One-dimensional moving polarons with extended coherent states

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Abstract. The general properties of one-dimensional large Fröhlich polarons in motion are investigated with the previous extended coherent states where two-phonon correlations are considered. As a result, the polaron energy, velocity, effective mass, and average number of virtual phonons as a function the polaron total momentum are evaluated in a wide range of the coupling constant. In addition, rich information about virtual phonons emitted by the electron in motion is obtained. More importantly, some intrinsic features of 1D moving polarons are presented for the first time, which may also be suited to moving polarons in more than one dimensions.

PACS. 71.38.+i Polarons and electron-phonon interactions – 63.20.Kr Phonon-electron and phonon-phonon interactions

1 Introduction

The problem of the one dimensional (1D) polaron has attracted much attention in the last decade for both its theoretical and practical interest. First, it is technologically possible to confine electrons in one direction [1] (*i.e.*, quantum-well-wires), and it had been reported that a 1D polaron emerges in the linear conjugative organic polymer conductors *cis*- and *trans*-polyacetylene $((CH)_x)$ [2]. Second, it is well known that the polaron effect is enhanced by reduced dimensionality [3–6], thus it can be selected as a extreme model to study the polaron physics. Third, due to the simplicity of the mathematics in 1D systems, some essential features of polarons and bipolarons in 1D could be clearly exhibited [7–13], which could supply a qualitative estimation for the polaron in more than one dimension.

In the modern literature, numerous investigations were devoted to the properties of static polarons. However, to our knowledge, only a little work [14–16] had been done about the dynamics of polarons in motion, which is also of great theoretical and practical importance. It is well known that the wave function and the energy-momentum relation of moving polarons are the fundamental ones in the calculation of the S-matrix in the scattering theory, which had been further developed to be the very famous Chew-Low scattering theory in fundamental particle physics [17]. In addition, the properties of dynamics of polarons have a close relation with the experimentally accessible quantities like the drift velocity, the Hall factor, and the mobility.

The aim of the present paper is to extensively study the properties of 1D moving polarons at zero temperature. The Hamiltonian selected in this paper is just that of the usual free one-dimensional polaron which has been used by many authors [7–13]. Within the framework of our earlier effective approach [9,18], where the phonon state is taken to be the extended coherent state, we can present a detailed investigation of the general properties of 1D moving polarons, such as the dependencies of the polaron energy, effective mass, velocity, the virtual phonon number, and the distribution of the phonon density on the polaron momentum in the intermediate-coupling regime. Self-consistent analyses of the obtained results are also presented.

2 General formalism of two-phonon correlation

Of the various intermediate-coupling polaron theories, except the Feynman path integral method and its extensions, most of them were developed on the basis of the pioneering work by Lee, Low, and Pines (LLP) [19], as does our previous scheme in this field [9,18]. Below we shall briefly summarize the main elements of our generalized method and refer the reader to reference [9] for the details.

The Hamiltonian large 1D Fröhlich polaron is given by [7–13]:

$$H = \frac{1}{2m}p^2 + \sum_q \hbar\omega_0 a_q^{\dagger} a_q + \sum_q v(a_q e^{iqx} + a_q^{\dagger} e^{-iqx}),$$
$$v = \hbar\omega_0 \left(\frac{\hbar}{2m\omega_0}\right)^{\frac{1}{2}} \left(\frac{2\alpha}{L}\right)^{\frac{1}{2}} \tag{1}$$

where m is the electron band mass, ω_0 is the frequency of the LO phonons, a_q^{\dagger} and a_q are respectively the creation

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and annihilation operators of the LO phonons with the wave vector q, and L is the length of the crystal lattice. Here the coupling constant α is equivalent to $\alpha' = \lim_{n \to 1} \frac{\alpha}{n-1}$ (α is the standard dimensionless electron-phonon coupling constant) in reference [8]. In doing so we can get the finite values of some observables such as energy and mass for finite value of α . The coupling constant α_{op} defined in reference [7] is equal to $\alpha/2\pi$ in the present paper.

First, performing the well-known LLP transformation [19] to the Hamiltonian (1), we have the following expression for the Hamiltonian in units of $2m = \hbar = \omega_0 = 1$

$$H = (Q - \sum_{q} q a_{q}^{\dagger} a_{q})^{2} + \sum_{q} a_{q}^{\dagger} a_{q} + \sum_{q} v (a_{q}^{\dagger} + a_{q}),$$
$$v = \sqrt{\frac{2\alpha}{L}}$$
(2)

where Q is the egenvalues of the total polaron momentum $\prod = p + \sum_{q} q a_{q}^{\dagger} a_{q}$. It is conserved and regarded as a cnumber, since the Hamiltonian is translationally invariant. For convenience we write Hamiltonian (2) in the following form

$$H = Q^{2} + \sum_{q} (1 - 2Qq + q^{2})a_{q}^{\dagger}a_{q} + \sum_{q} v(a_{q}^{\dagger} + a_{q}) + \sum_{q_{1},q_{2}} q_{1}q_{2}a_{q_{1}}^{\dagger}a_{q_{2}}^{\dagger}a_{q_{1}}a_{q_{2}},$$
(3)

here are only the creation and annihilation operators of phonons and the polaron momentum Q. The last term is the recoil term.

Next, we take the wave function of phonons in the new representation as the following extended coherent state form, straightforwardly [9]

$$\begin{aligned} |\rangle &= |\rangle_{0} + \sum_{q_{1},q_{2}} b_{2}(q_{1},q_{2}) a_{q_{1}}^{\dagger} a_{q_{2}}^{\dagger} |\rangle_{0}, \\ |\rangle_{0} &= \prod_{q'} e^{\alpha(q')a_{q'}^{\dagger}} | 0 \rangle, \\ q &|\rangle_{0} = \alpha(q) |\rangle_{0}, \end{aligned}$$
(4)

where $| 0 \rangle$ is the phonon vacuum state, $b_2(q_1, q_2)$ is the interchanging symmetrical function of q_1 and q_2 . It is implied that the correlation between wave vectors of two subsequently emitted phonons is under consideration in equation (4). Substitution of equation (4) into Schrödinger equation $H | \rangle = E | \rangle$, followed by collecting together the terms in (a^{\dagger}) , $(a^{\dagger})^1$, and $(a^{\dagger})^2$, and neglecting $(a^{\dagger})^3 | \rangle_0$ and $(a^{\dagger})^4 | \rangle_0$ -terms produces

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$$\begin{split} E(1 + \sum_{q_1,q_2} b_2(q_1,q_2) a_{q_1}^{\dagger} a_{q_2}^{\dagger}) \mid \rangle_0 &= \\ Q^2(1 + \sum_{q_1,q_2} b_2(q_1,q_2) a_{q_1}^{\dagger} a_{q_2}^{\dagger}) \mid \rangle_0 \\ &+ \sum_{q} v \alpha(q) \mid \rangle_0 + \sum_{q} [(1 - 2Qq + q^2)\alpha(q) \\ &+ v + 2 \sum_{q'} b_2(q',q) v] a_{q}^{\dagger}) \mid \rangle_0 \end{split}$$

$$+\sum_{q_1,q_2} \left\{ \sum_{q} v\alpha(q)b_2(q_1,q_2) + q_1q_2\alpha(q_1)\alpha(q_2) + [2 - 2Q(q_1 + q_2) + q_1^2 + q_2^2]b_2(q_1,q_2) + 2q_1q_2b_2(q_1,q_2) \right\} a_{q_1}^{\dagger}a_{q_2}^{\dagger} |\rangle_0.$$
(5)

Comparing the coefficients of the terms of $(a^{\dagger})^0 \mid_{0}$, $(a^{\dagger})^1 \mid_{0}$, and $(a^{\dagger})^2 \mid_{0}$ in both sides of equation (5) we have

$$E = \sum_{q} v\alpha(q) + Q^2, \tag{6}$$

$$v + (1 - 2Qq + q^2)\alpha(q) + 2\sum_{q'} vb_2(q', q) = 0, \quad (7)$$

$$\left\{\sum_{q} v\alpha(q) - E + Q^2 + [2 - 2Q(q_1 + q_2) + q_1^2 + q_2^2] + 2q_1q_2\right\} b_2(q_1, q_2) = -q_1q_2\alpha(q_1)\alpha(q_2).$$
(8)

According to equations (6, 8) it can be seen that $b_2(q_1, q_2)$ satisfies

$$b_2(q_1, q_2) = -\frac{q_1 q_2 \alpha(q_1) \alpha(q_2)}{2 - 2Q(q_1 + q_2) + (q_1 + q_2)^2}, \qquad (9)$$

inserting equation (9) into equation (7) we get the selfconsistent equation obeyed by $\alpha(q)$

$$\alpha(q) = -\frac{v}{1 - 2Qq + q^2} + \frac{2}{1 - 2Qq + q^2} \sum_{q'} v' \frac{qq'\alpha(q)\alpha(q')}{2 - 2Q(q + q') + (q + q')^2} \cdot (10)$$

Introducing the function

$$F(q) = \left(\frac{\alpha L}{2\pi^2}\right)^{1/2} \alpha(q), \tag{11}$$

and transforming the summation into an integral, then equations (6, 10) can be respectively simplified to

$$E = \int_{-\infty}^{\infty} F(q)dq + Q^2, \qquad (12)$$

$$F(q) = -\frac{\alpha}{\pi(1 - 2Qq + q^2)} + \frac{2}{1 - 2Qq + q^2} \times \int_{-\infty}^{\infty} dq' \frac{qq'F(q)F(q')}{2 - 2Q(q + q') + (q + q')^2}.$$
 (13)

It can be noticed from equation (12) that F(q) is the distribution function of the 1D polaron energy $E(\alpha, Q)$ in terms of q, and equation (13) is its self-consistent integral equation, which can be solved by the iteration method.

It is recalled from our previous paper [9] that all static polaron observables (Q = 0) obtained by the first two iterations in equation (13) are identical to those within the fourth-order perturbation theory [8]. Moreover, the exact self-consistent calculation of equation (13) yields very good polaron results in the intermediate-coupling regime compared to the very famous path integral ones [7]. It should be pointed out that the 3D polaron energies obtained within this approach [22] are in good agreement with the exact Monte-Carlo ones [20] for a wide coupling range, which should illustrate the high quality of our method in polaron physics.

In the next section, based on the same formulation, setting $Q \neq 0$, we can further study the general properties of moving polarons.

3 Numerical results and discussions

Before performing any numerical calculations, we will show that the non-degenerate perturbation theory, such as the second-order Rayleigh-Schrödinger perturbation theory, gives the wrong results for polarons in $Q \rightarrow 1$ or > 1. Within this method, we can easily obtain

$$E(\alpha, Q) = \int_{-\infty}^{\infty} -\frac{\alpha}{\pi(1 - 2Qq + q^2)} dq + Q^2, \qquad (14)$$

For convenience, we rewrite the above equation as

$$[(E(\alpha, Q) - Q^2]/\alpha = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{1 - Q^2 + x^2} dx, \quad (15)$$

It is found that this integral diverges if $Q \to 1$ or > 1. But this property for $Q \to 1$ or > 1 is not the intrinsic property in the the moving problem of large polarons, which had been well demonstrated in reference [15] for the 3D polaron and in reference [16] for the 2D polaron. In references [15,16], the authors had shown that for $Q \to 1$ or Q > 1 one has to use degenerate perturbation theory, such as Wigner-Brillion perturbation theory, to obtain the correct energy momentum relation. Their remarks are also true for the 1D polarons. Therefore, all the results in the present paper, which can cover those by the second-order Rayleigh-Schrödinger perturbation theory, should be restricted to Q < 1. The problem of moving 1D polarons for $Q \to 1$ or > 1 will be attempted by Wigner-Brillion perturbation theory in a forthcoming paper.

We will present some numerical results to discuss the behavior of the distribution of phonon number, total phonon momentum, the average of virtual phonon numbers, polaron energy, velocity, and effective mass with nonzero polaron momentum in a wide coupling range.

3.1 Distribution of phonon density

Given values of coupling constants is α and Q, solving for equation (13), we can determine the phonon wave function (4) by means of equations (9, 11), then, the distribution of the density of the phonon number (DPN) in terms of the phonon momentum q can be calculated by

$$n(q) = \frac{\langle \mid a_q^{\dagger} a_q \mid \rangle}{\langle \mid \rangle}$$
(16)



Fig. 1. The density of phonon number n(q) as a function of the phonon momentum q with different total polaron momentum Q at coupling constant $\alpha = 1$.

This expression is rather complicated and not presented here. After tedious but straightforward calculation, we display the numerical results in Figures 1 and 2. By the way, for a 1D system, eonly by the abscissa can we readily indicate the phonon momentum vector q.

It is shown in Figure 1 that, for given coupling constant, such as $\alpha = 1.0$, the value of DPN increases with the increase of the total polaron momentum Q if the phonon momentum q is along the Q-direction, and decreases when in the opposite direction. It follows that the phonons emitted by the electron along the moving direction outnumber those in the opposite direction. It is also easily found from each curve that a peak appears around q = Q, and the value of DPN decreases rapidly while away from the peak. This is to say, the contribution to the polaron observables are mainly attributed to the phonons with momentum around Q, although we usually take account of the phonons with all momentum q in the calculation of observables. Besides, the maximum value of DPN increases with Q-value, and the displacement is approximately proportional to Q for all Q-values.

From Figure 2, it can be seen that, for a given polaron total momentum, such as Q = 0.2, the value of DPN increases with the increasing coupling constant α for all phonon momentum q, and the height of the peak for DPN is approximately proportional to α for all α -values. It is physically reasonable, because the enhancement of the electron-phonon coupling results in many more virtual phonons emitted by the electron.

It is of some interest to note from both Figures 1 and 2 that for the most part phonons are in the momentum regime $|q - Q| \leq 2$, and are only weakly sensitive to the modulation of α and Q.



Fig. 2. The density of phonon number n(q) as a function of the phonon momentum q with different coupling constant α at total polaron momentum Q = 0.2.



Fig. 3. The phonon momentum P_T vs. the total polaron momentum Q relation with $\alpha = 0.5$ and 1, respectively.

3.2 Total phonon momentum

By means of the results for n(q) obtained in equation (16), the total phonon momentum can be readily calculated by

$$P_T = \sum_q qn(q). \tag{17}$$

In Figure 3 we present the total polaron momentum dependence of the total phonon momentum P_T with different coupling constant α . It is clear that the P_T increases with Q and α . All curves of P_T versus Q for a given α show a nonlinear behavior. According to the relation $P_T + P_e = Q$ where P_e refer to the momentum of the electron, it is learned that as the Q or α increases, the proportion of the



Fig. 4. The dependence of the total average number of virtual phonons N on total polaron momentum Q with different coupling constants α .

phonon momentum occupied in the total polaron momentum increases gradually.

3.3 Average number of virtual phonons

The average number of virtual phonons can be calculated by the formulae $N = \sum_{q} n(q)$. Alternatively, it can also be obtained from the energy $E(\alpha, Q)$ directly,

$$N = \left(1 - \frac{3}{2}\alpha \frac{\partial}{\partial \alpha} - \frac{1}{2}Q \frac{\partial}{\partial Q}\right) E(\alpha, Q)$$
(18)

which has ever been proved exactly in reference [21]. The latter method is more concise than the former one, and is employed in the present calculation.

We exhibit the numerical results in Figure 4. For a given coupling constant, it is demonstrated that N increases with Q in a nonlinear way. This tendancy is much more evident with larger α .

It is very necessary, by Figure 4, to link the average number of virtual phonons in the phonon field with the valid range of our method, where only two-phonon correlations are taken into account.

From the highest curve, we find that when $\alpha = 2.0$, the total phonon number N is greater than 2 for all Q, so the present method where only two-phonon correlations are taken into account fails to describe this system, and a improved state where correlations among wave vectors of more than 2 phonons in the field are under consideration should be proposed; this is not attempted here. Thus we should restrict the following discussion of the energy, velocity, and effective mass up to $\alpha = 1.5$. Even for $\alpha = 1.5$, from the second higher curve, one can see the value of N becomes greater than 2 when Q > 0.6, therefore our



Fig. 5. The dependence of the polaron energy $E(\alpha, Q)$ on the total momentum Q with different coupling constants α (the corresponding $E(\alpha, Q) - Q^2$ vs. Q relations are indicated by dashed lines).

method can not yield reasonable results for Q > 0.6 either. If one really wishes to study some observables in the region of Q > 0.6, one might find that the calculated results deviate drastically from the common tendancy and diverge rapidly.

3.4 Polaron energy

By means of equations (12, 13), the dependence of the polaron energy on the polaron total momentum with different coupling constants are plotted in Figure 5. It is shown from all the curves that the energy only increases slightly with increasing Q, in a nonparabolic way. Although the polaron kinetic energy considerably increases with Q as Q^2 , the decrease of the electron-phonon coupling energy caused by the resultant increase of the total phonon number will depress this effect in the total energy, and keep the energy almost unchanged with Q. This point can also be clearly demonstrated in the following quantitative analysis.

It is known that the energy for Fröhlich optical polarons in the intermediate-coupling regime can be expanded in powers of α [22]. From equations (12, 13), we can obtain the energy expansion analytically as

$$E(\alpha, Q) = Q^2 + \sum_{i=1}^{\infty} E_i(Q)\alpha^i$$
(19)

where $E_i(Q)$ is independent of α . The coefficient of the leading term $E_1(Q)$ is just identical to the left-hand side of equation (15). It is evident that $E_1(Q)$ decreases with increasing Q, and then it will offset the increasing polaron



Fig. 6. The total momentum Q dependence of two coefficients $E_1(Q)$ and $E_2(Q)$ in the energy expansion.

kinetic energy Q^2 to a considerable degree. The numerical results for $E_1(Q)$ are displayed in Figure 6.

In principle, we can also get the expansions of the energy including all subsequent terms. But only the coefficient $E_2(Q)$ of α^2 -terms is exactly calculated, as had been proven in our previous paper [9]. Here, we also present the numerical results for $E_2(Q)$ in Figure 6. It is very interesting to note that $E_2(Q)$ increases smoothly with Q, in contrary to the behavior of the Q-dependence of $E_1(Q)$. This is to say, the energy originated from the recoil term increases with the total polaron momentum. We have also found that the coefficients of terms after the α^2 -term display a similar behavior. Although these coefficients are incompletely calculated, it is to expected that their unknown exact results will show similar features because they are all originated from the recoil term. However, all these coefficients of the terms after the leading term in the energy expansions are, at least, two orders of magnitude smaller than that of the leading term, so they do not play an important role in modifying the E(Q) behavior.

We can also explain the reason that the E(Q) curves in Figure 5 are truncated at a critical value of Q_c , which is smaller than 1. According to equation (19), for a given α , whether this series converges or not depends on the Qdependence of the coefficient of $E_i(Q)$. It is observed in Figure 6 that although $E_2(Q)$ is considerably smaller than $E_1(Q)$ for a wide region of Q values, it diverges before the divergence of $E_1(Q)$ in larger Q values. Similar discussions may also be suited for higher-order coefficients. So in practical calculations, beyond a critical value of Q_c , the results based on solving equations (12, 13) deviate drastically from the common tendance and diverge rapidly. The decrease of the critical value of Q_c with the larger α can be naturally explained by equation (19). This analysis is also consistent with the discussions of the total phonon number in Section 3.3.

In Figure 5, we have also presented the curves of $E(\alpha, Q) - Q^2$ versus Q. It is learned from the two groups of curves that two inequalities $E(\alpha, Q = 0) < E(\alpha, Q \neq 0)$ and $E(\alpha, Q \neq 0) - Q^2 < E(\alpha, Q = 0)$ are always met. These are just two theorems proved by Gerlach *et al.* [23] (note the unit m = 1 in Ref. [19] and the unit m = 2 in this paper). It follows that our treatment is trully convincing and reliable.

3.5 Velocity and effective mass

In order to study the dynamics of the 1D polarons in motion, it is also significant to evaluate the polaron velocity and the effective mass as a function of the momentum Q. The definition of polaron velocity is given by [16]

$$V(Q) = \frac{\partial E}{\partial Q}.$$
 (20)

Figure 7 indicates these numerical results. It is learned form this figure that for a given polaron momentum, the velocity decreases with the coupling constant. This is physically reasonable, because the enhancement of the electron and lattice interaction will hinder the motion of the polarons. This tendancy may hint at a localization of polarons in the strong-coupling regime, which, however, is beyond the scope of the present intermediatecoupling theory. More interestingly, we find that the velocity monotonously increases with the total polaron momentum in $\alpha = 0.5$ and 1.0 curves, and a non-monotonous behavior is clearly shown in the lowest curve for $\alpha = 1.5$. Thus it is safe to say that the velocity grows more slowly with larger Q, if not decreasing. Generally, the polaron velocity should increase with Q for fixed α . On the other hand, the average number of virtual phonons does also increase with increasing Q, as stated before, then the electron-phonon coupling becomes enhanced, this effect may depress the trend of the velocity to increase. This may account for the downward trend of the curves for $\alpha = 0.5$ and 1.0. Especially for relatively a large coupling constant, say $\alpha = 1.5$, this effect is substantially strengthened and results in the decline of the velocity with larger Q-value as shown in Figure 7. In addition, the nonlinearity of the velocity-momentum relation clearly exhibits a nonparabolic dependence of the energy on the momentum.

The polaron effective mass $m^*(Q)$ can be obtained with the uses of the polaron velocity

$$m^*(Q) = \frac{2Q}{V(Q)}$$
 (2m = 1). (21)

The numerical results are presented in Figure 8. One may find that $m^*(Q)$ increases with the total polaron momentum, and this trend is more pronounced with larger α . It is consistent with the fact that the increase of α and Qleads to the increase of the total phonon numbers, which in turn raise the effective mass.



Fig. 7. The dependence of the polaron velocity V(Q) on the total momentum Q with different coupling constants α .



Fig. 8. The dependence of the polaron effective mass $m^*(Q)$ on the total momentum Q with different coupling constants α .

4 Conclusions

The previous effective method to static polarons is successfully generalized to study the dynamics of 1D polarons. As a result, we have obtained some properties of moving polarons, such as the distribution of the density of phonon numbers, the total phonon momentum, the total phonon number, the ground-state energy, the velocity, and the effective mass. The main results are listed as follows.

1 The phonons emitted by the electron along the polaron moving direction outnumber those in the opposite direction. The maximum value of DPN appears around q = Q, and away from the peak the value of DPN decreases rapidly. In addition, the value of DPN increases with larger α .

- 2 The proportion of the phonon momentum occupied in the polaron total momentum increases with α and Q.
- 3 The total phonon number increases with the momentum Q, which is more evident with larger coupling constant. This quantity can act as a criterion to judge the range of validity of the present method.
- 4 The energy increases slightly with increasing Q in a nonparabolic way. Moreover, two inequalities proved by Gerlach *et al.* [23] are readily checked in our numerical calculations. Alternatively, the coefficient of the α^2 -term in the energy expansion increases smoothly with Q, just contrarily to that of the leading term.
- 5 For given polaron momentum, the polaron velocity V(Q) decreases with the coupling constant, and for given coupling constant, the polaron velocity grows more slowly with larger Q, if not decreasing.
- 6 The effective mass of moving polarons $m^*(Q)$ increases with the total momentum Q, and this trend is more pronounced with larger α .

It should be stressed that the above conclusions are completely self-consistent. Compared to the famous theorem by Gerlach *et al.*, we can say that our treatment is effective and reliable. By the way, if setting Q=0, all the results for static 1D polarons can be recovered. So we believe our results within the present scheme are reliable in both the weak- and intermediate-coupling regimes. The comparison to other approaches can not be made in the present paper owing to the fact the investigations on 1D moving polarons are still lacking to date. To the best of our knowledge, we study, for the first time, the 1D moving polarons and clearly present some intrinsic features, which may also be suited to describe moving polarons in more than one dimension.

Finally, we would like to point out that the present paper is only intended to preliminarily obtain some essential features of moving polarons within a simple but well-used model in a theoretical sense. Hamiltonian (1)in this paper is too simple to represent real quasi-onedimensional systems, such as polarons in quantum wire, where the confining potential should be presented, several existing sub-bands should be discussed, and the two bulk confining phonon modes as well as two interface phonon modes should be considered. The extensions to this more realistic system will be presented in a forthcoming paper. On the other hand, if we neglect the inter-band transition and only take bulk-phonon approximation (*i.e.* neglecting the coupling of the electron to other phonon modes), the Hamiltonian of polarons in a quantum wire with symmetrical potential may be approximately mapped into

Hamiltonian (1) used in this paper, due to the fact that this system is of axial symmetry (we take the wire direction as the axis). Then, in our opinion, the general properties of moving polarons in such a system are not essentially different from those obtained in the present paper in some aspects.

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