Effects of the Lattice Discreteness on a Soliton in the Su-Schrieffer-Heeger Model

RYÕEN SHIRASAKI *

Department of Physics, Faculty of Education, Yokohama National University, Yokohama, Kanagawa 240

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Abstract

In this paper we analytically study the effects of the lattice discreteness on the electron band in the SSH model. We propose a modified version of the TLM model which is derived from the SSH model using a continuum approximation. When a soliton is induced in the electron-lattice system, the electron scattering states both at the bottom of the valence band and the top of the conduction band are attracted to the soliton. This attractive force induces weakly localized electronic states at the band edges. Using the modified version of the TLM model, we have succeeded in obtaining analytical solutions of the weakly localized states near the bottom of the valence band and the top of the conduction band. This band structure does not modify the order parameters. Our result coincides well with numerical simulation works.

*E-mail: sirasaki@ed.ynu.ac.jp
§1. Introduction

The trans-polyacetylene is an ideal material which bears a non-linear excitation. A soliton is the non-linear excitation which changes the arrangement of double bonds of carbons. Su-Schrieffer-Heeger model (SSH model) is the most simple lattice model which clarifies the soliton. In this paper, we study effects of the lattice discreteness on the electron band and the order parameter of the soliton in the SSH model. The Takayama-Lin-Liu-Maki model (TLM model) is known as a continuum version of the SSH model and gives a analytical solutions for the soliton, the polaron, and the soliton lattice. Takayama et al. derived this model from the SSH model retaining only the lowest order term with respect to $a/\xi$, where $a$ is the lattice constant in the direction of a polymer chain and $\xi$ is the soliton width. To take into account the discreteness of the SSH model, it would be a correct way to include higher order terms which will be treated in a perturbational way, the TLM model being the unperturbed Hamiltonian. Obtained results have to satisfy a selfconsistency condition between the order parameters and the single-electron wave functions.

There were several works which determined an acoustic component of the order parameter. For example, Maki obtained the order parameters up to the first order of $a/\xi$ using the TLM model. At low temperature, soliton friction motion is dominated by the interaction between the acoustic phonon and the order parameter. Some workers used his result to study the soliton diffusion. Kurita, Ono, and Wada have taken into account the fact that the band width is finite, using a model introduced by Gammel. It retains the property that the electronic wave number is confined in the first Brillouin zone. Thus, the finiteness of the electron band reappears in a natural way even in the continuum limit. Kurita et al. have obtained the first order corrections to the electronic wave functions and the order parameters by the perturbation method. They have found that there is a divergence in the second order calculations.

It has been pointed out that the first order acoustic component of the order parameter is working as an attractive potential to give rise to electronic localized levels at the bottom and the top of the band. There have been several works which have solved the SSH model numerically. Kurita et al. have pointed out that there are two electronic levels which are localized at the soliton or at the polaron, in addition to the well-known mid-gap states. The structure of the electron band for a soliton is shown in Fig.1. One of them is below the bottom of the valence band and the other above the top of the conduction band. Fu, Shuai, Liu, Sun, and Hicks have obtained the two localized levels for the soliton together with two more levels in the energy gap. Kurita et al. have analyzed the phase shifts of the electronic wave functions of the SSH model numerically in ref. and showed that there are two types of electronic states which are classified according to a property roughly corresponding to parity. There are accordingly two types of the phase shift. They
agree with each other except at band edges. The present author and Wada showed in ref. [9] that the weakly localized states at the edges of the band can be determined analytically by solving equations given by the sum of the TLM Hamiltonian and the first order correction terms without using the perturbation method [4].

The purpose of this paper is to develop the method to obtain the scattering states of electrons near the band edges as well as the localized states analytically up to the first order of $a/\xi$. We propose a modified version of the continuum model which is constructed introducing the electronic wave functions at the edges of the band in addition to the electron wave functions at the fermi level. The derived equation for the electron wave function contains the acoustic component of the order parameter as the attractive potential. The self-consistency condition is reconstructed using both the electron wave functions at the edges of the band and at the fermi level. Solving the equation, we obtained analytical expressions of the electronic wave functions. Using this model, we will show that the behavior of the phase shift of the extended electronic states for a soliton and the existence of the weakly localized states are consistent with the small distortion of the acoustic component of the order parameter.

In §2, the formulation of the modified version of the TLM model is constructed. The self-consistency between the lattice order parameter and the electron wave function will be shown in §3. We solve the equations in §4 and obtain the structures of electronic bands. The phase shifts of the extended states are also derived.

§2. Continuation of the Su-Schrieffer-Heeger model

The Hamiltonian of the SSH model [1] is

$$H_{\text{SSH}} = \sum_{n,s} t_{n+1,n} (C_{n+1,s}^\dagger C_{n,s} + C_{n,s}^\dagger C_{n+1,s}) + \frac{1}{2} K \sum_n (u_{n+1} - u_n)^2 + \frac{1}{2} M \sum_n \ddot{u}_n; \quad (2.1)$$

where the overlap integral $t_{n+1,n}$ is given by $t_{n,n+1} = t_0 - \alpha (u_{n+1} - u_n)$. $t_{n,n+1}$ is a linear function of the bond length between the $n$ and $n+1$ sites. The quantity $C_{n,s}^\dagger$ is the creation operator of a $\pi$ electron at site $n$ with spin $s$, and $u_n$ is the displacement of the $n$-th site in the polymer chain. The second term is the harmonic potential for the bond between the $n$ and $n+1$ sites with the spring constant $K$ due to the $\sigma$ electrons. The third term is the kinetic energy of the unit, $M$ being the mass of the unit.

The bond variable $y(n)$ is defined by

$$y(n) = u_{n+1} - u_n. \quad (2.2)$$

Considering that the dynamics of lattice is sufficiently slow in comparison to that of the electrons at the Fermi level, we have, in the adiabatic limit,

$$\dot{u}_n = 0.$$
Then, the set of electronic wave functions $\Phi_{k,s}(n)$ is determined as eigen-functions of the equations

$$E_k \Phi_{k,s}(n) = -\{t_0 - \alpha y(n - 1)\} \Phi_{k,s}(n - 1) - \{t_0 - \alpha y(n)\} \Phi_{k,s}(n + 1), \quad (2.3)$$

with energy $E_k$. This equation is derived by the variational principle with respect to $C_n^\dagger$. Using $\Phi_{k,s}$, the total energy is given by $\sum'_{k,s} \langle \Phi_{k,s} | H_{SSH} | \Phi_{k,s} \rangle$. This is minimized when $y(n)$ satisfies

$$y(n) = -\frac{\alpha}{K} \sum_{k,s} \{ \Phi_{k,s}(n) \Phi_{k,s}(n + 1) + c.c \} + \frac{\alpha}{NK} \sum_{n} \sum'_{k,s} \{ \Phi_{k,s}^*(n) \Phi_{k,s}(n + 1) + c.c \}, \quad (2.4)$$

where $\sum'$ means a summation over the occupied states. The second term comes from the constraint

$$\sum_n y(n) = 0. \quad (2.5)$$

As is shown by Su-Schrieffer-Heeger, this model bears the bond order wave (BOW) state, which has the bond alternation of the wave number $\pi/a$. In this state, the bond variable $y(n)$ is given by

$$y_n = \frac{1}{2\alpha} (-)^n \tilde{\Delta} \quad (2.6)$$

where $\tilde{\Delta}$ is the optical component of the order parameter. In the SSH model, the quantity $\tilde{\Delta}$ is determined by the selfconsistency equation,

$$1 = 2\lambda \int_0^{k_F a} \frac{2t_0 \cos^2 ka}{\sqrt{(2t_0)^2 \cos^2 ka + \tilde{\Delta}^2 \sin^2 ka}} d(ka). \quad (2.7)$$

When the non-linear excitation is induced in the BOW state, the order parameter $\tilde{\Delta}$ is distorted near the center of the excitations. Maki had pointed out that the acoustic component of the order parameter also suffers a distortion around the non-linear excitation. The bond variable is written as follows:

$$y_n = \frac{1}{2\alpha} \left\{ \tilde{\zeta}(na + \frac{a}{2}) + (-)^n \tilde{\Delta}(na + \frac{a}{2}) \right\}, \quad (2.8)$$

where $\tilde{\zeta}$ is the acoustic component of the order parameter. Takayama-Lin-Liu-Maki have written the electron wave function nearly at the Fermi level by the summation over the left-going and the right-going waves,

$$\Phi_{k,s}(na) = [W_s(na) \exp\{ik_F na\} - iV_s(na) \exp\{-ik_F na\}] \sqrt{a}, \quad (2.9)$$
with the Fermi wave number \( k_F = \pi/2a \). On the other hand, near the bottom or the top of the electron band, the electron wave function should be given by

\[
\Phi_{k,s}(na) = \{Z_s(na) - iY_s(na)e^{i2k_F(na)}\}\sqrt{a}.
\]  

(2.10)

for \(|E| \sim 2t_0\),

where \( Z \) and \( Y \) are slowly varying functions. Using \( W, V, Z \) and \( Y \), the electronic states in the presence of the non-linear excitation will be analyzed. Substituting eqs.(2.8) and (2.9) into eq.(2.3), and introducing \( \psi_{k,s}(x) \) by

\[
\psi_{k,s}(x) = \left( \frac{W_s(x)}{V_s(x)} \right),
\]

(2.11)

we obtain the equation for the electron,

\[
E_k\psi_{k,s}(x) = -i\Delta_0\sigma_3\partial\psi_{k,s}(x) + \bar{\Delta}(x)\sigma_1\psi_{k,s}(x)
\]

\[
+ m_1\left\{ \frac{1}{2}(\partial\bar{\zeta}(x))\sigma_3\psi_{k,s} + i\bar{\zeta}(x)\sigma_3(\partial\psi_{k,s}(x)) \right\} + \ldots,
\]

(2.12)

where \( x = na \), and \( 2\Delta_0 \) being the electron band gap. The quantity \( m_1 = a/\xi = \Delta_0/(2t_0) \) is the smallness parameter. The differentiation \( \partial \) is defined by \( \partial = \frac{\xi}{\partial x} \) where \( \xi = 2t_0a/\Delta_0 \) is soliton width. In the calculation, \( \psi_{k,s}(x \pm a) \), the functions \( \bar{\Delta}(x \pm a/2) \) and \( \bar{\zeta}(x \pm a/2) \) were expanded around \( x \).

Substituting eqs.(2.8) and (2.10) into eq.(2.3) and introducing \( \varphi_{q,s}(x) \) by

\[
\varphi_{q,s}(x) = \left( \frac{Z_s(x)}{Y_s(x)} \right),
\]

(2.13)

we obtain the equation for the electron near the edges of electron band,

\[
E_q\varphi_{q,s}(x) = \left( -2t_0 - \frac{\Delta_0}{2}m_1\partial^2 + \bar{\zeta}(x) \right)\sigma_3\varphi_{q,s}(x)
\]

\[
- im_1\left\{ \frac{1}{2}(\partial\bar{\zeta}(x))\sigma_3\varphi_{q,s} + i\bar{\zeta}(x)\sigma_3(\partial\varphi_{q,s}(x)) \right\} + \ldots
\]

(2.14)

The functions \( \varphi_{q,s}(x \pm a) \), \( \bar{\Delta}(x \pm a/2) \) and \( \bar{\zeta}(x \pm a/2) \) were expanded around \( x \).

Equations(2.11), (2.12), (2.13) and (2.14) are the equations of the electron wave function.

Substituting eqs.(2.9) and (2.10) into eq.(2.4), we obtain the self-consistency relation between the electron and the bond variable \( y(n) \). Using eq.(2.8) and equating the slowly varying term and fast oscillating term by \((-)^n\), we obtain the equations for the order parameters \( \bar{\Delta}(x) \) and \( \bar{\zeta}(x) \)

\[
\bar{\Delta}(x) = -\frac{4\alpha^2a}{K} \sum_{k,s}^\prime \psi_{k,s}^\dagger(x)\sigma_1\psi_{k,s}(x)
\]

\[
- m_1\frac{2\alpha^2a}{K} \sum_{q,s}^\prime i\{ (\partial\varphi_{q,s}^\dagger(x))\sigma_1\varphi_{q,s}(x) - \varphi_{q,s}^\dagger(x)\sigma_1(\partial\varphi_{q,s}(x)) \},
\]

(2.15)
\[
\tilde{\zeta}(x) = -\frac{4\alpha^2 a}{K} \sum_{q,s}' \varphi_{q,s}^\dagger(x) \sigma_3 \varphi_{q,s}(x) \\
+ m_1 \frac{2\alpha^2 a}{K} \sum_{k,s}' i \{ (\partial \psi_{k,s}^\dagger(x)) \sigma_3 \psi_{k,s}(x) - \psi_{k,s}^\dagger(x) \sigma_3 (\partial \psi_{k,s}(x)) \},
\]
where the summation \(\sum'\) is performed over the occupied states. \(\varphi_{q,s}(x \pm a/2)\) and \(\psi_{k,s}(x \pm a/2)\) were expanded around \(x\).

Equation (2.12) determines the wave function of the electron at the Fermi level, while eq. (2.14) is the wave function of the electron near the top of the conduction or the bottom of the valence band. Equations (2.15) and (2.16) are the selfconsistency conditions for the order parameters \(\tilde{\Delta}\) and \(\tilde{\zeta}\).

The zeroth order terms of the expansion with respect to \(m_1\) in eqs. (2.12) and (2.15) give the TLM model. Equations (2.14), (2.16) and the higher order terms with respect to \(m_1\) in eqs. (2.12) and (2.15) come from the lattice discreteness of the SSH model.

The order parameter of soliton in the TLM model is given by
\[
\tilde{\Delta}(x) = \Delta_0 \tanh \kappa x,
\]
with \(\kappa = 1/\xi\). The electron wave function for the scattering state is
\[
\psi_\gamma(x) = \frac{N_\gamma}{2} \left( \frac{E_\gamma + \gamma + i \tanh(\kappa x)}{i(E_\gamma - \gamma - i \tanh(\kappa x))} \right) e^{i\gamma x}
\]
\[
N_\gamma = (L(1 + \gamma^2) - 1/\kappa)^{(-1/2)},
\]
\[
E_\gamma = \pm \sqrt{1 + \gamma^2},
\]
\[
\gamma = \xi k,
\]
where \(k\) is the wave number. In eq. (2.18), the plus sign corresponds to the conduction band and the minus sign to the valence band. The energy of the electron is given by
\[
E_k = \Delta_0 E_\gamma.
\]
The electronic localized state inner side of the band gap is given by
\[
\psi_{B0}(x) = \frac{1}{2\sqrt{\xi}} \text{sech} \ \kappa x \left( \begin{array}{c} 1 \\ -i \end{array} \right),
\]
\[
E_M = 0.
\]
The quantity \(\Delta_0\) is determined by the lowest order term of the selfconsistency equation (2.13). This condition becomes
\[
1 = 2\lambda \log \left( \frac{2 \times 2t_0}{\Delta_0} \right),
\]
with $\lambda = 4\alpha^2/(2t_0K\pi)$.

Maki had analyzed the soliton using eqs. (2.12), (2.15) and (2.16) neglecting the terms related to $\varphi_{q,s}$ and retaining terms up to the first order with respect to $m_1$. He obtained the acoustic order parameter

$$\tilde{\zeta}(x) = -\frac{m_1}{2}\Delta_0\text{sech}^2\kappa x, +O(m_1^2).$$

(2.24)

The optical order parameter and the electronic wave function were unchanged. Numerical and analytical works in the SSH model have pointed out that there are weakly localized states around the soliton in addition to the mid-gap state. Their energy levels are located at the top of the conduction band and the bottom of the valence band. The acoustic component of the order parameter $\tilde{\zeta}$ works as an attractive potential at the soliton center, making one weakly localized state at each of the band edges. As shown in Fig.1, the level structure is different from that obtained in ref.[4]. Therefore, it is important to see whether the selfconsistency between eq.(2.24) and the electronic states is satisfied or not. In the next section, we obtain the electron wave function near the edges of the electron bands and the selfconsistency will be confirmed up to the first order with respect to $m_1$.

§3. Selfconsistency

In the present section, the electronic states and the lattice configuration are self consistently determined, using eqs. (2.12) ~ (2.16). We expand the electron wave function by the smallness parameter $m_1$,

$$\psi_{k,s}(x) = \psi_{k,s}^{(0)}(x) + m_1\psi_{k,s}^{(1)}(x) + \ldots,$$

$$\varphi_{q,s}(x) = \varphi_{q,s}^{(0)}(x) + m_1\varphi_{q,s}^{(1)}(x) + \ldots,$$

(3.1)

and the order parameters, in the same way,

$$\Delta(x) = \Delta^{(0)}(x) + m_1\Delta^{(1)}(x) + \ldots,$$

$$\tilde{\zeta}(x) = \zeta^{(0)}(x) + m_1\zeta^{(1)}(x) + \ldots.$$

(3.2)

Then, the equations for electrons, eqs. (2.12) and (2.14), become

$$E_k^{(0)}\psi_{k,s}^{(0)} = H^{(0)}\psi_{k,s}^{(0)},$$

(3.3)

$$E_k^{(1)}\psi_{k,s}^{(0)} + E_k^{(0)}\psi_{k,s}^{(1)} = H^{(1)}\psi_{k,s}^{(0)} + H^{(0)}\psi_{k,s}^{(1)},$$

(3.4)

$$E_q^{(0)}\varphi_{q,s}^{(0)} = h^{(0)}\varphi_{q,s}^{(0)},$$

(3.5)

$$E_q^{(1)}\varphi_{q,s}^{(0)} + E_q^{(0)}\varphi_{q,s}^{(1)} = h^{(1)}\varphi_{q,s}^{(0)} + h^{(0)}\varphi_{q,s}^{(1)},$$

(3.6)
where the Hamiltonian $H^{(i)}$, $h^{(j)}$ ($i, j = 0, 1$) are given as follows:

\[
H^{(0)} = -\Delta_0 \sigma_3 \partial + \Delta^{(0)}(x) \sigma_1, \tag{3.7}
\]

\[
H^{(1)} = i\left\{\frac{1}{2}(\partial \zeta^{(0)}(x)) + \zeta^{(0)}(x) \partial\right\} \sigma_3, \tag{3.8}
\]

\[
h^{(0)} = \left\{-2t_0 - \frac{m_1}{2} \Delta_0 \partial^2 + \zeta^{(0)}(x) + m_1 \zeta^{(1)}(x)\right\} \sigma_3, \tag{3.9}
\]

\[
h^{(1)} = -i\left\{\frac{1}{2}(\partial \Delta^{(0)}(x)) + \Delta^{(0)}(x) \partial\right\} \sigma_1. \tag{3.10}
\]

Because the electrons near the edges of the electron bands suffer the attractive potential given by the acoustic component of the order parameter $\tilde{\zeta}(x)$, the second and the fourth term in the right-hand side of eq.(3.9) is included in the unperturbed Hamiltonian $h^{(0)}$. Substituting eqs.(3.1) and (3.2) into eqs.(2.15) and (2.16), the selfconsistency equations become

\[
\Delta^{(0)}(x) = -\frac{4\alpha^2}{K} a \sum_{k,s} \psi_{k,s}^{(0)}(x) \sigma_1 \psi_{k,s}^{(0)}(x), \tag{3.11}
\]

\[
\Delta^{(1)}(x) = -\frac{4\alpha^2}{K} a \sum_{k,s} \psi_{k,s}^{(0)}(x) \sigma_1 \psi_{k,s}^{(1)}(x) + \psi_{k,s}^{(1)}(x) \sigma_1 \psi_{k,s}^{(0)}(x) \tag{3.12}
\]

\[
\zeta^{(0)}(x) = -\frac{4\alpha^2}{K} a \sum_{q,s} \varphi_{q,s}^{(0)}(x) \sigma_3 \varphi_{q,s}^{(0)}(x), \tag{3.13}
\]

\[
\zeta^{(1)}(x) = -\frac{4\alpha^2}{K} a \sum_{q,s} \varphi_{q,s}^{(0)}(x) \sigma_3 \varphi_{q,s}^{(1)}(x) \tag{3.14}
\]

Using eqs.(3.3), (3.5), (3.7), (3.9), (3.11) and (3.13), an unperturbed solution is obtained.

Equations (3.7) and (3.11) are the same equations as in the TLM model. Thus, in the soliton case, the unperturbed solution $\psi^{(0)}(x)$ for the scattering state is given by eq.(2.18) and the solution for the mid-gap state is given by eq.(2.21). Our model does not modify the electron wave function near the Fermi level which is given by the TLM model.

The optical component of the order parameter is given by

\[
\Delta^{(0)}(x) = \Delta_0 \tanh \kappa x. \tag{3.15}
\]
The band gap $\Delta_0$ is given by the equation
\[
1 = 2\lambda \log \left( \frac{2v_F\Lambda}{\Delta_0} \right),
\]
(3.16)
where $\Lambda$ is introduced as the cut off of the wave number $k$.

The wave function of the electron near the bottom of the valence band or the top of the conduction band is obtained by eqs. (3.5) and (3.9). The wave function $\varphi$ is given by
\[
\varphi_q^{(0)}(x) = \begin{pmatrix} \phi_q(x) \\ 0 \end{pmatrix},
\]
(3.17)
\[
E_q = -2t_0 + \varepsilon_q,
\]
(3.18)
for the valence band, and by
\[
\varphi_q^{(0)}(x) = \begin{pmatrix} 0 \\ \phi_q(x) \end{pmatrix},
\]
(3.19)
\[
E_q = 2t_0 - \varepsilon_q,
\]
(3.20)
for the conduction band. The functions $\phi_q(x)$ are solutions of the Schrödinger equation
\[
\varepsilon_q \phi_q(x) = \left( -\frac{m_1}{2} \Delta_0 \partial^2 + \zeta^{(0)}(x) + m_1 \zeta^{(1)}(x) \right) \phi_q(x),
\]
(3.21)
where $\zeta^{(0)}(x)$ and $\zeta^{(1)}(x)$ is the real function given by the selfconsistency equation (3.13) and (3.14). The quantity $\varepsilon_q$ is the eigen-value of eq.(3.21). As it will be shown later, the forms of $\zeta^{(0)}(x)$ and $\zeta^{(1)}(x)$ do not depend on the structure of $\phi_q(x)$. Because $\phi_q(x)$ is the solution of the second order differential equation, there is a completeness relation,
\[
\sum_q \phi_q^*(x) \phi_q(y) = \delta(x - y).
\]
(3.22)
where $\phi_q(x)$ is renormalized as $\int \phi_q^*(x) \phi_q(x) dx = 1$. In eq.(3.22), the summation is taken over all eigen-functions $\{\phi_q(x)\}$. From the selfconsistency equation (3.13) and the completeness relation (3.22), the zeroth order part of the acoustic component of the order parameter, $\zeta^{(0)}(x)$, is the constant. Since, from eq.(2.5), the integration over $x$ of $\zeta(x)$ is zero, we obtain
\[
\zeta^{(0)}(x) = 0.
\]
(3.23)
Therefore, substituting eq.(3.23) into (3.3), the first order Hamiltonian $H^{(1)}$ is zero. From eq.(3.4), the first order wave function is zero.
\[
\psi^{(1)}(x) = 0.
\]
(3.24)
Substituting eqs.(3.19) and (3.24) into eq.(3.12), the first order term with respect to \( m_1 \) of the optical component of the order parameter, \( \Delta^{(1)}(x) \), is given by

\[
\Delta^{(1)}(x) = 0. \tag{3.25}
\]

From eqs.(3.6) and (3.10), the first order electron wave function \( \varphi^{(1)}_q(x) \) is given by the perturbation.

\[
\varphi^{(1)}_q(x) = -i \int_{-\infty}^{\infty} dy Q_q(x, y) \left( \frac{1}{2} \text{sech}^2 \kappa x + \tanh \kappa x \partial \right) \sigma_1 \varphi^{(0)}_q(y), \tag{3.26}
\]

where we used eq.(3.15). \( Q_q(x, y) \) is the perturbation kernel,

\[
Q_q(x, y) = \sum_{q'}'' \frac{\Delta_0 \varphi^{(0)\dagger}_q(x) \varphi^{(0)}_q(y)}{E_q - E_{q'}}. \tag{3.27}
\]

In the summation \( \sum'' \) over \( k' \), the wave number \( q = q' \) where \( \text{sgn}(E_q) = \text{sgn}(E_{q'}) \) is excluded. Substituting eqs.(3.17) and (3.19) into eq.(3.27), the kernel \( Q_q(x, y) \) for the valence band becomes

\[
Q_q(x, y) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \Delta_0 \sum_{k', E_{q'} < 0}'' \frac{\phi_{q'}(x) \phi_{q'}^*(y)}{\varepsilon_q - \varepsilon_{q'}} \Delta_0 \sum_{k', E_{q'} > 0}'' \frac{\phi_{q'}(x) \phi_{q'}^*(y)}{|E_q| + |E_{q'}|} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \frac{\Delta_0}{2} \delta(x - y), \tag{3.28}
\]

where \( \varepsilon_q \) is the eigenvalue of the Schrödinger equation (3.21). In the calculation from the first line to the second, we approximated \(|E_q| + |E_{q'}|\) by \( 2 \times (2t_0) \), since \( \varepsilon_q/(2t_0) \) is the quantity of the order of \( m_1^2 \). We used the completeness of \( \phi_k(x) \), eq.(3.22). As in the same way as eq.(3.28), substitution of eq.(3.17) into eq.(3.27) gives the kernel \( Q(x, y) \) for the conduction band,

\[
Q_q(x, y) \simeq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \frac{m_1}{2} \delta(x - y) - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \Delta_0 \sum_{k', E_{q'} > 0}'' \frac{\phi_{q'}(x) \phi_{q'}^*(y)}{\varepsilon_q - \varepsilon_{q'}}. \tag{3.29}
\]

From eqs.(3.26), (3.28) and (3.29), the first order wave function is

\[
\varphi^{(1)}_q(x) = -i \text{sgn}(E_q) \frac{m_1}{2} \left( \frac{1}{2} \text{sech}^2 \kappa x + \tanh \kappa x \partial \right) \sigma_1 \varphi^{(0)}_q(x). \tag{3.30}
\]

The perturbation Hamiltonian \( h^{(1)} \) is expressed by using \( \sigma_1 \). As we can see from eqs.(3.17) \sim (3.20), this matrix causes the mixture of the electron wave functions at the valence band and the wave functions at the conduction band. Because the
energy difference between eqs. (3.18) and (3.20) is the order of $4t_0$, the perturbation term $\varphi^{(1)}_q(x)$ is the order of $\Delta_0/(4t_0) \times \varphi^{(0)}_k(x) \sim m_1 \varphi^{(0)}_q(x)/2$. Then, the perturbation Hamiltonian $h^{(1)}$ gives the second order contribution to the electron wave function $\varphi_q(x)$. Substituting eqs. (2.21), (3.17) and (3.30) into eq. (3.14), $\zeta^{(1)}(x)$ is given by

$$\zeta^{(1)}(x) = -\frac{\Delta_0}{2} \text{sech}^2 \kappa x,$$  (3.31)

while $\varphi^{(1)}_q(x)$ gives no contribution to the acoustic component of the order parameter $\tilde{\zeta}(x)$. This result is the same as eq. (2.24). Because of the completeness of the electron wave function $\varphi_q(x)$, the electronic states near the edges of the band do not modify the order parameter up to the first order with respect to $m_1 = a/\xi$. The order parameters are determined by the electrons near the Fermi level.

§4. Electronic States at the Band Edges

The electron wave function near the edges of the electron band is given by eq. (3.17), where the function $\phi_q(x)$ is the solution of the Schrödinger equation (3.21). Because the acoustic component of the order parameter, in the soliton case, is given by eq. (3.31), this equation is written as follows:

$$2\varepsilon \frac{\Delta_0}{m_1 \Delta_0} \phi(x) = \left( -\frac{d^2}{d(x \kappa)^2} - \text{sech}^2 \kappa x \right) \phi(x).$$  (4.1)

Using the hypergeometric function, $\phi(x)$ for a positive $\varepsilon$ is written by

$$\phi_q(x) = e^{i\xi q} F[1 + \beta_0, -\beta_0, 1 + i\xi q; \frac{1 + \tanh(\kappa x)}{2}],$$

$$\frac{2\varepsilon}{m_1 \Delta_0} = (\xi q)^2.$$  (4.2)

where $q$ is the wave number. $\beta_0$ is defined by eq. (A.6). The details of the calculation are given in the Appendix A. From eqs. (3.17) and (1.2), the electron energy $E_q$ is given by

$$E_q = \pm 2t_0 \left( 1 - \frac{m_1^2 (\xi q)^2}{2} \right).$$  (4.3)

As eq. (4.1) is symmetric under the transformation $x \rightarrow -x$, $\phi_q(-x)$ is also a solution with $(2\varepsilon)/m_1 \Delta_0 = (\xi q)^2$. We use combination of $\phi_q(x)$ and $\phi_q(-x)$, which are defined by

$$\phi_{q,i}(x) = \frac{1}{\sqrt{L([1 \pm b(\xi q)]^2 + |a(\xi q)|^2)}} [\phi_q(x) \pm \phi_q(-x)].$$  (4.4)
where the upper sign corresponds to \( i = e \) (even) and the lower sign to \( i = o \) (odd).

The normalization factor is calculated in the Appendix B. A negative \( \varepsilon \) corresponds to the localized solution. It is given by

\[
\phi_{\ell}(x) = \sqrt{\frac{\Gamma(1 + 2\beta_0)}{\xi \Gamma(1 + \beta_0) \Gamma(\beta_0)}} \left( \frac{\text{sech} (\kappa x)}{2} \right)^{\beta_0}.
\]  

From eqs. (3.17) and (4.5), the energies of the weakly localized states are

\[
E_{\ell} = \pm 2t_0 \left( 1 + \frac{m_1^2}{2} \beta_0^2 \right). \tag{4.6}
\]

This form is the same as the eq.(4.28) given in ref. [9]. In the finite band version of the TLM model, the quantity \( \beta_0 \) is given by

\[
\beta_0 \approx \sqrt{\frac{5 - 7\lambda - 1}{2}}. \tag{4.7}
\]

In the present theory, the electron cosine band is linearized. Then, the contribution of the order \( \lambda \) is dropped from \( \beta_0 \) and the quantity \( m_1 \) in the present theory is a little larger than that obtained in the finite band version of the TLM model.

Substituting eqs. (4.4), (4.5), (3.17) and (3.19) into eq. (2.10), we obtain the electron wave function \( \Phi_q \),

\[
\Phi_{q,i}(x) = \sqrt{a\phi_{q,i}(x)} \times \begin{cases} 
1 & \text{for } E_q < 0, \\
e^{2ik_Fx} & \text{for } E_q > 0,
\end{cases} 
\]

\[
\Phi_{\ell}(x) = \sqrt{a\phi_{\ell}(x)} \times \begin{cases} 
1 & \text{for } E_{\ell} < 0, \\
e^{2ik_Fx} & \text{for } E_{\ell} > 0,
\end{cases} \tag{4.8}
\]

with \( i = e, o \). The wave function \( \Phi_{\ell}(x) \) of the electron at the bottom of the valence band is shown in Fig.2. The band structure is schematically shown in Fig.3. We have selected the cut off of the wave number \( q \) as \( \Lambda_\phi = k_F/2 = \pi/(4a) \) and the cut off of \( k \) as \( \Lambda = k_F/2 \).

§5. Phase Shift of the Extended States in the Electron Band

The localized states corresponding to those discussed in the previous section were also obtained by the numerical calculation of the soliton in the SSH model. It was shown that there were two branches in the phase shift of the electron wave function in the SSH model. The phase shift for the electron wave function with even parity approached \(-\pi\) as \( q \to 0 \), while that for the wave function with odd parity approached 0 as \( q \to 0 \).
The behavior of the phase shift is reproduced by our analytic wave function, eq.(4.4). As $|x| \to \infty$, the electron wave function, eq.(4.4), behaves like

$$
\Phi_{q,i}(x) = \sqrt{a}L(1 \pm b(q)) + |a(q)| \times [a(q)e^{iq|x|} + (b(q) \pm 1)e^{-iq|x|}],
$$

(5.1)

where $i = e, o$ denotes even or odd parity. $D_n$ is defined as

$$
D_n = \begin{cases} 
1, & \text{for the valence band} \\
\exp(2ik_Fx), & \text{for the conduction band}. 
\end{cases}
$$

(5.2)

Equation (5.1) is rewritten as

$$
\Phi_{q,e}(x) = \sqrt{a}L(1 + b(q)) + |a(q)| D_n \cos(q|x| - \delta_e / 2),
$$

$$
\Phi_{q,0}(x) = \sqrt{a}L(1 - b(q)) + |a(q)| D_n \sin(q|x| - \delta_o / 2),
$$

(5.3)

where

$$
e^{i\delta_e} = \frac{1 + b(q)}{a(q)},
$$

$$
e^{i\delta_o} = \frac{1 - b(q)}{a(q)}.
$$

(5.4)

We plot the phase shifts $\delta_e$ and $\delta_o$ in Fig.4(a). They are drawn in the region from $q = 0$ to $q = \Lambda_\phi$, where we selected $\Lambda_\phi$ as $k_F/2$. Figure 4(b) shows the phase shifts obtained by the numerical calculation in the SSH model. The agreement between the analytical result and the numerical one is remarkably good. The $\delta_e$ approaches $-\pi$ as $q \to 0$, while $\delta_o$ approaches 0 as $q \to 0$. The both phase shifts, $\delta_e$ and $\delta_o$, increase and approach to 0 at the cut off $q \sim \Lambda_\phi$. These behaviors indicate that of the electron plane waves near the edges of the electron band are pulled into the soliton center by the attractive potential $\zeta(x)$. This result is consistent with Levinson’s theorem. The theorem says that the number of localized states at the bottom of the band reflects the phase shift. If the numbers of localized states with even and odd parities are $n_e$ and $n_o$, respectively, the phase shifts of the even and odd extended states go to $-(2n_e - 1)\pi$ and $-2n_o\pi$, respectively, as $q \to 0$. The present case corresponds to $n_e = 1$ and $n_o = 0$.

The phase shift near the Fermi level is given by

$$
e^{i\delta} = \frac{E_\gamma}{1 + \gamma},
$$

(5.5)
where $\gamma$ is the quantum number defined by eq. (2.19). This phase shift (5.5) is the same as that obtained in the TLM model. We have to be careful about the definition of the wave number. At the Fermi level, $k(=\gamma/\xi)$ is zero. Thus $k$ is considered as the deviation of the wave number from $k_F$. Therefore,

$$k = q - k_F.$$

The phase shift $\delta$ in the valence band is plotted as the function of $q$ in Fig. 4(a). $k = 0$ corresponds to $q = k_F$ and the cut off $k = -\Lambda = -k_F/2$ corresponds to $q = k_F - \Lambda = k_F/2$, respectively. The phase shift $\delta$ increases as $q$ becomes larger, approaching to $\pi/2$ as $q \to k_F$. This behavior is also in good agreement with the numerical result shown in Fig. 4(b). There is a discontinuity of the phase shift at $q = \Lambda$. This is because we have used eq.(2.11) for $0 \leq q < \Lambda$ and eq.(2.13) for $\Lambda < q \leq k_F$.

§6. Summary and Discussion

We have studied the effects of lattice discreteness on a soliton in the SSH model using a modified version of the continuum (TLM) model. We solved this model in the adiabatic limit.

When there is a soliton in the SSH model, the arrangement of the double bonds is changed and the ions near the soliton are shifted to the soliton center. Then, the acoustic component of the order parameter, $\tilde{\zeta}(x)$, has non-zero amplitude near the soliton center and it acts as a potential for the electrons at the band edges. Since $\zeta(x)$ acts as an attractive potential, weakly localized states appear at the band edges. The levels are very close to the corresponding band edges. Because the amplitude of the acoustic component is very small (of the order $\kappa a/\Delta_0$), the states are more weakly localized than the mid-gap state. In the TLM model, this effect (the acoustic component) is not included because the interaction between the acoustic component $\zeta(x)$ and the electrons at the bottom of the valence band is omitted in the continuum limit.

To improve the TLM model, we have taken into account the electronic wave function at the bottom of the valence band and the top of the conduction band in addition to the electron wave function at the Fermi level. We have considered the discreteness by taking into account the terms of higher order in $a/\xi$, when the expansion parameter $a/\xi$ is sufficiently small. We have studied the electronic states of electrons, using the unperturbed Hamiltonian eqs.(3.7) and (3.9), which are composed of the zeroth and a part of the first order terms with respect to $m_1$. The selfconsistency between the electrons and the order parameters have been satisfied up to the first order of $m_1$.

The wave functions of weakly localized states are given by eq.(4.8). The energy levels of the localized states are given by eq.(4.6). This result has the same form as
given in the finite band version of the TLM model. Concerning the scattering states, we have obtained the dispersion relation, eqs. (2.20) and (4.3), which corresponds to the scattering states in the SSH model.

\[ E_q = \pm \sqrt{(2t_0)^2 \cos^2(qa) + \Delta_0^2 \sin^2(qa)}. \] (6.1)

The wave functions are given by eqs. (4.2) and (4.4). Using these wave functions, the phase shift analysis has been performed for the two groups of the electronic states, with even and odd parities respectively. The two phase shifts coincide with each other over a wide range of the wave number. In the regions of small wave numbers, the two take different values which are consistent with the fact that there are localized states with even parity.

Using the present model, the order parameters, eqs. (2.17) and (2.24), which were given by ref. [4], have been reproduced. In the expression of the electron wave functions near the band edges, eq. (4.8), the complete set of the function \( \{ \phi_{q,i}(x) \} \) have been introduced. Because of the completeness of \( \{ \phi_{q,i}(x) \} \), the acoustic component of the order parameter, \( \tilde{\zeta}(x) \), is unmodified by the weakly localized states at the edges of the band. The order parameters are determined by the electrons near the Fermi level.

We have made a modified version of the TLM model and solved it perturbationally up to the first order with respect to \( a/\xi \). The present model has a merit that it can deal with the electrons near the bottom of the band as well as those near the Fermi level. It has another advantage that we can treat the interaction between the electron and the acoustic component of the order parameter. Thus, this model is suitable for analyzing the interaction between the acoustic phonon and the non-linear excitation. It is interesting to study the diffusion motion of the nonlinear excitation induced by the interaction using this model.

To obtain the exact result up to the second order of \( \kappa a \), we should make a higher order perturbation calculation. However, since the cosine band in the SSH model is linearized by the continuation procedure, the contributions of the order \( \lambda \cdot m_1, m_1^2 \) and higher which come from the scattering states are omitted. Kurita et al. obtained the acoustic component, \( \tilde{\zeta}(x) \), using the finite band version of the TLM model. \( \tilde{\zeta}(x) \) was given by

\[ \tilde{\zeta}(x) \sim -m_1 \left( \frac{1}{2} - \frac{7}{8} \lambda \right) \Delta_0 \cosh^{-2} \kappa x + O(m_1^2). \] (6.2)

Then, our result of the acoustic component, eq. (3.31), is a bit larger than that of the SSH model. To make higher order perturbation selfconsistently, we should construct the unperturbed Hamiltonian using the finite band version of the TLM model. It is a bit tedious but important problem to explore.

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APPENDIX

Appendix A: Solutions of the Differential Equation (4.2)

In this Appendix, we will consider the differential equation

\[ \varepsilon' \phi(x) = -\frac{d^2}{d(\kappa x)^2} \phi(x) - \text{sech}^2(\kappa x) \phi(x). \]  

(A.1)

First, the localized solution with a negative \( \varepsilon' \) will be considered. Introducing \( t(\theta) \) and \( \theta \) by

\[ \phi_\ell(x) = \left(1 - \tanh^2 \kappa x\right) \sqrt{-\varepsilon'} \theta t(\theta), \]

(A.2)

\[ \theta = 1 + \tanh \kappa x. \]

(A.3)

We write eq.(A.1) in the form

\[ \left[ \theta(1 - \theta) \frac{d^2}{d\theta^2} + (1 + \sqrt{-\varepsilon'})(1 - 2\theta) \frac{d}{d\theta} - (2R - \varepsilon' + \sqrt{-\varepsilon'}) \right] t(\theta) = 0. \]

(A.4)

This is the hypergeometric differential equation. \(^3\) With the help of eqs.(A.2) and (A.3), the solution \( \phi_\ell(x) \) is given by a hypergeometric function

\[ \phi_\ell(x) = \left[4\theta(1 - \theta)\right]^\frac{\sqrt{-\varepsilon'}}{2} F\left[\sqrt{-\varepsilon'} - \beta_0, \sqrt{-\varepsilon'} + \beta_0 + 1, \sqrt{-\varepsilon'} + 1, \theta\right], \]

(A.5)

where

\[ \beta_0 = (\sqrt{5} - 1)/2. \]

(A.6)

As we can see from eq.(A.2), \( \phi_\ell(x) \) approaches zero, as \( x \) goes to \(-\infty\). In order that \( \phi_\ell(x) \) is finite in the limit of \( x \to \infty \), the hypergeometric function \( F \) should be a polynomial. So we can put \( \sqrt{-\varepsilon'} - \beta_0 = -n \) with a non-negative integer \( n \). Since \( \beta_0 \) is about 0.6, \( n \) should be zero. Then we have

\[ \sqrt{-\varepsilon'} = \beta_0. \]

(A.7)

As \( \beta_0 \) is positive, we have a localized solution

\[ \phi_\ell(x) = \left[\theta(1 - \theta)\right]^{\beta_0} F\left[0, 2\beta_0 + 1, \beta_0 + 1, \theta\right] \]

\[ = \left(\text{sech} \kappa x\right)^\beta_0. \]

(A.8)

The eigen value \( \varepsilon' \) is given by

\[ \varepsilon' = -\beta_0^2/2. \]

(A.9)
To obtain the solutions of scattering states with a positive $\varepsilon'$, we replace $\sqrt{-\varepsilon'}$ in eq. (A.3) by $i\gamma$, that is $\varepsilon' = \gamma^2$, to get

$$\phi_\gamma(x) = [\theta(1 - \theta)]^{i\gamma} F[-\beta_0 + i\gamma, \beta_0 + 1 + i\gamma; \theta].$$ (A.10)

The hypergeometric function has the following relations

$$F[\alpha, \beta, \gamma; \theta] = (1 - \theta)^{-\alpha - \beta} F[\gamma - \alpha, \gamma - \beta, \gamma; \theta],$$ (A.11)

$$F[\alpha, \beta, \gamma; \theta] = \frac{\Gamma(\alpha + \beta - \gamma)\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}(1 - \theta)^{-\alpha - \beta} F[\gamma - \alpha, \gamma - \beta, \gamma - \alpha - \beta + 1; 1 - \theta]$$

$$+ \frac{\Gamma(\gamma)\Gamma(\gamma - \alpha - \beta)}{\Gamma(\gamma - \alpha)\Gamma(\gamma - \beta)} F[\alpha, \beta, \alpha + \beta - \gamma + 1; 1 - \theta].$$ (A.12)

We write $\phi_\gamma$ as a function of $1 - \theta$, using eqs. (A.11) and (A.12) and the relation $e^{-2x} = \frac{1 - \theta}{\theta}$ to get

$$\phi_\gamma(x) = e^{i\gamma x} F[1 + \beta_0, -\beta_0, 1 + i\gamma; \theta]$$

$$= b(\gamma)\phi_\gamma(-x) + a(\gamma)\phi_{-\gamma}(-x),$$ (A.13)

where

$$a(\gamma) = \frac{\Gamma(1 + i\gamma)\Gamma(i\gamma)}{\Gamma(1 + \beta_0 + i\gamma)\Gamma(-\beta_0 + i\gamma)},$$

$$b(\gamma) = \frac{\Gamma(1 + i\gamma)\Gamma(-i\gamma)}{\Gamma(1 + \beta_0)\Gamma(-\beta_0)}.$$ (A.14)

We rewrite $\phi_\gamma(x)$ by $q = \gamma/\xi$,

$$\phi_q(x) = \phi_\gamma(x) = e^{iqx} F[1 + \beta_0, -\beta_0, 1 + i\xi q; \theta],$$ (A.15)

$q$ is the wave number of the electron at the band edges. From eqs. (A.13) and (A.15), we can see that the function $\phi_\gamma$ has the asymptotic forms

$$\phi_\gamma(x) = \begin{cases} 
  e^{iqx} & \text{as } x \to -\infty, \\
  a(\xi q)e^{iqx} + b(\xi q)e^{-i\xi q} & \text{as } x \to \infty.
\end{cases}$$ (A.16)

Appendix B: Calculation of Normalization Factor

Consider an hermitian operator $L_0$ and its eigen function $u_\gamma(x)$

$$L_0 = -\frac{d^2}{dz^2} + U(z),$$

$$L_0 u_\gamma = E(\gamma) u_\gamma,$$ (B.1)
where the eigenvalue $E(\gamma)$ is related to the quantum number $\gamma$ by $E(\gamma) = \gamma^2$. We differentiate eq. (B.1) by $\gamma$ and multiply by $u^*_{\gamma}$ from the left to obtain
\[
 u^*_{\gamma}(L_0 - \gamma^2)u_{\gamma} = 2\gamma u^*_{\gamma}u_{\gamma}. \tag{B.2}
\]
The hermitian conjugate expression of eq. (B.1) gives
\[
 (L_0u^*_{\gamma} - \gamma^2u^*_{\gamma})u'_{\gamma} = 0. \tag{B.3}
\]
The difference between the two is integrated to give
\[
 \left[ \frac{d}{dz}u^*_{\gamma} - u^*_{\gamma}\left(\frac{d}{dz}u'_{\gamma}\right) \right] = 2\gamma \int_b^a u^*_{\gamma}d\gamma. \tag{B.4}
\]
Suppose we put
\[
 u_{\gamma} = \phi_{\gamma}(x) \pm \phi_{\gamma}(-x), \tag{B.5}
\]
which give $\phi_{\gamma, i}(x)$. With the help of eq. (A.16), we get
\[
 \int_{-L/2}^{L/2} |\phi_{\gamma, i}(x)|^2 dx = \int_{-L/2}^{L/2} |u_{\gamma}(x)|^2 dx = (|1 \pm b(\gamma)|^2 + |a(\gamma)|^2)L + O(1) \tag{B.6}
\]
The wave functions of the localized states eq. (A.5) can be obtained from $u_{\gamma}(x)$, if we perform an analytic continuation
\[
 \gamma \to \gamma_1 = i(\alpha - n), \tag{B.7}
\]
where $n$ is a non-negative integer. Equation (B.4) becomes
\[
 \left[ \frac{d}{dz}u_{\gamma_1} - u_{\gamma_1}\left(\frac{d}{dz}u'_{\gamma_1}\right) \right] = 2\gamma_1 \int_b^a (u_{\gamma_1})^2 dz. \tag{B.8}
\]
Since eq. (A.14) gives
\[
 a(\gamma_1) = 0, \quad b(\gamma_1) = i(-1)^n, \quad \text{for } \gamma_1 = i\beta_0
\]
substitution of eq. (A.16) with $\gamma = \gamma_1$ into eq. (B.8) gives
\[
 N^{-2} = \int_{-L/2}^{L/2} (\phi_{1, \gamma_1}(x))^2 dx
 = ia'(\gamma_1)b(\gamma_1)/\kappa
 = \frac{n! \Gamma(\beta_0 + 1 - n)\Gamma(\beta_0 - n)}{\kappa \Gamma(1 + 2\beta_0 - n)}. \tag{B.9}
\]
In particular, for $\phi_{\ell}$
\[
 \int_{-L/2}^{L/2} \cosh(\kappa x)^{-2\beta_0} dx = \frac{2^{2\beta_0} n! \Gamma(\beta_0 + 1)\Gamma(\beta_0)}{\kappa \Gamma(1 + 2\beta_0)}. \tag{B.10}
\]
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Figure Captions

Fig. 1: Levels of localized states of a soliton. Two states, B and C, are close to the band edges and weakly localized. The energy of these two states are given by eq. (1.0). The state A is a mid-gap state.

Fig. 2: Electron density distributions of the bound state wave functions for the coupling constant $\lambda = 0.2$. The ordinate is scaled by $1/\xi$. The abscissa is $x/\xi$. $|\Phi_\ell|^2$ is the electron density at the bottom of the valence band. $|\Phi_M|^2$ is the electron density in the mid-gap localized state.

Fig. 3: Schematic electronic band structure of a soliton. The dispersion relation at the Fermi level, eq. (2.20), is plotted as the function of $k = q - k_F$, which is identical with that of the TLM model. The dispersion relation at the band edges, eq. (1.3), have a parabolic form, which is plotted as the function of $q$. We selected the cut off as $\Lambda = \Lambda_\phi = k_F/2$.

Fig. 4: Phase shifts of the wave functions as a functions of $q$. The dimensionless coupling constant $\lambda$ is selected as 0.2. The ordinate is scaled by $1/\pi$. The abscissa is $q/k_F$.
   a) The phase shifts $\delta_e$ and $\delta_o$ given by eq. (5.4). $\delta$ is the phase shift of electrons near the fermi level. We selected the cut off as $\Lambda = \Lambda_\phi = k_F/2$.
   b) The phase shift of electrons in the SSH model obtained in ref. 7.