tag{3}$$

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$k \in [-\pi, \pi]$ being the quasi-momentum within the first Brillouin zone. This procedure gives rise to the single-particle lattice dispersion

$$\epsilon_k^\alpha = -t[\mathrm{Li}_\alpha(e^{ika}) + \mathrm{Li}_\alpha(e^{-ika})], \tag{4}$$

where $\mathrm{Li}_\alpha(z) = \sum_{n=1}^\infty z^n/n^\alpha$ is the polylogarithm function. Notice that ϵ_k^α is always real since is of the form $z + z^*$ with z a complex number and z^* its complex conjugate. Furthermore, for $\alpha \gg 1$, the lattice dispersion approaches to the well-known result of a lattice with nearest-neighbor hopping, that is $\epsilon_k^{\alpha\to\infty} \simeq -2t\cos ka$. Using that $\mathrm{Li}_\alpha(1) = \zeta(\alpha)$ with $\zeta(\alpha)$ the Riemann zeta function, one can recognize that the energy of the zero-momentum mode is $\epsilon_{k=0}^\alpha = -2t\zeta(\alpha)$. Since $\zeta(\alpha)$ converges when the real part of α is greater than one, finite energies in the thermodynamic limit are obtained when $\alpha > 1$. In the upper panels of Figure 1, we illustrate the lattice dispersion as a function of the quasi-momentum k for several values of α, the NN case corresponds to a lattice with nearest-neighbor hopping. As one can notice, for nearest-neighbor hops, the dispersion is a smooth function of k, while it becomes sharp-pointed at $k = 0$ as α decreases. The lower panels of Figure 1 show the density of states (DOS) $\rho_\alpha(\omega) = -\frac{1}{\pi}\Im m[\sum_k(\omega - \epsilon_k^\alpha)^{-1}]$ as a function of the energy $\omega = (\epsilon_k^\alpha - \epsilon_{k=0}^\alpha)/\Delta_\alpha$ with $\Delta_\alpha = \epsilon_{k=\pi}^\alpha - \epsilon_{k=0}^\alpha$ the lattice bandwidth and $\Im m$ denotes the imaginary part. As α decreases, the DOS loses its symmetry at the band edges, becoming smaller at the bottom of the band. That is, low-energy states become less dense compared to high-energy states. As we will see later, this characteristic has consequences on the physics of the polaron.

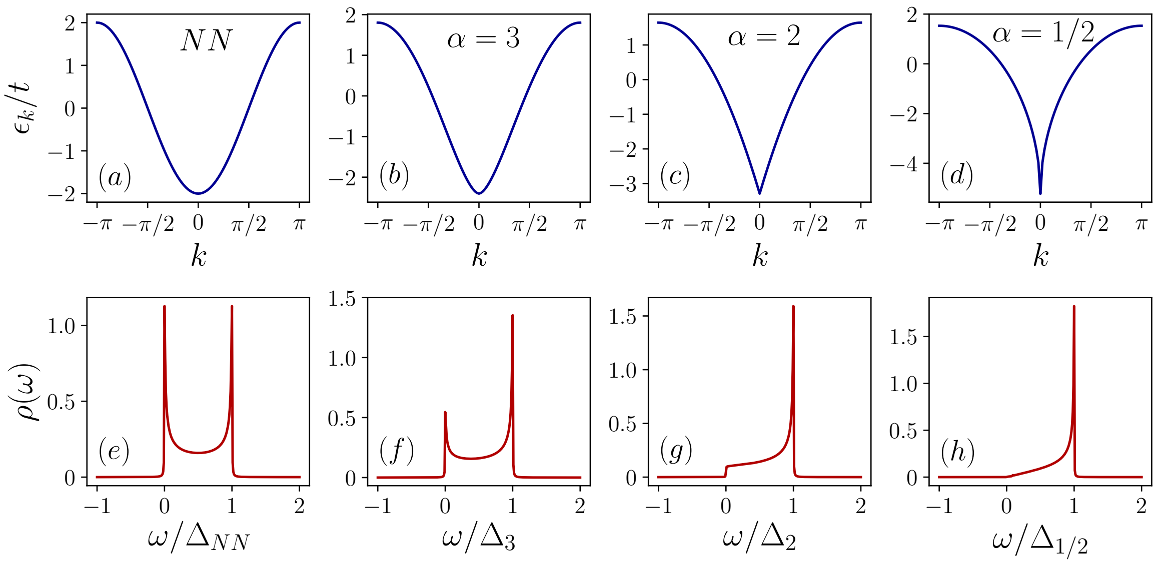

Figure 1. Panels (**a**)-(**d**) show the lattice dispersion ϵ_k/t as a function of the quasi-momentum in the first Brillouin zone $k \in [-\pi, \pi]$. Panels (**e**)-(**h**) illustrate the density of states ρ as function of $\omega = (\epsilon_k^\alpha - \epsilon_{k=0}^\alpha)/\Delta_\alpha$ with $\Delta_\alpha = \epsilon_{k=\pi}^\alpha - \epsilon_{k=0}^\alpha$ the lattice bandwidth. Panels (**a**) and (**e**) are associated with a lattice with nearest-neighbor hopping.

4. Two-body Scattering

In this section, we focus on the scattering of an impurity atom and a single boson in an empty lattice. For on-site interactions, the scattering matrix $\mathcal{T}$ of the two-body problem depends only on the total center-of-mass momentum P and on the energy ω of the pair. Its explicit simple form is

$$\mathcal{T}(P,\omega) = \frac{U_{BI}}{1 - U_{BI}\Pi(P,\omega)}, \tag{5}$$

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where $\Pi(P,\omega)$ is the pair propagator in an empty lattice which is given as follows

$$\Pi(P,\omega) = \frac{1}{L}\sum_k \frac{1}{\omega - \epsilon^{\alpha}_{BP/2+k} - \epsilon^{\alpha}_{IP/2-k}}. \tag{6}$$

The subscripts B and I indicate boson and impurity species, respectively. In Figure 2, we plot the spectral function $\mathcal{A}_{\mathcal{T}} = -2\Im m\mathcal{T}(k=0,\omega)$ as a function of U_{BI} and ω for several values of α. As it is well-known, the poles of the scattering matrix $\mathcal{T}$ are associated with bound states, in this context a bound state between one boson and one impurity. Since in lattice systems, the two-body scattering continuum is bounded above and below, the $\mathcal{T}$ matrix shows bound states for both negative and positive interactions. The former states are called attractively bound pairs and the latter repulsively bound pairs. In contrast to attractive dimers, a repulsively bound pair is not the ground state of the two-body system. However, due to energy constraints, the repulsively bound dimer is unable to decay by converting the interaction energy into kinetic energy, and therefore the repulsively bound state is dynamically stable. Repulsively bound pairs have been experimentally demonstrated in ultracold atomic gases confined in optical lattices with nearest-neighbor hoppings [55]. As one can notice from Figure 2, the branch of repulsively bound states is pushed towards the continuum as α decreases however, it is not absorbed. In contrast, the branch of attractively bound dimers is incorporated into the continuum as the range of the hopping increases, in fact, when $\alpha = 1.5$ there is no bound state branch for $-8 < U_{BI} < 0$. The incorporation of bound states into the continuum has been also observed in spin and disordered systems with power-law couplings [45,50].

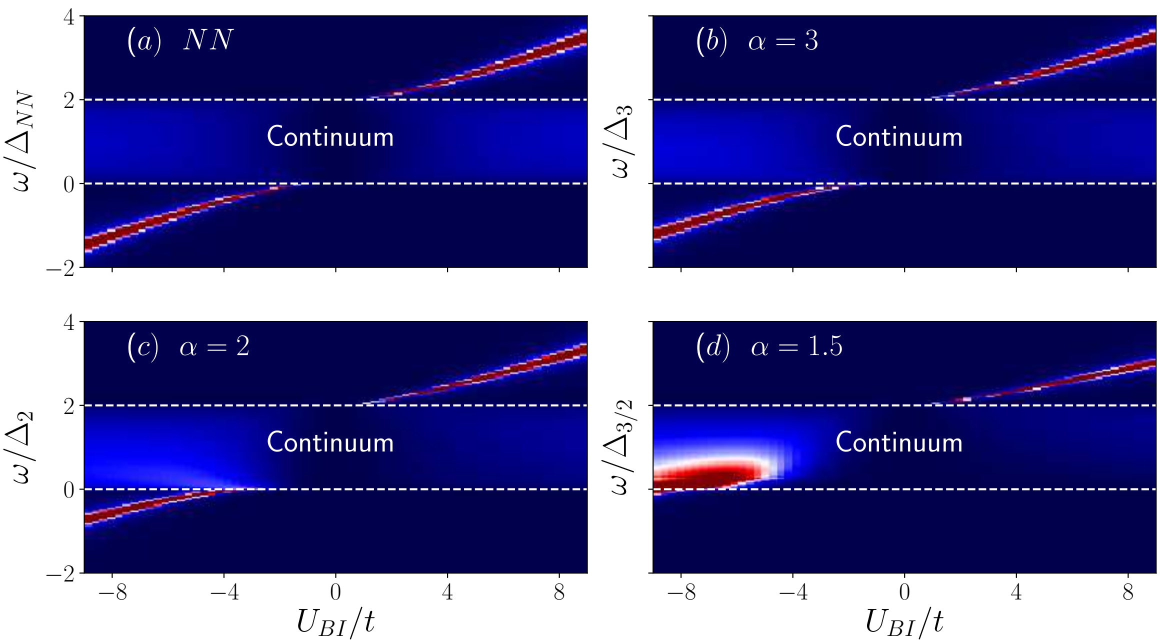

Figure 2. Spectral function $\mathcal{A}_{\mathcal{T}} = -2\Im m\mathcal{T}(k=0,\omega)$ as a function of the interaction strength U_{BI} and the energy ω for vanishing quasi-momentum k. In each panel, the dashed white lines enclose the two-body scattering continuum. (**a**) Spectral function for nearest-neighbor hopping, (**b**) $\alpha = 3$, (**c**) $\alpha = 2$, and (**d**) $\alpha = 3/2$.

5. Impurity in a Bose-Einstein Condensate

We now analyze the physics of a single impurity immersed in the BEC and the formation of the polaron. The spectral properties of an impurity with quasi-momentum k can be described by the impurity Green's function

$$G_I(k,\omega) = \frac{1}{\omega - \epsilon^{\alpha}_{Ik} - \Sigma(k,\omega)} \tag{7}$$

where $\Sigma(k,\omega)$ is the self-energy of the impurity. Due to the great complexity of many-body systems, an exact calculation of the self-energy is not feasible, for this reason, one has to make certain approximations. To calculate the self-energy, we employ the T-matrix approximation which has been successfully used to describe Bose polaron experiments [10,12,56–58]. In this approximation, the self-energy of the impurity is simply the product of the matrix $\mathcal{T}_{BEC}$ and the equilibrium density of the bosons n_0, that is $\Sigma(k,\omega) = n_0\mathcal{T}_{BEC}(k,\omega)$. In contrast to the two-body problem, the scattering matrix $\mathcal{T}_{BEC}$ has to include the presence of the BEC. To do so, we assume that the BEC can be accurately described by the Bogoliubov theory. This procedure gives the chemical potential $\mu_B = \epsilon^{\alpha}_{Bk=0} + n_0 U_B$, the excitation spectrum $E^{\alpha}_k = \sqrt{\epsilon^{\alpha}_{Bk}(\epsilon^{\alpha}_{Bk} + 2n_0 U_B)}$, and the modified two-particle propagator

$$\Pi_{BEC}(P,\omega) = \frac{1}{L}\sum_k \frac{u_k^2}{\omega - \epsilon^{\alpha}_{IP-k} - E^{\alpha}_k}, \tag{8}$$

where u_k is the usual Bogoliubov coherence factor

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\epsilon^{\alpha}_{Bk} + n_0 U_B}{E^{\alpha}_k}\right). \tag{9}$$

Substitution of $\Pi_{BEC}(P,\omega)$ into Equation (4) gives the scattering matrix $\mathcal{T}_{BEC}$. As expected, for $U_B = 0$, the scattering matrix $\mathcal{T}_{BEC}$ is identical to the two-body scattering matrix $\mathcal{T}$. In Figure 3, we plot the spectral function of the polaron $A_I = -2\Im m G_I(k=0,\omega)$ as a function of the impurity-boson interaction U_{BI} for vanishing quasi-momentum $k=0$ and several values of the power α. In each panel, the yellow curve is associated with the energy of the dimer states, that is the poles of the $\mathcal{T}$ matrix shown in Figure 2, the white dashed lines enclose the Bogoliubov continuum with energies $\epsilon^{\alpha}_{Ik} + E^{\alpha}_{-k}$, which is essentially indistinguishable from the two-particle continuum. For the numerical calculations, we take the value $n_0 = 1$ and $U_B/t = 0.02$. The reason for considering a small boson-boson interaction is to ensure that the bosonic system is far from the transition to the Mott phase. In all numerical calculations, it was ensured that the spectral function is properly normalized

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ A(k=0,\omega) = 1. \tag{10}$$

As one can notice from Figure 3, there are well-defined quasi-particle branches for both, positive and negative interactions. The poles of $G_I(k,\omega)$ are associated with the energies of the polaron E_{Pk}. This energy can be found by solving the following self-consistent equation

$$E^{\alpha}_{Pk} = \epsilon^{\alpha}_{Ik} + \Re e[\Sigma(k, E^{\alpha}_{Pk})], \tag{11}$$

where $\Re e$ denotes the real part. For $U_{BI}/t > 0$, the quasiparticle has a higher energy than the repulsive dimer and, like the latter, it is dynamically stable since there are no available states in which it can decay by converting the interaction energy into kinetic energy. As the range of the hopping increases, the energy of the impurity approaches the energy of the dimer for small U_{BI}/t, that is, the polaron becomes a dimer into a BEC. For $U_{BI}/t < 0$, the quasiparticle branch has a smaller energy than the attractively bound pair. Remarkably, the attractive polaron is still well-defined even when the attractively bound pair is already absorbed into the continuum (see Figure 3(d)). Furthermore, as

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α decreases, the broadening of the attractive polaron inside the Bogoliubov continuum is reduced. This can be physically understood from the asymmetry of the density of states (see Figure 1(d)). As the range of the hopping increases, the density of available states into which the polaron can decay decreases, and therefore the broadening of the impurity inside the Bogoliubov continuum is reduced.

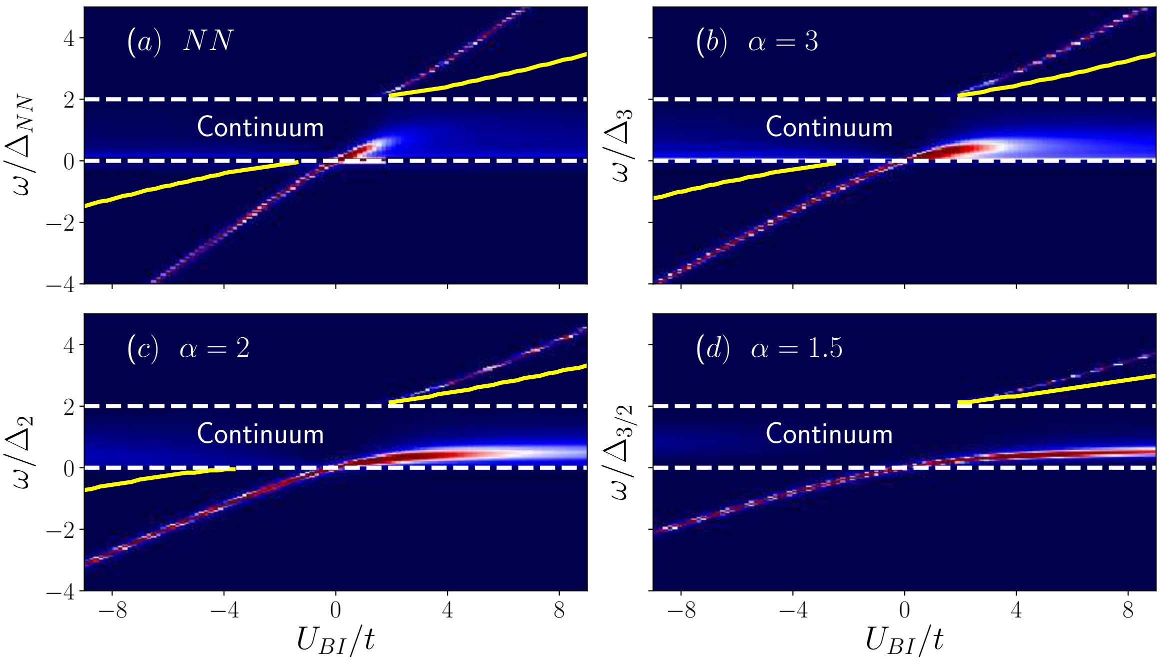

Figure 3. Spectral function of the impurity $A_I = -2\Im m G_I(k=0,\omega)$ as a function of the interaction strength U_{BI} and the energy ω. We consider $n_0 = 1$ and $U_B/t = 0.02$. The dashed white lines enclose the Bogoliubov continuum, the yellow curve is associated with the energy of the dimer states. (**a**) Spectral function for nearest-neighbor hopping, (**b**) $\alpha = 3$, (**c**) $\alpha = 2$, and (**d**) $\alpha = 3/2$.

Within the quasiparticle picture and in the vicinity of a pole, the impurity Green's function in Equation (7) can be approximated as follows [59]

$$G_I(k,\omega) \approx \frac{Z_k}{\omega - E_{Pk} + i\gamma_k}, \tag{12}$$

where Z_k is the quasiparticle residue and γ_k is the damping rate. These quantities are given by

$$\begin{aligned} Z_k^{-1} &= \left(1 - \frac{\partial \Re e[\Sigma(k,E_k)]}{\partial\omega}\right)\Bigg|_{\omega=E_{Pk}}, \\ \gamma_k &= -Z_k \Im m[\Sigma(k,E_k)]. \end{aligned} \tag{13}$$

In Figure 4, we show the residue and damping rate of a zero-quasi-momentum polaron as a function of the impurity-boson interaction for several values of α. The residue of the repulsive branch decreases as the range of the hopping increases, this behavior is in agreement with the previous observation that the polaron branch is pushed towards the bound state branch. Since $Z_0 \ll 1$, it is not possible to discern this branch in current experiments. In stark contrast, the residue of the attractive branch increases when the hopping range increases, making the polaron picture more robust and feasible to be observed. As shown in Figure 4b, the damping rate for the attractive polaron branch decreases as α decreases, that is, the polaron becomes more long-lived. The damping of the repulsive branch does not change significantly with the tunneling range.

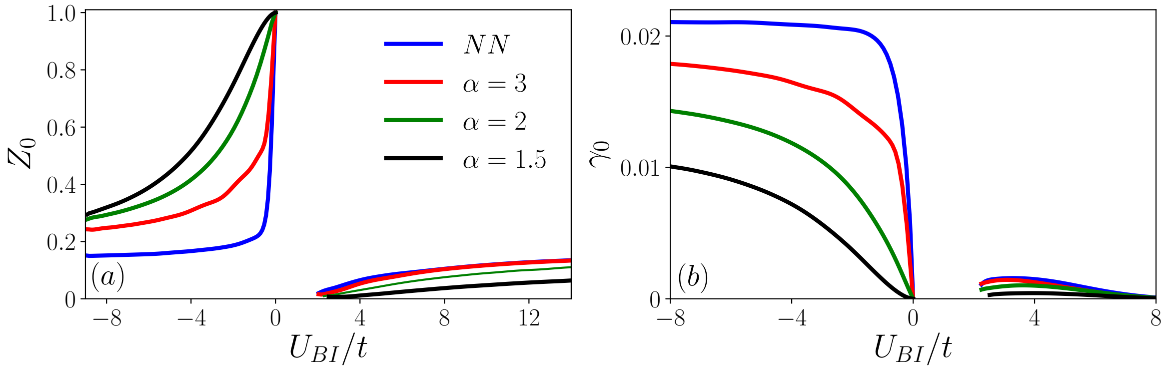

Figure 4. (**a**) Quasiparticle residue as a function of the impurity-boson interaction for vanishing crystal momentum $k = 0$ and several values of the power hopping α. (**b**) Damping rate as a function of the impurity-boson interaction for vanishing crystal momentum $k = 0$ and several values of the power hopping α.

6. Conclusions

In conclusion, we have investigated the spectral properties of a mobile impurity mixed with identical bosons in a one-dimensional lattice with power-law hopping. To this end, we first address the scattering problem of a single impurity and a single boson. By means of the T-matrix formalism, we show that as the range of the hopping increases the attractively bound pair is incorporated into the two-body continuum, whereas the repulsively bound state stays out of the latter. Afterwards, we assume that the bosons can be described by the Bogoliubov approximation and modify the two-body scattering matrix to include the effects of the BEC on the impurity. Within this formalism, we illustrate the effects of tunneling range on the impurity dressed by the BEC excitations. In particular, we show the existence of polaron branches for repulsive and attractive interactions. Furthermore, we illustrate that the polaron branch for attractive interactions is well defined even when the impurity-boson bound state is absorbed into the Bogoliubov continuum and that as the hopping range increases the attractive polaron becomes more robust. Many-body physics in quantum systems with power-law interactions is of current theoretical interest and is under development in experimental platforms such as trapped ions, Rydberg atoms, and photons in crystal waveguides.

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