Polaron with disordered electron-phonon interaction

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A single electron in one dimensional lattice is considered within the framework of extended Holstein model at strong-coupling limit. Disordered density-displacement type electron-phonon interaction is proposed. Basic parameters of small polaron formed due to disordered electron-phonon interaction are calculated. It is shown that disordered electron-phonon interaction substantially influences all properties of the polaron. Depending on disordered electron-phonon interaction polaronic effect might be enhanced or diminished. It turns out that all parameters of the polaron are site dependent. Further application of proposed model is briefly discussed.

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I. INTRODUCTION

Polaron concept was introduced in the 30th years of XX century by Landau [1] and later was theoretically developed by a number of researchers (see review [2]). Though in the field of polaron physics there are substantial understanding of main features of polaron related phenomena in a variety of solids, there still remain open issues to be clarified. One of them is the application of the theoretical models to the real solids, in particular the various disordered systems. An interplay of lattice disorder and electron-phonon interaction in such systems, as it is well known, determines charge carrier dynamics. In the past decades Holstein polarons [3] were studied in a variety of medium, including near an impurity [4,5] and in a disordered lattice [6,7,12]. The all mentioned works except of Ref.[3] deal with local electron-phonon interaction, in which charge carrier interacts only with onsite intramolecular vibrations. In reality, charge carrier interacts simultaneously with all ions of the lattice and the range of this electron-phonon interaction extends over many lattice units. At the same time disorder influences coupled electron-phonon system too. Noteworthy that in work [6] it was shown opposite effect namely that electron-phonon interaction renormalizes disorder potential and that disorder seen by a polaron is different from the bare disorder[12]. In this sense, an electron sees the disordered ions and as a consequence it interacts with them via electron-phonon interaction which is spatially disordered as well. Such type of disordered electron-phonon interaction and its role in polaron formation was not studied yet. The objective of this paper is to remedy this shortcoming. In order to do this we further develop an idea of Ref.[14] with regard of polarons and apply it to disordered lattice.

Namely in Ref.[14] a model of a polaron with a long-range “density-displacement” type force was introduced. The model by itself represents an extension of the Fröhlich polaron model [15] to a discrete ionic crystal lattice or extension of the Holstein polaron model [3] to a case when an electron interacts with many ions of a lattice with longer ranged electron-phonon interaction. Subsequently, the model was named as the extended Holstein model (EHM) [14]. The model was introduced in order to mimic high – $T_c$ cuprates, where the in-plane ($CuO_2$) carriers are strongly coupled to the $c$-axis polarized vibrations of the apical oxygen ions [17]. In the last decades the model was studied in great detail in Refs.[16, 18–39].

II. THE MODEL

In this paper we deal with the extended Holstein model in one dimensional lattice in which electron-phonon interaction is disordered. The Hamiltonian of the model is

$$H = H_e + H_{ph} + H_{e-ph}$$  \hspace{1cm} (1)

where

$$H_e = -t \sum_n (c_n^{\dagger}c_{n+1} + H.c.)$$  \hspace{1cm} (2)

is the electron hopping energy,

$$H_{ph} = \sum_m \left( -\frac{\hbar^2 \partial^2}{2M \Omega_m^2} + \frac{M \omega_n^2 u_m^2}{2} \right)$$  \hspace{1cm} (3)

is the Hamiltonian of the vibrating ions,

$$H_{e-ph} = \sum_{n,m} f_m (n) \cdot u_m c_n^{\dagger}c_n$$  \hspace{1cm} (4)

describes interaction between the electron that belongs to a lower chain and the ions of an upper chain (see below). Here $t$ is the nearest neighbor hopping integral, $c_n^{\dagger}(c_n)$ is a creation (destruction) operator of an electron on a cite $n$, $u_m$ is the $c$-polarized displacement of the $m$-th ion and $f_m (n)$ is an interacting density-displacement type force between an electron on a site $n$ and the $c$-polarized vibration of the $m$-th ion. $M$ is the mass of the vibrating ions and $\omega$ is their frequency.

We consider an electron performing hopping motion on a lower chain consisting of the static sites, but interacting with all ions of an upper chain via a long-range
density-displacement type force, as shown in Fig. 1. So, the motion of an electron is always one-dimensional, but a vibration of the upper chain’s ions is c-polarized (perpendicular to the chains). There is no doubt that an explicit analytical form of the force \( f_m(n) \) is one of crucial aspects determining polaron parameters. Of cause, it depends on structural elements that located on sites \( m \). Whether the structural elements are neutral, charged (positively or negatively) or dipoles (electrical or magnet) this force may have different origin and may lead to different polaronic states. As in Refs. [19, 24, 31, 34] here it is also assumed that the structural elements are electrically charged (positive or negative) and thus the force has Coulombic nature. Now let’s try to simulate a disorder in the lattice. There are many ways to simulate a disorder in the lattice. One of them is allocation driven disorder where positions of upper chain’s ions are randomized. Of course, if allocation of the ions throughout the upper chain is disordered then density-displacement type force \( f_m(n) \) is also disordered. An another way to simulate a disorder in the lattice is randomize the charge value of the upper chain’s ions. There are a lot of examples for the systems where such type of charge fluctuations or modulations occurs (see for example [10, 42]). Modulations of charge states of structural elements of the lattice may occur in many other systems like cuprates, manganites, organic semiconductors and it has become possible owing to modern crystal growth technology. Here we consider only charge modulation (fluctuation) driven disorder of electron-phonon interaction and its consequences in polaron formation. So, our consideration is relevant to all compounds where polaron formation is possible and it occurs in the presence of charge modulation’s (fluctuation) driven electron-phonon interaction.

Considering the above said opinions without loss of generality one writes explicitly a discrete form of the density-displacement type electron-phonon interaction force as:

\[
f_m(n) = \frac{c \cdot \kappa_m}{(|n - m|^2 + c^2)^{3/2}}
\]  

where \( \kappa_m \) is some force coefficient, which characterizes charge states of the upper chain’s ions, and \( |n - m| \) is measured in units of \( |a| \). In this work we choose \( \kappa_m \) as uniformly distributed random number in the interval of \((0,1)\), so \( \kappa_m \neq \kappa_{m'} \) and \( \kappa_m \in (0,1) \). For this reason the value of \( \kappa_m \) changes randomly in passing \( m \) from one site to another site.
III. RESULTS AND DISCUSSION

The possible ways of changing the value of $k_m$ are illustrated in Fig. 2. In turn density-displacement force Eq. (3) acquires a peculiarity of randomized (i.e. disordered) electron-phonon interaction force. From now the force Eq. (3) has two features: (i) it is still longer-ranged and descends as $r^{-3}$, where $r$ is the distance between the electron and ion under consideration, and (ii) it is randomized (disordered). In Fig. 3 the plots of the dependence of the value of density-displacement electron-phonon interaction force Eq. (3) on site indexes $m$ are presented. As it is seen from the plots randomization of the electron-phonon interaction force changes the picture of the phenomenon drastically (qualitatively and quantitatively). Indeed, for a regular lattice we have $f_{|m|}(|n|) > f_{|m|'}(|n|)$ if $|m| > |m'|$. But for our case of the lattice with the disordered electron-phonon interaction the above relation is not always true i.e. on some sites $f_{|m|}(|n|) < f_{|m|'}(|n|)$ even if $|m| < |m'|$. This is the effect of considering disorder on the density-displacement type electron-phonon interaction. As a result of all parameters of the polaron will be affected by the disorder. In order to show this explicitly we calculate just some basic polaron’s parameters like $E_p$- polaron shift, $g^2$- band-narrowing factor, $\gamma$- a numerical factor that depends on crystal structure and binds the polaron energy $E_p$ to band-narrowing factor $g^2$ via relation $g^2 = \gamma E_p / h\omega$ and $\Phi(m-n')$- whose gradient in corresponding direction is important to determine the mass of the polaron in a regular lattice.

In strong electron-phonon coupling limit and nonadiabatic regime one uses the standard procedures such as Lang-Firsov transformation that eliminates electron-phonon interaction term. Subsequent use of perturbation expansion of the transformed Hamiltonian $H_F$ with respect to parameter $\lambda^{-1} = 2t/E_p$ up to the first order in the hopping integral yields

$$E_p(n) = \frac{1}{2M\omega^2} \sum_m f_{m}^2(n),$$

FIG. 4: The value of polaron shift $E_p$ at sites $n$ due to disordered electron-phonon interaction.

FIG. 5: The value of band-narrowing factor $g^2$ at sites $n$ due to disordered electron-phonon interaction.

FIG. 6: The value of $\gamma$ at sites $n$ due to disordered electron-phonon interaction.

FIG. 7: The value of $\Phi(n)$ at sites $n$ due to disordered electron-phonon interaction.
sented the plots of values of laron’s parameters. In Fig.4, Fig.5 and Fig.6 we pre-
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Randomization undergoes also polaron’s hopping inte-
pendent i.e disordered. Something similar ideas, namely
it is appears that all polaron’s parameters are site de-
values for different disorders, Fig.8. One can observe the
values of \( \Phi(n) = f_m(n) \cdot f_m(n+a) \) (9)

Though these parameters were obtained by perturba-
tion theory under certain assumptions we accept them
as starting point expressions for the discussion of the in-
fluence of disordered electron-phonon interaction on po-
laron’s parameters. In Fig.4 Fig.5 and Fig.6 we pre-
sented the plots of values of \( E_p(n) \), \( g^2(n,a) \) and \( \gamma(n,a) \),
respectively, on different sites \( n \). As it is seen from the
presented date all these parameters are randomized too.
Depending on disordered electron-phonon interaction pola-
ronic effect might be enhanced or diminished. The
values of \( \Phi(n) \) on different sites \( n \) are given in Fig.7
Randomization undergoes also polaron’s hopping integ-
ral from one site to on another site of the lattice. Within
the used framework one can estimate the value of hop-
ning integral from ratio \( t' / t \simeq \exp(g^2) \) and plot its val-
ues for different disorders, Fig.8. One can observe the
same tendency for hopping integral. Findings indicate
that disorder changes a picture of polaron formation, and
it is appears that all polaron’s parameters are site de-
pendent i.e disordered. Something similar ideas, namely
about site dependence of polaron energy (shift) and lo-
cal electron-phonon interaction’s coupling constant on \( n \),
can be found in [44].

The above results were obtained under assumption
that the values of \( \kappa \) are uniformly distributed within
the interval \( (0,1) \). But our model can be straightfor-
wardly generalized to the case when the values of \( \kappa \) be-
long to an arbitrary interval \( (p,q) \) and is defined within
it by some function of distribution (Gaussian, Poisson,
Bernoulli and so on). There are a great variety of op-
tions for simulation here. In our model it is also possible
to simulate string like structures and study a polaron
formation in such structures. For this purpose it is suf-
cient to select a required set of values of \( \kappa_m \), for example
\( \kappa_m = (\ldots, 0, 0, 1, 1, 1, 1, 1, 1, 1, \ldots) \). There are also
other possibilities.

Another question that we would like to discuss here
concerns the size of the polaron in the lattice where
electron-phonon interaction is disordered. As for the
Hamiltonian \( (1) \) there are two points of view on this mat-
ter. Ref.[14] treats the polaron of the model \( (1) \) as small
Fröhlich polaron, while Ref.[16] treats the polaron of the
model \( (1) \) as large Holstein polaron. Here we follow the
definition in which small polaron is formed at \( t/E_p \ll 1 \)
and large polaron is formed at \( t/E_p \gg 1 \) [14]. Since in our
model the ratio \( t/E_p \) fluctuates from site to site one can
not say clearly about size of polaron even it formed by
long-rang electron-phonon interaction [5]. For some sites
the condition of small (large) polaron formation is satis-
fied, while for other sites it is ruled out. Then one may
say that in the systems with disordered electron-phonon
interaction polaron’s size also modulated by the disor-
dered electron-phonon interaction. It seems that such
property of polarons in disordered structures is common
since in Ref.[5] a mixed behavior typical for large (away
impurity) and small (near impurity) polarons was also
expected for a crystal with impurities. The results ob-
tained here suggest further study of polaron formation
in disordered structures taking into an account not only on-
diagonal and off-diagonal aspects of the disorder, but also
the disordered nature of the electron-phonon interaction
as well.

**IV. CONCLUSION**

In conclusion we have studied one dimensional lattice
within the framework of the extended Holstein model.
Considering the case when charge fluctuations can oc-
cur in the system we have applied the extended Holstein
model to study polaron formation in the system. In do-
ing this we introduce a disordered density-displacement
type electron-phonon interaction by randomizing force
constant that describes charge state of the ions. We have
calculated the basic parameters of polaron with the dis-
ordered electron-phonon interaction and have found that
all parameters of polaron are drastically affected by the
disordered electron-phonon interaction. It turns out that
all parameters of polaron are site dependent. This is true
with respect to ratio \( t/E_p \) that determines a polaron size.
Then one can not say definitely about size of polaron in
such system. The size of the polaron depends on its po-
position and from the disorder seen by polaron from this
location. So, the size of the polaron is modulated (disor-
dered) i.e. site dependent in the system with disordered
electron-phonon interaction.
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