

## SOLITON-IMPURITY INTERACTIONS IN THE PEIERLS MODEL

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The interaction of amplitude soliton with an impurity in a one dimensional Peierls system is investigated. The total energy is calculated. It is shown that bound soliton-impurity states may be formed. The soliton reflection coefficient and the transition frequencies between the bound states are estimated.

The conductivity properties of most quasionedimensional Charge Density Waves (CDW) systems are varied in wide limits by doping. It is known that due to the selftrapping of the doped electron or the hole amplitude solitons are formed. Up to date the problem of soliton-impurity interaction (the interaction of soliton with the dopand ion in the case of doping) has not solved finally. The dynamic of CDW is considered usually in the frameworks of the phase CDW Hamiltonian [1-3]. Therefore only phase solitons can be taken into account. In this work we study the interaction of the amplitude soliton with the impurity, localized near the chain. We suppose that the interaction potential width is much smaller than the soliton size, therefore we considere a local interaction.

The Hamiltonian of the 1d Peierls model is

$$H_0 = \int dx \Psi^\dagger [-iv_F \frac{\partial}{\partial x} \sigma_z + \Delta(x) \sigma_+ + \Delta(x)^* \sigma_-] \Psi + \frac{\Delta^2}{g^2}, \quad (1)$$

where  $\Psi^\dagger(x) = (\Psi_+^\dagger(x), \Psi_-^\dagger(x))$  are components of electron operators with momenta near right and left Fermi points,  $v_F$  is the Fermi velocity;  $\sigma_x, \sigma_\pm = \sigma_x \pm i\sigma_y$  are Pauli matrixes,  $g$  is the electron-phonon interaction constant.

The interaction Hamiltonian has the form

$$H_{int}(x) = \Psi^\dagger(x) V_1(x) \Psi(x) + \Psi^\dagger(x) V_2(x) \sigma_+ \Psi(x) + \Psi^\dagger(x) V_2^*(x) \sigma_- \Psi(x). \quad (2)$$

The first term in (2) describes the forward scattering, the second is due to the backscattering. We will suppose that the interaction is localized on distances more less than the soliton width  $\xi_0$ , therefore

$$V_1(x) = V_1 \delta(x - x_i), \quad V_2(x) = V_2 \delta(x - x_i),$$

where  $x_i$  is the impurity position, and  $V_2 = |V_2| e^{i\beta}$ . For the sake of simplicity we omit spin indexes and consider the spin diagonal scattering only. By introducing the Green function of the nonperturbated Schrodinger equation

$$\begin{aligned} (i\partial/\partial t + iv_F \sigma_z \partial/\partial x - \Delta(x) \sigma_+ - \Delta(x)^* \sigma_-) G(x, x', t - t') = \\ = \delta(x - x') \delta(t - t') \end{aligned} \quad (3)$$

it is easily to obtain in mixed representation  $(x, \omega)$

$$G(x, x', \omega) = \sum_{\lambda} \frac{\varphi_{\lambda}(x) \otimes \varphi_{\lambda}^{\dagger}(x')}{\omega - \epsilon_{\lambda} + i\delta}$$

where  $\{\varphi_{\lambda}(x)\} = \{\varphi_{+, \lambda}(x), \varphi_{-, \lambda}(x)\}$  is the complete set of nonperturbed Hamiltonian eigenfunctions for a given function  $\Delta(x)$ .

From (1) - (3) we have that eigenfunctions of the Hamiltonian  $H = H_0 + H_{int}$  are determined from the following equation:

$$\Psi(x, E) = \int dy G(x, y, E) H_{int}(y) \Psi(y, E) = G(x, x_i, E) \hat{V} \Psi(x_i, E), \quad (4)$$

where

$$\hat{V} = \begin{pmatrix} V_1 & V_2 \\ V_2^* & V_1 \end{pmatrix}.$$

The eigenvalues  $E$  are determined from (4):

$$\det(G(x_i, x_i, E) \hat{V} - 1) = 0$$

or

$$(|V_2|^2 - V_1^2) \det G + V_2^* G_{12} + V_2 G_{21} + V_1 \text{tr} G - 1 = 0. \quad (5)$$

Let us assume that in the absence of an impurity there is one amplitude soliton in the chain. In this case we take as a nonperturbed set of wavefunctions  $\{\varphi_{\lambda}(x)\}$  the one soliton solution [4]:

$$\begin{aligned} \varphi_{+, \epsilon} &= \frac{\Delta_1 + \epsilon + v_F p + i\Delta_2 \tanh[\Delta_2(x - x_s)/v_F]}{\sqrt{2L\epsilon(\epsilon + \Delta_1)}} \exp(ipx) \\ \varphi_{-, \epsilon} &= \frac{\Delta_1 + \epsilon - v_F p - i\Delta_2 \tanh[\Delta_2(x - x_s)/v_F]}{\sqrt{2L\epsilon(\epsilon + \Delta_1)}} \exp(ipx) \end{aligned} \quad (6)$$

for a continuum spectrum with the dispersion  $\epsilon^2 = v_F^2 p^2 + \Delta^2$ ,  $\Delta^2 = \Delta_1^2 + \Delta_2^2$ ,  $L$  is the chain length, and

$$\varphi_+ = -\varphi_- = \frac{\sqrt{\Delta_2}}{2 \cosh[\Delta_2(x - x_s)/v_F]}, \quad \epsilon = -\Delta_1 \quad (7)$$

for the local level. The deformation  $\Delta(x) = \Delta_1 + i\Delta_2 \tanh[\Delta_2(x - x_s)/v_F]$  consists of the constant term due to the polymer structure and the Peierls deformation  $\Delta_2(x)$  ( $x_s$  is the soliton position).

After substituting (6), (7) to (5) we have the following equation for the shifts of valent band levels  $\delta\epsilon = E - \epsilon(p)$ :

$$\begin{aligned} 0 = (\delta\epsilon L)^2 - (\delta\epsilon L) \{ & V_1 (2 - \frac{\Delta^2 \cosh^{-2}(z)}{\epsilon(\epsilon + \Delta_1)}) + |V_2| \cos \beta (\frac{2\Delta_1}{\epsilon} + \frac{\Delta_2^2 \cosh^{-2}(z)}{\epsilon(\epsilon + \Delta_1)}) + \\ & + |V_2| \sin \beta \frac{2\Delta_2 \tanh(z)}{\epsilon} \} + (V_1^2 - |V_2|^2) (\frac{\epsilon^2 - \Delta^2}{4\epsilon^2}), \end{aligned} \quad (8)$$

where  $z = (x_i - x_s)\Delta_2/v_F$ . We obtain from (8) that

$$\begin{aligned} \delta\epsilon(p)L + \delta\epsilon(-p)L = V_1\left(2 - \frac{\Delta^2 \cosh^{-2}(z)}{\epsilon(\epsilon + \Delta_1)}\right) + \\ + |V_2| \cos\beta \left(\frac{2\Delta_1}{\epsilon} + \frac{\Delta_2^2 \cosh^{-2}(z)}{\epsilon(\epsilon + \Delta_1)}\right) + |V_2| \sin\beta \left(\frac{2\Delta_2 \tanh(z)}{\epsilon}\right). \end{aligned} \quad (9)$$

For the local level  $E_0$  shift we have by the similar way that

$$\delta\epsilon_0 = E_0 + \Delta_1 = -(V_1 + |V_2| \cos\beta) \frac{\Delta_0}{2v_F \cosh^2(z)}. \quad (10)$$

The total energy shift  $\delta W = W - W_0$  is found from (9), (10)

$$\begin{aligned} \delta W(x_s - x_i) = \sum_{\text{cont}} \delta\epsilon + \delta\epsilon_0 = \\ = (V_1 + |V_2| \cos\beta) \frac{\Delta_2}{2v_F \cosh^2(z)} (\nu_0 - 2\frac{\theta}{\pi}) - \\ - |V_2| \sin\beta \frac{2\Delta_2}{g^2} \tanh(z), \end{aligned} \quad (11)$$

where  $\nu_0$  is the filling factor of the local level ( $\nu_0 = 0, 1, 2$ ),  $\theta = \tan^{-1}(\Delta_2/\Delta_1)$ .

For the pure Peierls model ( $\Delta_1 = 0$ ,  $\theta = \pi/2$ ) we have from (11) that

$$\begin{aligned} \delta W(x_s - x_i) = (V_1 + |V_2| \cos\beta) \frac{\Delta_2}{2v_F \cosh^2(z)} (\nu_0 - 1) - \\ - |V_2| \sin\beta \frac{2\Delta_2}{g^2} \tanh(z). \end{aligned} \quad (12)$$

In the case

$$(V_1 + |V_2| \cos\beta)(\nu_0 - 1) < -|V_2| \sin\beta |4v_F/g^2| \quad (13)$$

we have the bond state of the soliton and the impurity. In other cases the energy minimum is achieved at  $z \rightarrow \infty$  or  $z \rightarrow -\infty$

When obtaining the expression (9), (10), we have supposed that the energy level shift is much smaller than the distance between the neighbour levels of the quasicontinuous spectrum. It is right if  $V_1/v_F, |V_2|/v_F \ll 1$  for all levels in the valence band except a small vicinity of the valence band edge. But the contribution of this vicinity to the total energy (11) is small by the additional factor of order of  $\Delta/\epsilon_F$ .

Now we estimate the transition frequencis between the soliton bound levels and the soliton reflection coefficient on the impurity potential. We consider the soliton as the quantum particle, which is discribed by the Hamiltonian [5]:

$$H_s = -\frac{1}{2M_s} \frac{\partial^2}{\partial x_s^2} + \delta W(x_s - x_i), \quad (14)$$

where  $M_s$  is the soliton effective mass,  $x_s$  is the solitone coordinate and  $\delta W(x_s - x_i)$  is given by (12). In order to facilitate the problem we consider the forward

scattering only (i.e. put  $V_2 = 0$ ) and suppose that  $V_1(\nu_0 - 1) < 0$ . Then we obtain for the energy levels:

$$E_n = -\frac{1}{8M_s \xi_0^2} (\sqrt{1 + 8M_s |U_0| \xi_0^2} - 1 - 2n)^2$$

and for the reflection coefficient

$$R = \frac{\cos^2(\pi/2 \sqrt{1 + 8M_s |U_0| \xi_0^2})}{\sinh^2(\pi \xi_0 k) + \cos^2(\pi/2 \sqrt{1 + 8M_s |U_0| \xi_0^2})}$$

where

$$|U_0| = |\Delta_2 V_1(\nu_0 - 1)/2|, \quad \xi_0 = v_F/\Delta_2,$$

$n$  is the integer,  $0 \leq n < (\sqrt{1 + 8M_s |U_0| \xi_0^2} - 1)/2$  and  $k$  is the wavevector of the soliton. For the effective mass of the soliton we have from [4] that

$$M_s = \frac{4\Delta_2^2}{\xi_0 \omega_0^2 g^2},$$

where  $\omega_0$  is the phonon frequency with momentum near  $2p_F$ .

Taking into account the data for the polyacetylene [5]:  $\Delta_2 \simeq 0.7 \text{ eV}$ ,  $v_F \simeq 6 \text{ eV}\text{\AA}$ ,  $\omega_0^2 \simeq 6 \cdot 10^{28} \text{ sec}^{-2}$ ,  $g^2 \simeq 8 \text{ eV}\text{\AA}$  and  $V_1 \sim 1 \text{ eV}\text{\AA}$  we find that  $M_s \simeq 9m_0$  ( $m_0$  is electron mass) and frequencies:

$$\omega_{nm} = E_n - E_m \sim 10^2 - 10^3 \text{ cm}^{-1}.$$

For the reflection coefficient we obtain:

$$R \sim 10^{-6}. \quad (15)$$

The coefficient  $R$  has been calculated for the thermal wavevector at  $T = 300 \text{ K}$ . From (15) we see that the solitons can put very essential contribution into the conductivity of the system, and the transitions between bound states of the soliton can put a contribution into the infrared absorption coefficient.

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