Dynamics of an Acoustic Polaron in One-Dimensional Electron-Lattice System

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The dynamical behavior of an acoustic polaron in typical non-degenerate conjugated polymer, polydiacetylene, is numerically studied by using Su-Schrieffer-Heeger’s model for the one dimensional electron-lattice system. It is confirmed that the velocity of a polaron accelerated by a constant electric field shows a saturation to a velocity close to the sound velocity of the system, and that the width of a moving polaron decreases as a monotonic function of the velocity tending to zero at the saturation velocity. The effective mass of a polaron is estimated to be about one hundred times as heavy as the bare electron mass. Furthermore the linear mode analysis in the presence of a polaron is carried out, leading to the conclusion that there is only one localized mode, i.e. the translational mode. This is confirmed also from the phase shift of extended modes. There is no localized mode corresponding to the amplitude mode in the case of the soliton in polyacetylene. Nevertheless the width of a moving polaron shows small oscillations in time. This is found to be related to the lowest odd symmetry extended mode and to be due to the finite size effect.

Keywords: acoustic polaron, polydiacetylene, SSH model, saturation of velocity, Levinson’s theorem
1 Introduction

Polydiacetylene (PDA) is one of typical quasi-one-dimensional materials, which can exist as perfect single crystals with parallel straight chains of polymers separated by a rather long distance (\(\sim 0.7\) nm). About one and a half decades ago, Donovan and Wilson [1] studied experimentally the dynamical properties of excess charges created by photo-excitation. What they found was unexpectedly interesting: the excess charges have very high mobility larger than \(20 m^2s^{-1}V^{-1}\), yet their velocity is a constant of about half of the sound velocity for the field range \(10^2\text{–}10^6\) \(Vm^{-1}\). Wilson [2] later proposed the transport mechanism due to an acoustic polaron in order to explain these experimental facts. He discussed the dynamics of the acoustic polaron in terms of Su-Schrieffer-Heeger’s (SSH) model. [3] The acoustic polaron is created as the ground state when there is one electron in the conduction band. The electron is trapped by the local lattice distortion which is introduced by the presence of the electron itself. The electronic state and the lattice distortion are determined by solving a self-consistent equation. Wilson solved this self-consistent equation analytically within the continuum approximation for the SSH model. In solving the equation for a moving polaron, he assumed the space and time dependence of the lattice distortion and/or the electronic wave function could be described in terms of \(x - vt\) with \(v\) the velocity of the polaron. Wilson’s solution indicates that the velocity shows a saturation at the sound velocity of the system, that the total energy diverges as a function of the velocity at the saturation velocity, and that the polaron width decreases with increasing velocity and vanishes at the saturation velocity. These results are consistent with the experimental ones by Donovan and Wilson.

Recently Ono and co-workers [4, 5, 6, 7] have developed a method of a numerical simulation to study the dynamics of a soliton in polyacetylene (PA). In this formulation, we prepare the state bearing a soliton by numerically calculating the lattice distortions and the electronic wave functions by solving a set of self-consistent equations derived from the condition of minimizing the total energy of the system and the soliton is accelerated by a physical force. Therefore we need not employ any assumption about the functional shape of a moving soliton. The time development of the lattice distortions and the electronic wave functions are obtained by solving the equation of motion and the time-dependent Schrödinger equation. Application of this method to the dynamics of an acoustic polaron is straightforward. It will be worthwhile to study the dynamics of the acoustic polaron in the light of this method.

We have learned from the studies of dynamical behaviors of solitons and polarons in PA that the linear mode analysis is quite useful to understand the dynamics of such nonlinear localized excitations. [8, 9, 10, 11, 12, 13] In the present paper, we also carry out the linear mode analysis in the presence of an acoustic polaron and discuss the relation of the linear vibrational modes and the behaviors of a moving polaron. In the case of the solitons and polarons in PA, where they are related to the optical lattice vibrations due to the fact that the electrons are half-filling the \(\pi\)-band, the number of localized modes and the phase shift of the extended modes in the limit of vanishing wave number are related just as in Levinson’s theorem for the one-dimensional Schrödinger equation. [14, 15, 16] It will be discussed whether such an analogy is valid in the case of the acoustic polaron.

In the following section, the model and the method of calculation are briefly described.
The results of simulations are presented in § 3. In § 4, the results of the linear mode analysis are explained and particularly the relation between the number of localized modes and the behavior of the phase shift of extended modes is discussed. The role of linear modes in the dynamics of the polaron is considered. We present concluding remarks and discussions in the final section.

2 Model and Method of Calculation

Although we are bearing in mind the non-degenerate conjugated polymer, PDA, we employ the SSH model which is widely used in studying the degenerate conjugated polymer PA. This will be allowed since we are treating a single carrier excited in the bottom region of the conduction band. PDA has a much more complicated chemical structure than PA, but such details will not matter in discussing the basic dynamics of an acoustic polaron.

The SSH model Hamiltonian is expressed as follows,

\[ H_{\text{SSH}} = H_{\text{ele}} + H_{\text{lat}}, \]  

\[ H_{\text{ele}} = -\sum_n \left( t_0 - \alpha y_n \right) \left[ e^{i\gamma A} c_{n+1}^+ c_n + e^{-i\gamma A} c_{n+1} c_n \right], \]  

\[ H_{\text{lat}} = \frac{K}{2} \sum_n y_n^2 + \frac{M}{2} \sum_n u_n^2, \]

where \( y_n \equiv u_{n+1} - u_n \) and \( \gamma = ea/\hbar c \) with \( u_n \) the displacement of the \( n \)-th site, \( a \) the lattice constant, \( e \) the absolute value of the electronic charge and \( c \) the light velocity. The field operators \( c_n^+ \) and \( c_n \) annihilate and create an electron on the \( n \)-th site; the spin index is omitted since we consider single electron problem. \( K \) is the force constant mainly due to the \( \sigma \)-bond, \( M \) the mass of a unit cell, \( t_0 \) the nearest neighbor transfer integral of a \( \pi \)-electron, and \( \alpha \) the electron-lattice coupling constant. Here we have introduced similarly as in ref. [4] a time dependent vector potential \( A \) which is related to a uniform electric field \( E \) as \( E = -\dot{A}/c \).

The standard values of parameters accepted generally for PDA [3] are \( t_0 = 0.64\text{eV}, K = 2.4\text{eV}/\AA^2, e = 0.38\text{eV}/\AA \text{and} a = 4.9\AA \). In this paper we basically use these values as far as we do not mention other values. For these values of parameters, the bare optical phonon frequency \( \omega_Q = \sqrt{4K/M} \) is equal to \( 1.47 \times 10^{13} \text{sec}^{-1} \) and the sound velocity \( v_s (= \omega_Q a/2) = 3.6 \times 10^5 \text{cm/sec} \). In the following, the time is scaled by \( \omega_Q^{-1} \), the velocity by \( v_s \) and the length by \( a \). It is most convenient to scale the strength of the field by

\[ E_0 \equiv \frac{\hbar \omega_Q}{ea}, \]

which is equal to \( 2.0 \times 10^5 \text{V/cm} \) for the aforementioned parameter values. Throughout the paper we assume the periodic boundary condition in order to avoid the end-point effects.

The static polaron solution is determined by solving the self-consistent equation for the bond variable \( y_n \) derived so as to minimize the total energy of the system in the absence
of the external field;
\[ y_n = -\frac{2\alpha}{K} \psi(n + 1)\psi(n) + \frac{2\alpha}{NK} \sum_{n'} \psi(n' + 1)\psi(n'), \]  
(5)

where \( \psi \) is the electronic ground state wave function for the Hamiltonian \( H_{\text{ele}} \) (with \( A = 0 \)) which involves bond variables \( \{y_n\} \). The second term on the right hand side is introduced in order to certify the relation \( \sum_n y_n = 0 \) caused by the periodic boundary condition.

The time evolution of the system in the presence of an external electric field is described by the time-dependent Schrödinger equation for the electronic wave function and the equations of motion for the lattice displacements \( \{u_n\} \). The former is written as
\[
\text{i} \hbar \frac{\partial}{\partial t} \psi(n, t) = -(t_0 - \alpha y_n)e^{i\gamma_A}\psi(n + 1, t) - (t_0 - \alpha y_{n-1})e^{-i\gamma_A}\psi(n - 1, t),
\]  
(6)

while the latter is expressed as
\[
M \frac{d^2 u_n}{dt^2} = -\frac{\partial}{\partial u_n} \left\{ \varepsilon_{\text{ele}}(\{y_n\}) + \frac{K}{2} \sum_{n'} y_{n'}^2 \right\},
\]  
(7)

where \( \varepsilon_{\text{ele}}(\{y_n\}) \) represents the electronic energy which is treated as a Born-Oppenheimer type adiabatic potential for the lattice motion.

The time dependent Schrödinger equation is solved by using the fractal path integral method. \cite{15, 16} The Hamiltonian matrix is divided into two parts, one of which involves only the transfer processes between \((2n - 1)\)-th and \(2n\)-th sites with \(n\) an arbitrary natural number and the other only those between \(2n\)-th and \((2n + 1)\)-th sites. As the fractal path integral formula, we adopt the simplest one which is correct up to the second order of the time mesh \( \Delta t \) for the numerical simulation, which is chosen to be sufficiently small compared to the characteristic time of the lattice vibration, \( \omega_Q^{-1} \). The electric field is slowly switched on and off with a certain duration time \( \tau \) in order to avoid disturbances due to sudden switching. \cite{5, 17} The details of the time dependence of the field are described in ref. \cite{4}.

3 Results of Numerical Simulations

The spatial structure of the static acoustic polaron is shown in Fig. \cite{4}, where the total number of the lattice sites is \( N = 200 \); the top is the electron density \( \rho_n = |\psi(n)|^2 \), the middle the lattice displacement \( u_n \), the bottom the bond variable \( y_n \) and the abscissa of all the figures being the site number \( n \). The center of the polaron is chosen to be at \( n = 100 \). Furthermore the center of mass of the lattice system is fixed at the same point; this is allowed because of the translational invariance of the SSH Hamiltonian. Note that the bond variable \( y_n \) takes a finite (non-vanishing) value even in the region far from the polaron center. This is due to the finiteness of the system size and the periodic boundary condition. This is reflected also in the behavior of the lattice displacement \( u_n \) which has
Figure 1: The spatial structure of an acoustic polaron obtained in a finite chain of the SSH model with periodic boundary condition. The electron density $\rho_n$ (the top), the lattice displacement $u_n$ (the middle) and the bond variable $y_n$ (the bottom) are plotted as functions of the site number $n$. The total number of sites is $N = 200$ and the values of parameters are given above eq. (2.4). $u_n$ and $y_n$ are both scaled by the lattice constant $a$.

Figure 2: The time dependence of the polaron velocity $v_p$ obtained from the electron density (the upper graph) and from the bond variable (the lower graph). The system size is $N = 200$ and the field strength is $0.005E_0$, which is slowly switched on with a duration time $200\omega^{-1}_Q$. The horizontal dashed line indicates the saturation velocity.

a finite slope in the region far from the polaron. Apart from this finite size effect, the behaviors of $u_n$ and $y_n$ are in good agreement with the analytic result by Wilson [2] in the continuum limit. The half width of the polaron is about 20 times the lattice constant. The charge density is well localized within the polaron width.

In the following we show mainly the results of numerical simulations where the acoustic polaron shown in Fig. 1 is accelerated by an electric field with strength $0.005E_0$. The time mesh $\Delta t$ is chosen to be $0.0025\omega^{-1}_Q$ and the duration time of switching-on is set to be $200\omega^{-1}_Q$.

3.1 Saturation of velocity

The velocity of the polaron is calculated from the time dependence of the center of mass, which can be obtained by regarding the electron density or the bond variable [18] as the probability weight for the position. Details on how to calculate the center of mass are described in ref. [4]. The velocity of the polaron shows saturation if we continue to apply the electric field, similarly as in the case of the soliton in PA. An example is depicted in Fig. 2 where the polaron velocity $v_p$ scaled by the sound velocity $v_s$ is given as a function of the time scaled by $\omega^{-1}_Q$; the upper graph is obtained from the electron density and the lower from the bond variable. The dashed line indicates the saturation velocity which is numerically estimated in the following way.

In order to estimate the saturation velocity we fit the numerical data to the following form,

$$v_p(t) = v_{sat} - v_0 \exp(-t/T_{sat}),$$

for the time interval $6 \times 10^3 < t\omega_Q < 11 \times 10^3$. The best fit curve is given by a thin line in Fig. 2. The data for the small $t$ region are not used since they would not fit to eq. (8), and those for very large $t$ region are also not used because of disturbances which may be due to excitations of vibrational modes created by the motion of the polaron. From this fitting, we obtain $v_{sat} = 0.90v_s$, $T_{sat} = 7.0 \times 10^3\omega^{-1}_Q$ for the upper graph of Fig. 2 and $v_{sat} = 0.87v_s$, $T_{sat} = 4.0 \times 10^3\omega^{-1}_Q$ for the lower graph. According to the analytic work by Wilson [2] and the semi-phenomenological treatment by Kuwabara et al., [19] the saturation velocity should be equal to $v_s$. The present simulation has given a smaller value. The reason will be discussed later. We have carried out similar simulations for different values of the electric...
Figure 3: The time dependence of the polaron width $\xi_{\text{ch}}$ obtained from the electron density profile and $\xi_{\text{lat}}$ obtained from the bond variable. Both are scaled by their static initial values. Data are taken from the simulation giving Fig. 2. Note that $\xi_{\text{lat}}$ is not well-defined for large values of $t$ because of lattice vibrational modes excited due to the motion of the polaron.

Figure 4: The velocity dependence of the polaron width obtained by combining Fig. 2 and Fig. 3. The upper graph is obtained from the electron density, and the lower from the bond variable.

Field strength (the same duration time) and confirmed that $v_{\text{sat}}$ is almost independent of the strength of the applied field. On the other hand, the saturation time $T_{\text{sat}}$ is found to depend linearly on the logarithm of the field strength, similarly as in the case of the soliton. [4]

3.2 Width of polaron

The width of the polaron can be estimated from the variance of the distribution function of the position which is given by the electron density or by the bond variable. [5] We denote the polaron width obtained from the electron density by $\xi_{\text{ch}}$ and that from the bond variable by $\xi_{\text{lat}}$. [20] The results of simulations are summarized in Fig. 3 where the width scaled by its initial (static) value is given as a function of time. The relative changes of the widths obtained from the electron density and from the bond variable are almost the same in contrast to the case of the soliton in PA where the relative change of the width obtained from the excess charge distribution was about a half of that obtained from the bond order parameter. [5] Since we have calculated both the velocity and the width as functions of time, it is possible to eliminate the time and express the width as a function of velocity. The results are given in Fig. 4. Both of $\xi_{\text{ch}}$ and $\xi_{\text{lat}}$ look to decrease to zero at the sound velocity, which is consistent with the analytical results. [2] [19]

3.3 Energy and effective mass

The energy of the system shows also an anomalous behavior when the polaron velocity approaches the sound velocity. The electronic energy decreases with increasing polaron velocity. This is consistent with the behavior of the width, which is a decreasing function of the velocity as seen in Fig. 4. The narrower the width, the deeper the effective potential felt by the electron and as a result the binding energy can be increased, which leads to the decrease of the electronic energy. This fact indicates that the polaron becomes more stable when it moves, at least from the electronic point of view. In contrast to the electronic energy, the lattice energy (the sum of the lattice potential and kinetic energies) increases with increasing velocity due to the increase of the lattice kinetic energy and the increase of the lattice deformations. The total energy of the system looks to diverge when the velocity is increased towards the saturation velocity.
Figure 5: The velocity dependences of various energies obtained from the simulation giving Fig. 2 and Fig. 3. The electronic energy \( \varepsilon_{\text{ele}} \), the lattice potential energy \( \varepsilon_{\text{lp}} \), the lattice kinetic energy \( \varepsilon_{\text{lk}} \) and the total energy \( \varepsilon_{\text{tot}} \) are plotted as functions of the polaron velocity \( v_p \) determined from the electron density; only the differences from the static values are given. Inset is \( \varepsilon_{\text{tot}} \) in the small \( v_p \) region, the dashed curve being the best fit in the region \( v_p / v_s < 0.5 \) to the sixth order polynomial; the coefficient of the quadratic term is proportional to the effective mass of the polaron.

Similarly as in the previous subsection, we can derive the relation between the energy and the velocity from the time dependences of the two quantities. The velocity dependences of the electronic energy \( \varepsilon_{\text{ele}} \), the lattice potential energy \( \varepsilon_{\text{lp}} \), the lattice kinetic energy \( \varepsilon_{\text{lk}} \) and the total energy \( \varepsilon_{\text{tot}} \) are shown in Fig. 5 where the difference from the static values are given as functions of the velocity calculated from the electron density. The lattice potential and kinetic energies correspond to the first and the second terms of eq. (3), respectively. According to the analytic works, \( \varepsilon_{\text{lp}} \) and \( \varepsilon_{\text{lk}} \) diverge as \( (v_s - v_p)^{-3} \) when \( v_p \) approaches \( v_s \), while \( |\varepsilon_{\text{ele}}| \) diverges as \( (v_s - v_p)^{-2} \). Therefore the total energy behaves as \( (v_s - v_p)^{-3} \) when \( v_p \) tends to \( v_s \). The overall behaviors of energies as functions of velocity are quite well described by these analytic predictions as discussed in ref. [19].

We can also estimate the effective mass of the polaron from the velocity dependence of the total energy. As shown in the inset of Fig. 5 we have made a fitting of the data for \( v_p / v_s < 0.5 \) to the form,

\[
\varepsilon_{\text{tot}} = \frac{m_p v_s^2}{2} \left( \frac{v_p}{v_s} \right)^2 + C_4 \left( \frac{v_p}{v_s} \right)^4 + C_6 \left( \frac{v_p}{v_s} \right)^6.
\]  

In this expression, \( m_p \) has a meaning as the effective mass of the polaron. From the least square fitting we obtain \( m_p = 1.0 \times 10^2 m_e \) where \( m_e \) is the bare electron mass. This value agrees quite well with what is expected from the analytic calculations. [2] [19] This rather heavy mass should be compared with the rather light effective mass of the soliton in PA which is \( 3 \sim 4m_e \). [3] [4] The main reason of this difference will be due to the large difference in the mass of an ion unit for one lattice site, although the effective mass of the localized nonlinear excitation such as the soliton in PA or the acoustic polaron treated here is not directly related to the mass of the ion unit. It would be worthwhile to note that the value of the transfer integral \( t_0 \) used in the present calculation is much smaller than that used in the similar calculations in PA; the latter is about four times larger than the former. This may be one of the reasons of the large difference in the effective masses of the present acoustic polaron in PDA and the soliton in PA.

4 Linear Mode Analysis

Linear modes around an acoustic polaron can be obtained similarly as those around a soliton or a polaron in PA. [8] [9] [11] [12] The explicit formulation for the linear mode analysis in the case of the SSH model has been precisely described in ref. [12]. Therefore we do not state it again here and express only the results for the case with \( N = 200 \).
In the following, the linear modes represent small deviations of the lattice displacements \( \{u_n\} \) from their static values in the presence of an acoustic polaron.

In the linear mode analysis, we obtain two degenerate zero-frequency modes; one is a uniform mode which exists in any case because of the translational invariance of the original Hamiltonian and the other is a so-called Goldstone mode which describes the translational motion of the acoustic polaron. The latter is shown in Fig. 6. It has an essentially localized character, although it has a finite flat value in the region far from the polaron because of the finite size effect discussed in the previous section. In fact we have confirmed that the finite value outside the polaron region decreases proportionally to the inverse of \( N \) by carrying out similar analyses for different system sizes. The fact that the eigenfrequency of this Goldstone mode is zero means that there is no pinning effect due to the discreteness of the lattice. This may be related to the very high mobility observed for the excess charges created by photo-excitation of PDA.

It is worthwhile to note that we could not find any other localized mode. This is in contrast to the case of the soliton in PA, where there are two more localized modes with optical character other than the Goldstone mode corresponding the translational motion of the soliton. In order to confirm that there is only one localized mode in the case of the acoustic polaron, we have performed the phase shift analysis of the extended modes. Although no direct analogy with the quantum mechanical potential problem is expected in this case, we can get a certain information about the localized mode from the wave number dependence of the phase shift, since it is related to the modification of the density of modes [21] due to the presence of the polaron.

4.1 Phase shift analysis

Extended modes are expressed in the form of plane waves in the region far from the polaron center, since the linear modes of the lattice vibration is affected by the presence of the polaron only in the region near to it. The extended modes with even and odd parity approach asymptotically to the following forms,

\[
g_e(n) = A_e \cos \left[ k \left( n - \frac{N}{2} \right) a + \frac{\delta_e}{2} \right],
\]

\[
g_o(n) = A_o \sin \left[ k \left( n - \frac{N}{2} \right) a + \frac{\delta_o}{2} \right],
\]

on the right hand side of the polaron, where we have chosen the center of the polaron at \( n = N/2 \). Here \( \delta_e \) and \( \delta_o \) are the phase shifts of the extended modes with even and odd parity, respectively. The phase shifts and the wave numbers are calculated through the least square fitting to the above-mentioned function with three parameters in the region \( 3N/4 \leq n \leq N \). In this way we can derive a relation between the phase shift and the wave number. The results are summarized in Fig. 7.
Figure 7: The wave number dependence of the phase shift of the extended modes with even parity $\delta_e$ and odd parity $\delta_o$.

The phase shift for the even parity modes is linearly approaching to $2\pi$ for $k$ tending to zero, while that for the odd parity modes has a maximum as a function of $k$ and decreases to zero as $k$ goes to zero. Levinson’s theorem for one-dimensional Schrödinger equation tells us that the zero limit value of the phase shift is related to the number of localized states as $\delta_e(0) = (2n_e - 1)\pi$ and $\delta_o(0) = 2n_o\pi$ for even and odd parity, respectively, where $n_e$ and $n_o$ represent the number of localized states with even and odd parity, respectively. [14] The present result for $\delta_e$ does not coincide with this. However this is not astonishing, since in the present problem the eigenvalue (=the square of the eigenfrequency) becomes never negative in contrast to the negative eigenenergies of localized states in the Schrödinger equation and since the localized mode in the present problem is strictly localized only in the infinite system and has a character as an extended mode in finite systems. In the linear mode analysis in the case of the soliton or the polaron in PA, the existence of the analogy with the Schrödinger equation was pointed out. [8, 9, 11, 12] The situation there is completely different from the present one, since the reference frequency in that case is the renormalized optical phonon frequency and the frequencies of the localized modes are smaller than this reference frequency. If we regard the Goldstone mode shown in Fig. 8 as an extended mode the behavior of $\delta_e$ near $k = 0$ is quite reasonable, because this mode can be regarded as a uniform extended mode with a phase shift $2\pi$ as is easily seen from Fig. 3. The behavior of $\delta_o$ is consistent with the fact that there is no localized mode with odd parity. It should be noted that phase shifts for even and odd parity coincide with each other for larger values of $k$. This means that the lattice vibrations with larger $k$ suffer reflectionless scatterings from the polaron. [22] This will be important when we consider the interactions between phonons and the acoustic polaron.

We have performed similar phase shift analyses for different values of the coupling constant $\alpha$ in order to check whether the above conclusion can be affected by the change of the coupling constant. The obtained results are qualitatively the same as Fig. 4. In general the stronger coupling pushes up the phase shifts for larger $k$ but does not change the behaviors near $k = 0$. The peak position of $\delta_o$ and the reflectionless region are moved to larger $k$ as the coupling constant increases.

4.2 Amplitude mode

As discussed in the previous subsection we could not find any localized mode with odd parity. This means that there is no amplitude mode which has been confirmed to exist in the case of the soliton or polaron in PA. The amplitude mode would determine the oscillation of the width of the acoustic polaron if any. The lack of the amplitude mode makes us expect that the moving polaron may not show any oscillation of its width. In order to see whether this is the case, we have carried out a simulation where the electric field is switched off at a certain time. [7]

In Fig. 8, the result for $\xi_{lat}$ is depicted. An electric field with a strength $E = 0.002E_0$ is switched on with a duration time $\tau = 125\omega_Q^{-1}$ and switched off with the same duration
Figure 8: The behavior of the polaron width $\xi_{\text{lat}}$ (obtained from the bond variable) after switching off the electric field. The vertical broken line indicates the time at which the field vanishes completely. The strength of the electric field is $0.002E_0$ and the field is switched on and off slowly with a duration time $125\omega_Q^{-1}$; as a result the field vanishes at $t = 250\omega_Q^{-1}$.

Figure 9: The lowest extended mode with odd parity (solid curve). The dash-dotted curve shows what would be expected if there were a localized amplitude mode.

time just after it reaches the stationary value; namely the field is completely switched off at $t = 250\omega_Q^{-1}$. Although the amplitude is not very large, we see an almost periodic oscillation of the width. This can be understood if we look at the lowest extended mode with odd parity shown in Fig. 9. Its shape is topologically the same as what is expected for the amplitude mode (the dash-dotted line in Fig. 9). Therefore if this mode is excited the polaron width will oscillate with time. This is confirmed by the following facts. First of all, the period $T_{\text{dyn}}$ of the width oscillation observed in Fig. 8 is equal to $390\omega_Q^{-1}$, while the period of the mode depicted in Fig. 9 is $T_{\text{lin}} = 400\omega_Q^{-1}$ which is obtained from the eigenfrequency calculated in the linear mode analysis. Secondly, in order to confirm that this agreement is not accidental, we performed similar calculations for different system sizes. The results are $T_{\text{lin}} = 210\omega_Q^{-1}$ and $T_{\text{dyn}} = 200\omega_Q^{-1}$ for $N = 100$, and $T_{\text{lin}} = 800\omega_Q^{-1}$ and $T_{\text{dyn}} = 840\omega_Q^{-1}$ for $N = 400$. The agreement between $T_{\text{lin}}$ and $T_{\text{dyn}}$ seems satisfactory. We can therefore conclude that the oscillation of the width will die out in the thermodynamic limit. If the effective chain length becomes finite e.g. by the presence of defects, however, it may be possible to observe the width oscillation.

5 Summary and Discussion

In this paper we reconsidered the dynamics of an acoustic polaron in PDA, which was analytically treated by Wilson. We carried out numerical simulations by using the SSH model and applying formulations developed for studying the soliton or polaron in PA. The main difference between the two problems lies in the number of electrons: When we consider the acoustic polaron, we assume there is only one electron in the conduction band, whereas the conduction band is half-filled by electrons in PA.

The saturation of the polaron velocity at the value near to the sound velocity has been confirmed in the simulation where the external electric field is kept to be applied. The reduction of the polaron width with increasing velocity has been also confirmed; the result of simulation indicates that the width will vanish at the sound velocity. The behavior of energy suggests a divergence at the saturation velocity, which is consistent with the analytic studies. Although the saturation velocity estimated from the time dependence of the velocity is slightly smaller than the sound velocity, the behaviors of the width and the energy as function of the velocity clearly indicate that the saturation velocity is exactly the sound velocity. The fact that the saturation velocity obtained in the dynamical simulation is smaller than the sound velocity is partly due to the friction created
by the interaction between the polaron and the lattice vibrations excited by the motion of the polaron, and partly due to that it takes very long time to reach the saturation velocity; it may be too long to be confirmed this type of simulations.

Furthermore in order to understand the dynamics of the acoustic polaron more deeply, we have performed the linear mode analysis. As a result we have found only one localized mode corresponding to the translational motion of the polaron. The phase shift analysis of the extended modes is found to be consistent with this. Although an exactly same relation between the zero-limit value of the phase shift and the number of localized modes as given in Levinson’s theorem for the one-dimensional Schrödinger equation was not found in the present phase shift analysis, it has been argued that this is not astonishing because of the difference between the two situations.

The acoustic polaron was introduced by Wilson [2] to explain the experimentally observed behaviors of the excess charge generated in PDA by means of photo-excitation. [1] These carriers have an ultra-high mobility and their velocity is constant (less than the sound velocity) in low electric field. These characteristics are essentially understood by the behavior of the acoustic polaron. In the experiment, more than one electrons may be excited per chain. In this case we have to consider bipolarons or more sophisticated objects, for which the mutual interactions between electrons cannot be neglected. It will be interesting to study the cases with two or more electrons in the conduction band by a similar method used in the present work. This is left for the future work along with the study of the electron-electron interaction effects.

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[18] In this case, we shift the bond variable so that the flat part far away from the polaron position may become zero.

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[20] In fact the estimation of $\xi_{lat}$ by the variance is not very reliable for long time lapse, because of disturbances in the bond variables appearing in the regions far from the polaron center due to the motion of the polaron. We have, therefore, estimated $\xi_{lat}$ by fitting the bond variable $y_n(t)$ to

$$y_n(t) = y_0 \text{sech}^{-2}[(n - n_0)a/\xi_{lat}] + c$$

with $y_0$, $\xi_{lat}$, $n_0$ and $c$ as fitting parameters. It has been confirmed that the two estimations are consistent for short time lapse.

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