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Localized electronic states: non-linearity versus single impurity

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Abstract. As a typical model exhibiting non-linear excitations, the continuum model for conjugated polymers is studied in the presence of a single impurity. Using the unperturbed Green functions the scattering matrix of the full problem is calculated and information about the mutual influence of non-linear and impurity intragap states is extracted. As the main difference we find that the localization length of the impurity state is determined mainly by the potential strength whereas for the non-linear state it is an intrinsic property.

1. Introduction

The Peierls mechanism as the driving instability for a metal-insulator transition in quasi-one-dimensional systems has attracted quite a lot of attention in recent years. The formulation of this mechanism as an intrinsic non-linear problem is of interest also from a more general point of view and has been quite successfully applied to the existence and physical properties of non-linear excitations in conjugated polymers (for a review see [1]). In these materials with semiconductor gap of the order of 1 eV these non-linear excitations are electronically characterized by a localized state deep within the gap, the signatures of which can be detected experimentally. It is the existence of these gap states which makes these systems so attractive, also from an application point of view.

On the other hand, it is well known that in more conventional semiconductor intragap states can be introduced by doping the material with impurities. Therefore, one might ask whether there is any mutual influence of both mechanisms for the formation of localized electronic states.

The problem of the Peierls instability in the presence of impurities has been studied before ([2, 3], for short reviews see [4]) with mainly averaged quantities being focused on. All averaging procedures used so far have the shortcoming of restoring full translational invariance for the system under consideration. Thus a detailed analysis of the interaction of a single impurity and single non-linear excitation, both of which break translational invariance, could not be performed. Some attempts in this direction have been made [5] through a numerical simulation, including even a mobile non-linear excitation. In addition a linear response calculation has been made [5] for the change of a homogeneous structure around the impurity. Also, the change of the structure of the kink in a dirty background has been studied [6], i.e. the

interaction with the impurities has been taken into account only as an average. Here we want to focus on the influence of a single impurity on the structures of both kink and polaron as typical non-linear excitations in these systems in a non-translational invariant situation.

Fortunately the widely used TLM model [7] as the long wavelength (continuum) limit of the underlying lattice description can be solved exactly, i.e. the wavefunctions for all electronic states (valence and conduction bands as well as localized intragap states) are known in all cases: homogeneous ground state, kink and polaron excitation. Consequently the Green function can be calculated, (the results are compiled in the appendix for reference). The interaction with a single impurity can consequently be treated with the help of the scattering matrix, which is done in section 2. From the full Green function one can then extract information about the impurity states (section 3) as well as the non-linear intragap states (section 4) and their mutual interference. We close with some prospects on the many-impurity problem.

2. Model and general formalism

The electronic part of the coupled electron-phonon system is described within the TLM model [7] by

$$H_0 = \int dx \psi^\dagger(x) h(x) \psi(x) \quad h(x) = -i\sigma_3 \partial_x + \Delta(x) \sigma_1 \quad (1)$$

if no impurities are present. Together with a potential $V(x)$ due to an impurity the electronic Green function satisfies the equation of motion

$$(iE - h(x))G(x, x'; E) = \delta(x - x') + V(x)G(x, x'; E). \quad (2)$$

The corresponding Dyson equation in reciprocal space (with the unperturbed functions ψ) then reads

$$G_{pp'} = \delta_{pp'} G_p^0 + G_p^0 \sum_{p''} \int dx \psi_p^\dagger(x) V(x) \psi_{p''}(x) G_{p''p'}. \quad (3)$$

Note that in the presence of a single kink or polaron the translational invariance is broken so that $G^0(x, x'; E)$ depends on both x and x' and not only on the difference $x - x'$. Since the Green function in reciprocal space is given by

$$G_{pp'} = \int dx dx' \psi_p^\dagger(x) G(x, x') \psi_{p'}(x') \quad (4)$$

with $\psi_p(x)$ the correct eigenfunctions, even with kinks or polarons present it is diagonal in the indices

$$G_{pp'}^0 = \delta_{pp'} G_p^0. \quad (5)$$

Now, for a single impurity located at $x = x_1$, i.e. $V(x) = V\delta(x - x_1)$ and iterating equation (3) we find

$$G_{pp'} = \delta_{pp'} G_p^0 + G_p^0 t_{pp'} G_{p'}^0 \quad (6)$$

with scattering matrix

$$t_{pp'}(x_1) = \psi_p^\dagger(x_1)V[1 - G^0(x_1, x_1; E)V]^{-1}\psi_{p'}(x_1). \quad (7)$$

Transforming back to real space with (A1) we obtain finally

$$G(x, x'; E) = G^0(x, x'; E) + G^0(x, x_1; E)\bar{t}(x_1; E)G^0(x_1, x'; E) \quad (8)$$

with

$$\bar{t} = V[1 - G^0(x_1, x_1; E)V]^{-1}.$$

From (8) we can now determine the existence of additional bound states in the presence of an impurity as poles of the t -matrix as a function of energy, as well as their spatial extension, through the x -dependence of the corresponding spectral weight. The necessary unperturbed Green function G^0 for all interesting cases: homogeneous ground state, kink and polaron excitation, respectively, are compiled in the appendix.

3. Impurity state

For simplicity we present a detailed discussion for the case of a bond impurity, i.e. $V = U\sigma_1$ in our notation. In the many-impurity situation this turned out to be the more interesting case, as we then have the possibility of suppression of localized impurity states [8].

Due to the property (A12) the poles of the t -matrix are given in this special case by

$$c = (1 + U^2/4)/2U = 1/2u \quad (9)$$

with different coefficients c of G^0 (A12) to be used for the homogeneous, kink and polaron cases, respectively.

Also the spatial extent in general is given through the unperturbed Green function $G^0(x, x_1)$. From the expressions for G^0 and the general formula (8) it is clear that the characteristic length of the localized impurity state is governed by the exponential in $G^0(x, x')$. Therefore once we have determined the position of the impurity state in the gap we know its localization length.

3.1. Ground state

For completeness we start with the results for an impurity in a homogeneously dimerized structure, which have been given earlier. With c from (A6) the impurity state at ω is given by [8]

$$\sqrt{(1 - \omega^2)} = -u \quad (10)$$

which has a solution only if the phase of the order parameter at the site of the impurity has the correct sign. If this is the case the impurity state is to be found close to the band edges at $\omega_i = \pm\sqrt{(1 - u^2)}$.

As said before the spatial extent is extracted from the exponential in (A5): $\exp(-2(x - x_1)\sqrt{(1 - \omega^2)})$. With ω given by (10) the localization length is

$$l_i^G = (2u)^{-1}. \quad (11)$$

For a weak impurity ($u \rightarrow 0$) it is apparent that this is rather large since correspondingly the localized state ω_i is close to the band of extended (i.e. $l \rightarrow \infty$) states.

3.2. *Kink*

Proceeding in the same manner with c from (A9) we find [9]

$$\sqrt{(1 - \omega^2)} = -u \tanh(x_1). \tag{12}$$

In view of the result in section 3.1 it is clear that the impurity level in the gap can exist only on one side of the kink (located at $x = 0$) with $\tanh x_1 < 0$ (for $u > 0$). Close to the centre of the kink ($x_1 \rightarrow 0$) this state approaches the band of extended states, whereas far away ($x_1 \rightarrow \infty$) it moves deeper into the gap, approaching the value of the homogeneous state.

From the discussion before it is now clear that also the corresponding localization length of the impurity level in the presence of a kink is increased:

$$l_i^k = (2u \tanh |x_1|)^{-1} > l_i^G \tag{13}$$

since $\tanh |x| < 1$. In summary the kink pushes the impurity state towards the band and broadens it (in space).

3.3. *Polaron*

For a polaron excitation (located at $x = 0$) with profile $\Delta(x) = 1 - K_0^2 / [\omega_0 \cosh(K_0(x+x_0)) \cosh(K_0(x-x_0))]$ ($\omega_0 = \sqrt{(1-K_0^2)}$, $x_0 = (1/4K_0) \ln[(1+K_0)/(1-K_0)]$) determining the spatial width of the polaron, i.e. the separation of kink and antikink located at $\pm x_0$, respectively, which as a bound pair form this polaron) we find from (A11)

$$\sqrt{(1 - \omega^2)} = -u(\omega^2 \Delta(x_1) - \omega_0^2) / (\omega^2 - \omega_0^2). \tag{14}$$

A solution exists only for $1 > |\omega| > \omega_0$, ω_0 being the localized level of the polaron. A detailed analysis shows that this requires $|x_1| \leq x_0$. This means that the impurity level we are looking for can exist only within the extension of the polaron. The impurity level ω_i moves toward the band of extended states as the impurity moves close to either kink or antikink, i.e. $x_1 \rightarrow \pm x_0$, whereas this level is well inside the gap if the impurity is located right at the centre of the polaron ($x_1 = 0$). The limiting cases $\omega_0 \rightarrow 0$ (kink) and $\omega_0 \rightarrow 1$ (ground state) coincide with the previous results.

Similarly, as in the kink case the spatial width is increased compared with the homogeneous case:

$$l_i^p = l_i^G / [\tanh(K_0(x_1 - x_0)) \tanh(K_0(x_1 + x_0))] \tag{15}$$

in lowest order in U . This can easily be interpreted as both kink and antikink constituents of the polaron contributing an enhancement factor of $1/\tanh$ according to (13).

4. *Non-linear state*

The full TLM model consisting of the electronic part (1) plus an additional elastic energy for the (lattice) order parameter $\Delta(x)$

$$H_e = \frac{1}{2\lambda} \int dx \Delta^2(x) \tag{16}$$

yields via a self-consistent treatment, i.e. minimizing to total energy with respect to $\Delta(x)$, an essentially non-linear problem even without impurities present (for details see, for example, [1]). This leads to localized electronic states in the gap for both kink and polaron excitations. From the corresponding Green functions $G^0(x, x; \omega)$ (cf appendix) one can easily see that for the kink this localized state is to be found at $\omega = 0$ with a spatial width of 1 (or $\xi_0 = 1/\Delta_0$ in rescaled units) whereas for the polaron there are two states at $\omega = \pm\omega_0$ with a characteristic width of $K_0 = \sqrt{1 - \omega_0^2}$.

It is clear that in the presence of an impurity these states will be modified. The additional contribution from the second term in (8) to these poles is quite lengthy, here we concentrate on the effects in lowest order in U . It is tempting to replace \tilde{t} in this case simply by $V = U\sigma_1$ but since we are dealing with localized, unperturbed states, i.e. poles in G^0 , special care is needed.

For the kink this replacement is indeed possible and collecting only the terms proportional to the unit matrix in (8) we find

$$\text{Tr } G(x, x) = 2(c_0(x, x) + 2U(c_0(x, x_1)c_1(x, x_1) + ic_2(x, x_1)c_3(x, x_1))) \quad (17)$$

using the symmetries in x and x' of the coefficients of the unperturbed Green function $G^0(x, x') = \sum c_i(x, x')\sigma_i$. The first term in (17) gives the unperturbed, non-linear local density of states whereas the second term is the first-order change due to the impurity at x_1 . Extracting all contributions to the pole at $\omega = 0$ we finally arrive at

$$\begin{aligned} \text{Tr } G(x, x; \omega) = & (1/\omega)[1/2 \cosh^2(x) + (U/4)(1 + \text{sgn}(x - x_1) \tanh x)^2 \\ & \times (1 - \text{sgn}(x - x_1) \tanh x_1) \exp(-2|x - x_1|)]. \end{aligned} \quad (18)$$

The modification of the spectral weight is quite complicated in the neighbourhood of the impurity, but falls off at large distances with the same rate as the unperturbed state.

An analogous calculation for the polaron is not as simple since the corresponding Green function ((A10) and (A11)) has poles at $\omega = \pm\omega_0$ in all coefficients c_i . Therefore the matrix inversion (8) which defines the scattering matrix t has to be performed in general, and only later the approximations for the behaviour in the neighbourhood of $\pm\omega_0$ can be inserted. Then one finds that in lowest order in U there are additional contributions besides the term $U\sigma_1$. This procedure is also necessary in order to exclude any poles of higher order in the full Green function. The final result is quite lengthy and will not be reported here. We only note that qualitatively a similar behaviour as in the kink case is found, namely that the asymptotic localization length is the same as in the unperturbed case.

5. Summary

Using the unperturbed Green function for a kink and polaron conformation we have studied the electronic structure of an inhomogenous Peierls system in the presence of an impurity. We then have two mechanisms for the formation of localized intragap states which exhibit a mutual influence. We have found that the non-linear lattice structure (kink and polaron) pushes the impurity level towards the band edges, at the same time the spatial extent of this state is increased. On the other hand an

additional contribution to the spectral weight of the non-linear electronic state is found, its localization length remaining unchanged.

We have demonstrated this interplay between disorder and non-linearity with the specific example of a bond impurity only. We expect that an analogous treatment in the case of a more general situation, i.e. additional site disorder, yields qualitatively similar results.

There is, of course, one shortcoming of the present approach: we have treated the electronic problems exactly for a given lattice structure (or order parameter $\Delta(x)$). A fully self-consistent treatment, however, needs a change of this structure due to the change of the electronic properties. Technically speaking one needs to solve, in addition to the equation for the Green function (equations (2) or (3)), the self-consistency equation

$$\Delta(x) = \frac{1}{\lambda} \int d\omega \operatorname{Tr} \sigma_1 G(x, x; \omega)$$

from the minimization of the total energy with respect to $\Delta(x)$. This problem is quite involved, a more simplified treatment using the quasi-classical Green function [6] seems to be more promising, although even in the case of a Born approximation for the impurity scattering, difficulties with the intragap states (poles) arise. Compared with previous results [5] we have nevertheless obtained some improvement as we have taken into account a non-homogeneous order parameter from the very beginning.

The physically more interesting situation of many impurities is certainly more difficult. As mentioned in section 1 any averaging procedure restoring translational invariance neglects any local electron-impurity interaction and will not be able to capture the essential physics which produce the effects reported here for the one-impurity situation. On the other hand any too detailed impurity-kink (or polaron) interaction is not tractable in the many-impurity case. An approach which is somehow between these two limiting treatments is needed.

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Appendix

For the electronic problem $h(x)\psi_p(x) = \epsilon_p \psi_p(x)$ the Green function can be computed using the (known) eigenfunctions $\psi_p(x)$ through

$$G(x, x'; E) = \sum_p \psi_p(x) \frac{1}{iE - \epsilon_p} \psi_p^+(x') \quad (\text{A1})$$

since the correctly normalized functions $\psi_p(x)$ satisfy $\sum_p \psi_p(x) \psi_p^+(x') = \delta(x - x')$. In a modified notation $f_{p,\pm} = u_p \pm iv_p$ (from $\psi_p(x) = \begin{pmatrix} u_p(x) \\ v_p(x) \end{pmatrix}$) (cf [10]) the

expression for the Green function can be simplified to

$$G(x, x'; E) = \sum_p \frac{1}{iE - \epsilon_p} \{ [(A_+ + A_-)/4] \mathbf{1} + [(B_+ + B_-)/4] \sigma_3 \\ + i[(B_- - B_+)/4] \sigma_1 - [(A_+ - A_-)/4] \sigma_2 \} \quad (\text{A2})$$

with

$$A_{\pm} = f_{p,\pm}(x) f_{p,\pm}^*(x') \quad (\text{A3})$$

$$B_{\pm} = f_{p,\pm}(x) f_{p,\mp}^*(x'). \quad (\text{A4})$$

This is convenient in view of the symmetries between positive and negative energy solutions f_p . Now, using the known expressions for the eigenfunctions, we obtain for all cases (with Δ_0 scaled to 1) the following.

(a) *Ground state* ($\Delta(x) = \Delta_0$)

$$G(x, x'; E) = -\frac{1}{2\sqrt{(1+E^2)}} [iE \mathbf{1} + \sigma_1 + i\sqrt{(1+E^2)} \text{sgn}(x-x') \sigma_3] \\ \times \exp(-|x-x'|\sqrt{(1+E^2)}). \quad (\text{A5})$$

From the derivation it is clear that the appropriate limit as $x \rightarrow x'$ of the last term vanishes (odd function of $(x-x')$), therefore we have ($\omega = iE$)

$$G(x, x; \omega) = -[1/2\sqrt{(1-\omega^2)}](\omega \mathbf{1} + \sigma_1) \quad (\text{A6})$$

such that the density of states given by the imaginary part of G reads

$$n(x; \omega) = (1/\pi)\omega/\sqrt{(\omega^2 - 1)} \quad |\omega| > 1. \quad (\text{A7})$$

(b) *Kink* ($\Delta(x) = \Delta_0 \tanh(x/\xi_0)$, $\xi_0 = 1/\Delta_0$)

$$G(x, x'; \omega) = -[1/4\sqrt{(1-\omega^2)}] \{ 2\omega \mathbf{1} + (1/\omega)[1 - tt' + \sqrt{(1-\omega^2)}|t-t'|](\sigma_2 - \mathbf{1}) \\ + (t+t')\sigma_1 + [t-t' + 2\sqrt{(1-\omega^2)}\text{sgn}(x-x')]i\sigma_3 \} \exp(-|x-x'|\sqrt{(1-\omega^2)}) \quad (\text{A8})$$

with the abbreviations $t = \tanh(x)$, $t' = \tanh(x')$, ξ_0 scaled to 1. (In a different notation this has been given already in [11].) For $x' \rightarrow x$ we obtain from this

$$G(x, x; \omega) = -[1/2\sqrt{(1-\omega^2)}][\omega \mathbf{1} + \tanh(x)\sigma_1 + (1/2\omega \cosh^2 x)(\sigma_2 - \mathbf{1})]. \quad (\text{A9})$$

Note that the last term gives an additional contribution to the density of states due to the pole at $\omega = 0$.

(c) Polaron ($\Delta(x) = \Delta_0 - K_0[\tanh(K_0(x + x_0)) - \tanh(K_0(x - x_0))]$)

$$\begin{aligned}
 G(x, x'; \omega) = & -[1/4\sqrt{(1 - \omega^2)}] \exp(-|x - x'|/\sqrt{(1 - \omega^2)}) \left[2[\omega \mathbf{1} + \sigma_1 + i \operatorname{sgn}(x - x')] \right. \\
 & \times \sqrt{(1 - \omega^2)} \sigma_3 + [K_0^2/(\omega_0^2 - \omega^2)] \left(\omega \{ [1 - t_- t'_- + \sqrt{(1 - \omega^2)} \right. \\
 & / K_0] |t_- - t'_-| \} (1 - \sigma_2) + \{ 1 - t_+ t'_+ + [\sqrt{(1 - \omega^2)}/K_0] |t_+ - t'_+| \} \\
 & \times (1 + \sigma_2) \}] + \sigma_1 \{ [(1 - \omega^2)/K_0] (t_- + t'_- - t_+ - t'_+) + (2 - t_- t'_+ - t_+ t'_-) \\
 & + \operatorname{sgn}(x - x') \sqrt{(1 - \omega^2)} [t_+ t'_- - t_- t'_+ + (1/K_0)(t_- - t'_- + t_+ - t'_+)] \\
 & + i \sigma_3 \{ \operatorname{sgn}(x - x') \sqrt{(1 - \omega^2)} [2 - t_- t'_+ - t_+ t'_- + (1/K_0)(t_- + t'_- - t_+ - t'_+)] \\
 & + [(1 - \omega^2)/K_0] (t_- - t'_- + t_+ - t'_+) + t_+ t'_- - t_- t'_+ \} \} \left. \right] \quad (\text{A10})
 \end{aligned}$$

with $t_{\pm} = \tanh(K_0(x \pm x_0))$.

For $x = x'$ we then have

$$\begin{aligned}
 G(x, x; \omega) = & -[1/2\sqrt{(1 - \omega^2)}] \{ [\omega \mathbf{1} + [K_0^2/(\omega_0^2 - \omega^2)](\omega/2) \\
 & \times [(1/\cosh^2 K_0(x + x_0))(\sigma_2 + 1) - (1/\cosh^2 K_0(x - x_0))(\sigma_2 - 1)] \\
 & + \{ 1 + (K_0^2/\omega_0)[\omega^2/(\omega_0^2 - \omega^2)](1/\cosh K_0(x + x_0)) \\
 & \times (1/\cosh K_0(x - x_0)) \} \sigma_1 \}. \quad (\text{A11})
 \end{aligned}$$

Here the additional poles are found at $\pm\omega_0$.

It is of further computational convenience that in all cases (a)–(c) the equal site Green functions have the property

$$G(x, x; \omega) = a \mathbf{1} + b \sigma_2 + c \sigma_1 \quad (\text{A12})$$

and

$$\det G = a^2 - b^2 - c^2 = -\frac{1}{4}.$$

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