

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 bond 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 quasi-one-dimensional charge density wave (CDW) systems can be varied by doping within wide limits. It is known that amplitude solitons are formed due to the self-trapping of the doped electron or the hole. The problem of soliton-impurity interaction (the interaction of soliton with the dopant ion in the case of doping) has not yet been solved completely. The dynamic of CDW is usually considered in the framework of the phase CDW Hamiltonian.¹⁻³ Only phase solitons can therefore be taken into account. In this work we study the interaction of the amplitude soliton with the impurity which is localized near the chain. We assume that the interaction potential width is much smaller than the soliton size. We therefore consider a local interaction.

The Hamiltonian of the 1D Peierls model is

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

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

The interaction Hamiltonian has the form

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

The first term in (2) describes the forward scattering, and the second term is due to the backscattering. We assume that the interaction is localized at distances greater or less than the soliton width ξ_0 . We therefore have

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

where x_i is the impurity position, and $V_2 = |V_2| e^{i\beta}$. For simplicity we omit the spin indices and consider the spin diagonal scattering only. By introducing the Green's function of the unperturbed Schrödinger equation

$$[i\partial/\partial t + iv_F \sigma_z \partial/\partial x - \Delta(x) \sigma_+ - \Delta(x)^* \sigma_-] G(x, x', t - t') = \delta(x - x') \delta(t - t') \quad (3)$$

it is easy to obtain in mixed representation (x, ω)

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

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

From (1)–(3) we find that eigenfunctions of the Hamiltonian $H = H_0 + H_{\text{int}}$ are determined from the equation

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

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 an unperturbed set of wave functions $\{\varphi_{\lambda}(x)\}$ 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).

Substituting (6) and (7) in (5), we obtain the following equation for the shifts of the valent band levels $\delta\epsilon = E - \epsilon(p)$:

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

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

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

For the local level E_0 shift we find by analogy with the above procedure 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) and (10):

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

where ν_0 is the filling factor of the local level ($\nu_0 = 0, 1, 2$), and $\theta = \tan^{-1}(\Delta_2 / \Delta_1)$.

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

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

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 in the limit $z \rightarrow \infty$ or $z \rightarrow -\infty$.

In deriving expressions (9) and (10) we assumed that the energy level shift is much smaller than the distance between the neighboring levels of the quasi-continuous spectrum. It is correct to assume that $V_1/v_F, |V_2|/v_F \ll 1$ for all levels in the valence band, except in a small vicinity of the valence band edge. However, the contribution of this vicinity to the total energy (11) is small, an additional factor on the order of Δ/ϵ_F .

Let us now estimate the transition frequencies between the soliton bound levels and the soliton reflection coefficient at the impurity potential. We assume that the soliton is a quantum particle which is described 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 soliton coordinate, and $\delta W(x_s - x_i)$ is given by (12). In order to simplify the problem, we consider the forward scattering only (i.e., we set $V_2=0$) and assume that $V_1(\nu_0 - 1) < 0$. We then obtain the following expression 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 an integer, $0 \leq n < (\sqrt{1+8M_s|U_0|\xi_0^2} - 1)/2$, and k is the wave vector of the soliton. For the effective mass of the soliton we see from Ref. 4 that

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

where ω_0 is the phonon frequency with the momentum near $2p_F$.

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

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

For the reflection coefficient we obtain

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

The coefficient R has been calculated for the thermal wave vector at $T=300$ K. From (15) we see that the solitons can contribute significantly to the conductivity of the system, and the transitions between bound states of the soliton can contribute to the infrared absorption coefficient.

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