Coulomb blockade effect in collision of two acoustic polarons

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Abstract

Collision between two acoustic polarons, which are complexes of an electron near the band bottom and lattice distortions around it, is numerically studied by using SSH model extended to include short-ranged electronic interactions. When the two polarons have opposite spins, their collision looks quite repulsive in the absence of electronic repulsive interactions. Contrary to intuition, this effective repulsion is reduced by relatively weak electronic interactions. Detailed analyses indicate that a kind of "Coulomb blockade effect" might explain this reduction.

Key words: acoustic polaron, SSH model, Coulomb blockade, resonant tunneling

1. Introduction

In the presence of electron-lattice (e-l) interactions, an acoustic polaron (ACP) is formed by an electron near the band bottom and lattice distortions around it. The relevant lattice distortions are mainly composed of acoustic modes. In one-dimensional systems, a stable ACP can be formed for any values of e-l coupling constant. E.G. Wilson [1] pointed out the possibility to explain photo-created high mobility charge carriers in Polydiacetylene (PDA) [2], which might be regarded as a one-dimensional electron-lattice system, in terms of ACPs. The structure and dynamical properties of an ACP have been studied analytically by continuum model [1] and numerically by discrete model [3,5]. The former model is appropriate when the e-l coupling is sufficiently weak. The lattice distortions yield an effective attractive potential for an electron. Although the energy of the lattice system increases due to these distortions, that of the electron system decreases because of the attractive potential. If the latter is larger than the former, stable polarons can be created and it is expected that this is the case in quasi-one dimensional systems such as PDA.

ACPs are not necessarily isolated. Therefore it is worthwhile to consider collision processes between polarons [5]. In the present work, we report the results of numerical studies with respect to the collision between two ACPs with opposite spin orientations based on Su, Schrieffer and Heeger's (SSH) model extended to include short-ranged electron-electron (e-e) repulsive interactions. Though the e-e interaction plays no role in a single isolated ACP, it can affect the collision between polarons.

2. Model and method

The model Hamiltonian used in the simulations is expressed as $H = H_{\rm SSH} + H_{\rm ee} + H_{\rm pot}$. The first term is the so-called SSH Hamiltonian [6],

$$H_{\rm SSH} = -\sum_{i,\sigma}(t_0 - \alpha y_i)(c^\dagger_{i+1,\sigma}c_{i,\sigma} + c^\dagger_{i,\sigma}c_{i+1,\sigma}) + \frac{K}{2}\sum_i y_i^2 + \frac{M}{2}\sum_i \dot{u}_i^2, \quad (1)$$

where $y_i = u_{i+1} - u_i$ with u_i the lattice displacement of i-th site from its equidistant position, t_0 the transfer integral of π-electrons in a regular lattice, α the electron-lattice coupling constant, $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ the cre-

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ation and annihilation operators of an electron with spin σ at the i-th site, respectively. The last two terms on the right hand side of eq. (1) represent the lattice harmonic potential energy and the lattice kinetic energy, where K the force constant and M the mass of an ion-unit.

The second term of H expresses the extended Hubbard-type short-ranged e-e interactions,

$$H_{\rm ee} = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_i n_i n_{i+1}, \qquad (2)$$

with $n_{i,\sigma} \equiv c^\dagger_{i,\sigma} c_{i,\sigma}$ and $n_i \equiv \sum_\sigma n_{i,\sigma}$. U and V are the on-site and nearest-neighbor Coulomb interaction strengths, respectively. In this paper, these interactions are treated within the unrestricted Hartree-Fock approximation.

The last term $H_{\rm pot}$ is an electrostatic energy due to a time dependent external scalar potential, which yields a non-uniform electric field to put the two polarons in motion [5]. Its details are omitted here because of lack of space.

In the beginning of simulations, two ACPs with opposite spins are prepared at two most apart positions in the system satisfying the periodic boundary condition, namely if the center of one polaron is located at the site i_0, then that of the other is at $i_0 + N/2$ with N the system size. The initial state is obtained from a set of self-consistent equations for the lattice distortions and the electronic wave functions. In the calculations discussed here, the two polarons are initially located at the sites $N/4$ and $3N/4$ with $N = 500$. The motion of the polarons is calculated by solving the time dependent Schrödinger equations for the electronic wave functions and the equations of motion for the lattice displacements. We use the simplest version of the fractal decomposition of exponential operators to solve the Schrödinger equation. The details of the method are given in ref. [5].

3. Effective repulsion between polarons due to resonant quantum tunneling

From the static calculations we understand that two ACPs with opposite spins attract each other when the e-e repulsive interactions are sufficiently weak and that they will combine themselves into an acoustic bipolaron [4]. Contrary to our intuition, the two polarons with opposite spins show a rather strong repulsion in the collision process for vanishing electron-electron interaction. Furthermore this anomalous repulsion disappears by introducing very small e-e interaction [4].

In order to clarify what is happening in this repulsion, we have studied the motion of up- and down-spin electrons separately. The result is shown in Fig. 1 where the up- and down-spin electron numbers ($\rho_{\rm left}$) in the left half of the system ($i < N/2$, $N = 500$) are given as functions of time which is scaled by inverse of ω_Q, the bare optical phonon frequency. In this example, the relative velocity controlled by the non-uniform external electric field is 0.21 $v_{\rm s}$ with $v_{\rm s}$ the sound velocity of the system and the two polarons come within the nearest distance at around $t = 3100\omega_Q^{-1}$. The values of parameters used in this calculations are $\lambda \equiv \alpha^2/t_0 K = 0.094$ (the dimensionless coupling constant), and $U = V = 0$.

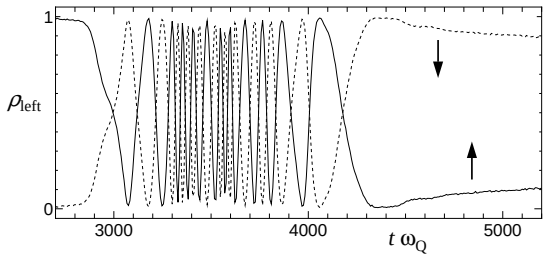

Fig. 1. The time dependence of the up(↑)- and down(↓)-spin electron numbers in the left half of the system in the collision process between two ACPs with opposite spins.

The strong back-and-forth motion of each spin is considered to be due to the resonant tunneling between the double minimum potential made by the lattice distortions related to the colliding polarons. Because of this fast motion an effective repulsion is created and the two polarons cannot be combined into a bipolaron. The situation is drastically changed when very weak repulsive interactions of the order of $0.001t_0$ is introduced. The quick back-and-forth motion of up- and down-spin electrons is disturbed by the presence of e-e interactions, and we confirm the formation of a bipolaron at the collision place. The excess energy is emitted as lattice vibrations. Although the strength of the repulsive electronic interactions does not play any essential role, the reduction of the effective repulsive force due to the resonant tunneling by introducing e-e interactions might be considered as a kind of ' Coulomb blockade' effect appearing between two ACPs which may be regarded as atomic scale moving quantum dots.

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