Localization and electron-phonon interaction in disordered systems

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Localization and electron-phonon interaction in disordered systems

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Yi Wan

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I. INTRODUCTION

The interactions between electrons and disorder, and between electrons and lattice vibrations, exist in any real solid state material. The impurities often appear in the electron system as random potentials whose distributions are described by models of disorder. Disorder modifies the motion of an electron in a rigid three-dimensional system in profound ways. The extended Bloch states develop phase incoherence and amplitude fluctuations. The sharp band edges disappear and tails of localized states emerge. The latter are separated from the extended states by mobility edges which move into the band with increasing disorder for dimensionality $2 < d < 4$. In the last two decades, our understanding of a number of important issues in the field of localization, such as the nature of the mobility edge, the energy dependence of the conductivity, the localization length and the amplitude fluctuation length, the basis for scaling arguments, and many others has been greatly advanced [1].

Electron-phonon interactions also have dramatic effects in some cases. For instance, in one-dimensional or quasi-one-dimensional systems, the interaction between electrons and lattice vibrations can give rise to a lattice distortion (the Peierls distortion) [2]. It is also well known [3], that in the case of one electron in a one-dimensional periodic lattice, a lattice distortion in the form of a polaronic state occurs in the presence of the electron-phonon interaction.

Very little has been done to study the combined effects of disorder and electron-phonon interaction. It has been argued that the electron-phonon coupling has profound effect on the characteristic fea-
tures of a disordered system. For example, it strongly enhances localization, inducing polaron formation at the mobility edge, even for vanishingly small coupling [4]. On the other hand, disorder also has important effect on the polaron formation. In a crystalline system, the states at the bottom of the energy band are the last to become unstable against polaron formation as the electron-phonon coupling increases. Yet, as soon as an infinitesimal amount of disorder is introduced, those states are among the first to become unstable. In this case, the impurities play the role of nucleation centers in the polaron formation [5].

It is clear, then, that the electron-phonon interaction and disorder are of comparable importance and should be so treated. However, as a matter of fact, this has not been done. In an effort to understand this problem, we will therefore study the effects of coupling between electrons and phonons in a one-dimensional disordered system. We choose one-dimensional system because considerable analytical and numerical work has been done for the localization problem in one-dimension. In addition, the Peierls distorted state in a one-dimensional electron-phonon system, as an approximation to the quasi-one-dimensional crystalline material, has been realized in experimental situations.

In this chapter, we discuss briefly the physical aspects of the Kohn effect, which is regarded as the cause of the Peierls instability in coupled electron-phonon system, and the electron localization in disordered system. Then we state the objective of our study and the models and methods to be discussed in subsequent chapters.
A. Kohn Effect and Peierls Instability

The Kohn effect \[6\] reflects the influence of electrons on the phonon dynamics in a coupled electron-phonon system. Its relation to the Peierls instability can be studied in a self-consistent scheme by taking into account both the electronic contribution to lattice dynamics and the phonon modification to the electron dynamics. The basic cause of the Kohn effect can be understood in elementary terms as the screening effect of the electrons. The polarization of the electron gas due to the excitation of electron-hole pairs with wave vector \(q\) and frequency \(\omega\) is written as

\[
\Pi_0(q, \omega) = \sum_k \frac{f_k - f_{k+q}}{\omega + \epsilon_k - \epsilon_{k+q}},
\]

where \(f_k\) is the Fermi distribution function, and \(\epsilon_k\) is the electron energy. At zero temperature the Fermi surface is sharp and \(q = 2k_F\) becomes the point where the Fermi surfaces corresponding to \(k\) and \(k + q\) no longer overlap. This results in a logarithmic singularity at \(2k_F\) in the electron polarization in one-dimensional system,

\[
\Pi_0(q, 0) \sim N_0 \ln \left| \frac{k_F}{q - 2k_F} \right|,
\]

where \(N_0\) is the electron density of states at the Fermi level.

Traditionally, the electron-phonon interaction is studied in the Fröhlich jellium model \[7\], whose Hamiltonian has the following one-dimensional form \((\hbar = 1)\),

\[
H = H_e + H_p + H_{ep}.
\]
\[ H_e = \sum_k \epsilon_k c_k^{\dagger} c_k, \]
\[ H_p = \sum_q \Omega(q)(B_q^{\dagger} B_q + \frac{1}{2}), \]
\[ H_{ep} = L^{-1/2} \sum_{kq} g(q) c_{k+q}^{\dagger} c_k (B_q + B_{-q}^{\dagger}), \quad (1.1) \]

where \( c_k, c_k^{\dagger} \) are the annihilation and creation operators for the conduction electron with wave vector \( k \) and band energy \( \epsilon_k \); \( B_q, B_q^{\dagger} \) are the corresponding operators for the phonon with wave vector \( q \) and frequency \( \Omega(q) \); \( g(q) \) is the electron-phonon coupling constant, \( L \) is the length of the system, and the summation over electron spin is implicitly included. The electronic and phonon dynamics can be described by the temperature Green's functions at temperature \( T \)

\[ G^{-1}(k, i\omega_n) = G_0^{-1}(k, i\omega_n) - \Sigma(k, i\omega_n), \quad (1.2a) \]
\[ D^{-1}(q, i\Omega_n) = D_0^{-1}(q, i\Omega_n) - \Pi(q, i\Omega_n), \quad (1.2b) \]

where \( \omega_n = (2n + 1)\pi/T, \Omega_n = 2n\pi/T, n = \text{integer} \) (Boltzmann constant \( k_B = 1 \)), and the bare electron and phonon Green's functions are, respectively

\[ G_0(k, i\omega_n) = \frac{1}{i\omega_n - \epsilon_k}, \quad D_0(q, i\Omega_n) = \frac{1}{\Omega^2(q) - (i\Omega_n)^2}. \]

The phonon contribution to the electron motion is described by the electron self-energy, \( \Sigma(k, i\omega_n) \). Likewise, the electron affects the phonon dynamics by modifying the phonon frequency through the phonon self-energy \( \Pi(q, i\Omega_n) \).
The electron and phonon self-energies can be calculated with perturbation method. From the Feynman diagrams shown in Fig. 1(a) and 1(b), we see that $\Pi(q, i\Omega_n)$ is given by the bare electron polarization

$$\Pi(q, i\Omega_n) = -2T \sum_{nk} |g(q)|^2 G_0(k, i\omega_n) G_0(k + q, i\omega_n + i\Omega_n) . \quad (1.3)$$

Its main effect is to renormalize the phonon frequency to

$$\tilde{\Omega}^2(q) = \Omega^2(2k_F) \left[ \ln \frac{T}{T_p} + \xi_0^2(q - 2k_F)^2 \right] , \quad (1.4)$$

where the dimensionless coupling constant $\lambda = N_0 |g(2k_F)|^2 / \Omega^2(2k_F)$, with $N_0$ the electron density of states at the Fermi level. $\xi_0$ is the coherent length and the Peierls temperature $T_p \propto \epsilon_F e^{-1/\lambda}$. The Kohn effect thus expresses the fact that the phonon is softened as a result of its interaction with the electron, and the $q = 2k_F$ phonon is the softest at a given $T$ above $T_p$. In the extreme case of one-dimension, the phonon frequency decreases to zero as $T$ approaches $T_p$, due to the logarithmic singularity at $q = 2k_F$, signifying a lattice instability which results in a phase transition to a distorted lattice, the Peierls state. In the Peierls state, the lattice displacement $u_{2k_F}$ assumes a finite mean-field value, $u_{2k_F} \propto \langle B_{2k_F} \rangle$. Its effect on the electrons can thus be treated in the mean-field approximation by writing the electron-phonon interaction term in Eq. (1.1) as

$$H_{cp} = \sum_k \Delta c_{k+2k_F}^\dagger c_k + h.c. , \quad (1.5)$$

where $\Delta = L^{-1/2} \langle u_{2k_F} \rangle$, neglecting all phonons with other wave vectors. The electron problem can be solved immediately with
Fig. 1. Feynman diagrams of electron self-energy and phonon self-energy
the result that a gap opens at the Fermi energy. The electronic energy is thus given by
\[ E_k = \pm (\epsilon_k^2 + \Delta^2)^{1/2}. \]
The order parameter in the Peierls transition, \( \Delta \), is in turn determined self-consistently in the mean-field treatment of the phonon terms in the Hamiltonian, Eq. (1.1), \( \Delta \propto \sum_k \langle c^\dagger_{k+2k_F} c_k \rangle \). In this way, the lattice distortion is sustained by the lowering of electronic energy through the creation of a gap at the Fermi level.

It should be remarked that the one-dimensional system represents an extreme of reality. Many other effects must be considered to reach sensible conclusions. For instance, it is well-known that thermal fluctuations suppress phase transitions in one-dimension. However, as shown by Sham and Patton [8], in the Peierls system, the phase transition at finite \( T_p \) is reinstated by the electron-phonon interaction involving interchain phonons. The one-dimensional chain considered here is always regarded as an approximation to a three-dimensional system with weak interchain interactions, and thus studying it at \( T = 0 \) will not lose physical relevance.

B. Localization in Disordered Systems

One of the most important concepts in the disordered electronic system is the Anderson localization, introduced by Anderson in 1958 [9]. He found by solving an essentially one-dimensional tight-binding model in the presence of random potential, that the electronic motion may be profoundly altered in the way that the envelope of the electron wave function decays exponentially with distance from some point in
space,

\[ |\Psi(r)| \propto e^{-|r-r_0|/l_c}, \quad (1.7) \]

where \( l_c \) is called the localization length. In the strong disorder limit, i.e., large random potential on the electronic energy scale (e.g., the energy band width), a localized state can be understood as an electron bound state in deep fluctuation of the random potential. The main point here is that the superposition of infinitely many such bound states does not give rise to extended states. The reason, which is very useful in understanding qualitatively many features of the localization problem, is that the localized states that are nearby in space, so that their wave functions overlap significantly, are in general very different in energy.

In weak disorder case, electron localization is understood starting from the traditional picture in which the Bloch waves loose phase coherence over a distance \( l_0 \), the mean free path, and the electrons move in the form of diffusion, characterized by a diffusion constant \( D_0 = v_F^2 \tau = v_F l_0 \) in one-dimensional system, where \( \tau \) is the mean collision time. As a result, the system has finite dc conductivity \( \sigma_0 \), or nonzero residue resistance, given by the Einstein relation \( \sigma_0 = e^2 N_0 D_0 \), with \( N_0 \) the electron density of states at Fermi level. However, when quantum effects are considered, the classical diffusion picture has to be changed. As illustrated in Fig. 2, the probability for an electron to reach point B from point A is given by the summation of the propagation amplitudes for different paths

\[ P = \sum_i |A_i|^2 + \sum_{i\neq j} A_i A^*_j. \quad (1.8) \]
Fig. 2. Paths of a particle:

(a) several possible paths of a particle diffusing from A to B;

(b) the constructive interference of two time-reversal paths
The quantum mechanical effects enter through the Heisenberg uncertainty principle such that each path has a finite width $\sim k_F^{-1}$, giving rise to the interference terms (the second term in Eq. (1.8)). In disordered systems, the classical diffusion picture with sharp paths is a good approximation, since these paths lack phase coherence and, therefore, the interference terms can be neglected. But this is not the case when the path returns to its starting point. Then the amplitudes for travelling in opposite directions along this path, corresponding to the time-reversed motion of each other, interfere constructively, doubling the contribution to $P$. Thus, a quantum mechanical particle is more localized than a classical one due to the enhanced probability of scattering back to its starting place. Such a picture based on the back scattering effects is called weak localization.

In strictly one-dimensional systems, it has been shown rigorously that all the states are localized [1,10], no matter how weak the disorder is. In the weak disorder case where perturbation method is valid, the localization length is explicitly given by

$$l_c^{-1}(E) = \frac{1}{96} \frac{W^2}{4t_0^2 - E^2} + O(W^4)$$  \hspace{1cm} (1.9)

for a tight binding band $\epsilon(k) = -2t_0 \cos k a$ and rectangular distribution of disorder (see Eq. (2.3)). For stronger disorders, there is no general expression for $l_c$. One way to describe the localized states in this case is by calculating the so-called participation ratio [1], defined by

$$p^{-1}(E) = L \sum_n |\psi_n(E)|^4 ,$$  \hspace{1cm} (1.10)
where $\psi_n(E)$ is the electron eigenfunction at energy $E$ in a discrete lattice. For extended states $p \sim 1$, while $p = L_e/L$ for localized states, with $L_e$ the effective size of the state (the number of sites where $\psi_n$ is appreciable). $L_e$ is often taken as a good estimate of the localization length, $l_c$. In one dimensional problems, $p$ can be approximately calculated by, for example, diagonalizing the Hamiltonian for a finite length system.

One of the most important quantities in the localization problem is the frequency dependent conductivity, $\sigma(\omega)$, which can be compared directly with experiments, such as in the photo-absorption measurements. The dc conductivity, $\sigma$, can be obtained as its limiting value, $\sigma = \lim_{\omega \to 0} \sigma(\omega)$. $\sigma$ vanishes if the electrons at the Fermi level are localized. Also, one can calculate or measure $\sigma$ as a function of the Fermi energy, as in the metal-insulator transition problem where $\sigma$ increases from zero when a particular energy, the mobility edge, $E_c$, is exceeded.

C. Purpose of This Study

As stated at the beginning of this chapter, the central question of our study is to understand the effects of coupling between electrons and phonons in a disordered system. In the following we introduce the one-dimensional model that we will later use, and discuss several general aspects of this problem and some previous related work.
1. Reduction of energy gap and static fluctuation of order parameter

Two major effects on the Peierls gap are expected which directly result from the scattering of the electrons by the random impurities. First of all, the electrons acquire a finite life-time $\tau$, the mean-collision time, so that the Bloch states and the associated energy band are no longer well-defined. More precisely, the life-time broadening destroys the perfectly nesting Fermi surface and thus sharpness of the Kohn effect and the Peierls transition. Secondly, since the gap formation can be viewed as the result of pairing and condensation of the electrons and holes near the Fermi surface, and since the impurity potential acts in opposite way on electrons and holes, the impurity scattering has a pair breaking effect which leads to the direct reduction of the Peierls gap. This situation is quite similar to the problems of impurities in excitonic insulators and magnetic impurities in superconductor alloys, where impurity moments tend to break the spin-singlet Cooper pairs.

In disordered systems, the order parameter $\Delta$ can no longer be identified as half the Peierls gap as in the pure system. The energy gap is given by the density of states, while the order parameter is related to the expectation value of the charge density. The local charge density couples directly to the local impurity potential, and is distorted by it. Thus, in addition to the averaged order parameter, we should also study the fluctuations of the order parameter, which is the disorder average of $|\Delta|^2$. The significance of this fluctuation in the one-dimensional electron-phonon system can be understood in the following way. The electron density response is particularly strong near
2\textit{k}_F. This causes the Kohn anomaly in the phonon frequency and the spontaneous lattice distortion discussed in Section A. As pointed out by Sham and Patton [8], the same effect can cause an impurity to induce a strong static Friedel oscillation of the electron charge density with wave vectors at or near 2\textit{k}_F, which in turn induced a static lattice distortion of the same wave vector where the lattice is particularly soft. These charge density oscillations and the corresponding lattice distortion have random phases due to the random distribution of the impurities, and they have zero average effect. However, their mean-square values can be finite. Another aspect of such random charge density oscillations is their nonlocal character, and in turn act like correlated disorder for the electrons.

2. The Su-Schrieffer-Heeger model and localized excitations

Recently, there have been a great interest in conjugated polymer systems due to their unusual electronic properties [11]. These systems exist basically in the form of parallel chains and have highly anisotropic electronic band structure such that they are electronically quasi-one-dimensional. In 1979, Su, Schrieffer and Heeger introduced a model [12] to describe Polyacetylene (\textit{trans-}(\textit{CH})_x), a particularly simple system in the class of conjugated polymers, given by the following Hamiltonian:

\begin{align}
H_{SSH} &= -\sum_n [t_0 + \alpha (u_n - u_{n+1})](c_n^+ c_{n+1} + h.c.) \\
&+ \frac{K}{2} \sum_n (u_n - u_{n+1})^2 + \frac{M}{2} \sum_n \dot{u}^2, \quad (1.11)
\end{align}
where $n$ is the lattice site index, $t_0$ is the hopping matrix element of the $\pi$ electrons in the tight-binding model, and $\alpha$ is the electron-phonon coupling constant. The last two terms are the elastic and kinetic energies of the (CH) molecule, the basic unit of the lattice, with $K$ and $M$ respectively the elastic constant and the mass.

The ground state of $H_{SSH}$ consists of a dimerized lattice, since the $\pi$ electron band is half-filled (one electron per site), and a Peierls gap at the Fermi level at the band center in the electron energy band $\epsilon_k = -2t_0 \cos ka$,

$$u_n = (-1)^n u_0, \quad E_k = \pm(\epsilon_k^2 + \Delta_0^2 \sin^2 ka)^{1/2}, \quad (1.12)$$

where the dimerization amplitude $u_0$ and the order parameter $\Delta_0$ are related by $\Delta_0 = 4\alpha u_0$ and given by the dimensionless coupling constant $\lambda$ (for $\lambda \ll 1$),

$$\Delta_0 = 8t_0 e^{-1-1/\lambda}, \quad \lambda = \frac{4\alpha^2}{\pi t_0 K}. \quad (1.13)$$

The electron density of states is nonzero for $\Delta_0 \leq |E| \leq 2t_0$,

$$N(E) = \frac{1}{\pi} \frac{|E|}{[(E^2 - \Delta^2)(4t_0^2 - E^2)]^{1/2}}. \quad (1.14)$$

The elementary excitation in this system, called soliton, is localized in the lattice and has an energy level at the center of the gap. The soliton state can be viewed as a domain wall separating the two degenerate dimerized phases of the system corresponding to $\pm u_0$, and is described in terms of the lattice distortion and the electron wave function, $\varphi_n = (-1)^n u_n$ and $\psi_{sn}$, respectively,

$$\varphi_n = u_0 \tanh \frac{(n - n_0)a}{\xi}, \quad \psi_{sn} = \xi^{-1/2} \text{sech} \frac{(n - n_0)a}{\xi} \cos \frac{\pi}{2} n. \quad (1.15)$$
where $\xi = 2t_0a/\Delta$ is the soliton coherence length.

The attractiveness of the soliton concept, in contrast to the usual coupled electron-phonon excitations such as polarons, lies in its topological nature associated with the degenerate dimerized ground states. Consequently, it has separate spin and charge degrees of freedom, i.e., neutral solitons with spin $-\frac{1}{2}$, and spinless charged solitons. These distinctive features have been supported by experiments [11]. In addition, the relatively large coherent length makes a soliton quite mobile in the lattice, thus a good candidate of charge carriers in the doped systems. However, as a coupled electron-lattice state, the soliton is likely susceptible to the disorder. Its spin and charge separation can be lost when the local charge conjugation symmetry is destroyed by the charged impurities. The large coherent length may also cause pinning of the soliton by impurity and the impurity induced local lattice distortions. One of our objectives is to investigate the stability of the soliton state in a disordered system.

The parameters values we will later use are typically for Polyacetylene, and we list them here,

$$t_0 = 2.5 \text{ eV}, \quad \alpha = 5.6 \text{ eV/Å}, \quad K = 34.3 \text{ eV/Å}^2, \quad a = 1.22 \text{ Å},$$

$$w_0 = 0.04 \text{ Å}, \quad \Delta_0 = 0.89 \text{ eV}, \quad \xi = 5.6a, \quad \lambda = 0.47.$$  

(1.16)

3. Previous related work

There have been a number of works on the the effects of impurity in the realm of the Su-Schrieffer-Heeger model or its continuum
approximation [13]. Here we briefly discussed some of those which moti-
tivated our own work.

Phillpot and coworkers studied in detail the single impurity ef-
fects using mainly molecular dynamical simulations [14]. They em-
phasized the impurity induced local lattice distortions which tend to
destroy the dimerization and is stablized by occupied electron levels in
the gap and below the band edge. They interpret these as polarons,
and as a result, they studied the interaction between a soliton and a
polaron, and its effect on the photo-excitation processes.

Gomez-Santos and Yndurain [15] used the coherent potential ap-
proximation, and Xu and Trullinger [16] used the supersymmetric-field
method to find the averaged electron density of states. However, they
assumed a uniform dimerization order parameter $\Delta$ which is in turn
determined from energy minimization, consequently they reached the
conclusion that at a critical disorder $\Delta$ drops to zero discontinuously.
This is not supported by ours and other groups' studies when the lat-
tice relaxation is allowed.

Numerical energy minimization, quite similar to the one that will
be described in Chapter II, was employed by Mele and Rice [17], and
by Bulka and Kramer [18]. The former group took a distorted charge
density wave as the Ansatz for the lattice distortion. This is reason-
able for weak impurity potential, $V \leq \Delta_0$, where extra electrons in-
trduced in the doping process exist in the form of distorted charge
density wave, and the system is slightly away from the half-filled en-
ergy band. The results of Mele and Rice agree in general with the
case of weak impurity potential for the binary distribution of disor-
der discussed in Section B of the next chapter. Bulka and Kramer
paid attention mainly to the weak disorder, and in that case, their results share the same basic features with ours, i.e., the reduction of the Peierls gap and the lattice distortion, and the electronic states become more localized as the electron-phonon coupling constant increases. However, for stronger disorder, we show that there are strongly localized states accompanied by large lattice displacements.

Another motivation to this study is our previous work on the one-dimensional discrete nonlinear Schrödinger equation [19], which describes the physical system corresponding to, in the continuum approximation, the Holstein model [3], of one tight-binding electron in the presence of nonlinear interactions. It was shown there that the stability of the large polaron solution is affected by the discrete nature of the lattice. Since the Su-Schrieffer-Heeger model is discrete and the soliton is a form of the nonlinear excitation, it is of interest to study stability of the soliton excitation in the presence of the disorder.

4. Format of dissertation

In this study we focus on the Peierls instability and treat the electron-phonon interaction in the static mean-field approximation, neglecting the kinetic energy of the lattice. Our results are obtained at zero temperature, though finite $T$ can be readily included through the Fermi function in both the numerical and analytical methods. In the numerical study we have checked the effects of temperature and they do not seem to change the basic features of our results.

In the next chapter, we study numerically the disordered $H_{SSH}$ for different types of impurities. We pay attention especially to the
interplay between the electron localization and the Peierls instability. After describing the method in Section A, results are presented and discussed for different cases in Section B.

The analytic perturbation method of Chapter III is partly motivated by the numerical results which indicate that the impurity induced lattice distortion play an important roles and may be treated as correlated disorder in a perturbation approach. The formalism developed in Section A and B is in close analogy to the theories of superconductor alloy [20, 21, 22] and excitonic insulator [23], and indeed some results have the same form. However, we show that the Umklapp scattering, which is particularly important in the half-filled case have important bearings on the results, which are given in Section C and compared with the numerical data in the weak disorder case. In Section D we discuss the physical meaning of the static order parameter fluctuation due to disorder and its contribution to the electron self-energy.

Finally, in Chapter IV, we conclude by briefly summarizing our results and pointing out some possible future development.
II. NUMERICAL METHOD

A. Model and Approach

In the numerical simulation we study the following model Hamiltonian which combines the Su-Schrieffer-Heeger Hamiltonian and the disorder,

\[ H = H_{SSH} + H_{imp} \]

where

\[ H_{imp} = \sum_n V_n c_n^\dagger c_n \]  

The site energies, \( V_n \), are random variables described by certain distribution function, \( P(V) \). We will use two types of distribution functions, namely, the rectangular distribution,

\[ P(V) = \frac{1}{2W}, \quad |V| \leq W \]

and the binary distribution,

\[ P(V) = c\delta(V - W) + (1 - c)\delta(V) \]

In the former case, \( V_n \) takes continuous values in a range \([-W, W]\). Its mean value is zero while its mean-square value is given by \( \langle V_n^2 \rangle_c = W^2/3 \). The rectangular distribution is widely used in the studies of localization problem. For the binary distribution, with \( \langle V_n \rangle_c = cW \) and \( \langle V_n^2 \rangle_c = c(1 - c)W^2 \). In experimental situations, the disorder is mainly introduced through doping of the system, where \( W \) describes the strength of the impurity potential, and might be as high as 5 eV.
if due to the Coulomb effects of the dopant ions. The binary distribution of disorder may be more relevant to reality, due to the usually dilute doping used in experiment.

We numerically solve the Schrödinger equation of the Hamiltonian in Eq. (2.1)

\[-t_{n+1,n} \psi_{n+1} - t_{n,n-1} \psi_{n-1} + V_n \psi_n = E \psi_n\ , \tag{2.5}\]

where \( t_{n+1,n} = t_0 - \alpha(u_{n+1} - u_n) \), and \( \psi_n \) is the normalized wave function at site \( n \). The eigenvalues and eigenfunctions depend on the particular values of the bond distortions \( \bar{u}_n \equiv u_n - u_{n-1} \) throughout the lattice. The total energy of the system is given by, including the factor 2 for the electron spins,

\[ E_t = 2 \sum_{E \leq E_F} E + \frac{K}{2} \sum_n \bar{u}_n^2 \ . \tag{2.6}\]

To determine the configuration of the bond distortions which minimizes the total energy, we impose the condition

\[ \frac{\partial E_t}{\partial \bar{u}_n} = 0 \ , \tag{2.7}\]

and use

\[ E = \sum_n \psi_n^* \left(-t_{n+1,n} \psi_{n+1} - t_{n,n-1} \psi_{n-1} + V_n \psi_n\right) \ , \]

the result is

\[ \bar{u}_n = -\frac{2\alpha}{K} \sum_{E \leq E_F} \left(\psi_{n-1}^* \psi_n + \text{c.c.}\right) \ . \tag{2.8}\]
Eq. (2.8) determines $\tilde{u}_n$ up to a constant, which can be fixed by requiring $\sum_n \tilde{u}_n = 0$, meaning that the length of the lattice remains unchanged during lattice relaxation.

The numerical procedure consists of self-consistent iteration of Eq. (2.5) and Eq. (2.8). For a given set of values of the random potential, $V_n$, we diagonalize the Schrödinger equation with periodic boundary conditions, choosing an initial configuration for the lattice bond distortions. Then we obtain the total energy in Eq. (2.6) and use the eigenfunctions and Eq. (2.8) to obtain the second generation of bond distortions, $\tilde{u}_n$, and use it as input of Eq. (2.5)) for the new eigenvalues and eigenfunctions. After convergence of the iteration, in terms of $E_t$, we calculate, from the resulting eigenvalues and eigenfunctions, various electronic properties such as the density of states, the effective size of the electronic state and the frequency dependent conductivity. The average over disorder is simply performed by repeating the above procedure for different sets of impurity potentials.

However, as expected, the results for a given set of impurity potentials depend on the initial lattice distortions used to start the iteration. The difference in $E_t$ for these metastable final states are typically less than 5%, and increases slightly for larger disorder. The resulting difference in the electron density of states is more appreciable, in terms of whether the Peierls gap is still open. We believe this is the cause of the discontinuous drop of the order parameter in some of the previous studies [15,16], which therefore might not represent the real physical behavior. This situation can be roughly seen in terms of the phase space of the lattice distortions spanned by $\tilde{u}_n$. Each final configuration corresponds a point where the total energy of the system
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reaches a minimum. There are many such local minima in the phase space separated by energy barriers with the typical size of the difference in total energies between relaxed and unrelaxed lattice configurations. The relaxation path of the system as the iteration proceeds will pass saddle points of the barriers so that different starting points in the phase space result in different relaxation paths and different local energy minima. This situation is somewhat like that in the spin glass problem. In an attempt to reach the lowest energy minima such that the final results represent those of ground state of the system, we tested different initial configurations of bond distortions including uniform lattice and dimerized lattice, as well as random bond distortions. Then use the state of the system which has the lowest total energy for a given set of random potentials in the disorder average.

B. Results and Discussions

From the numerical data gathered using the method of last section we calculate readily the averaged electron density of states and participation ratio given in Eq. (1.10). The frequency dependent conductivity is calculated by

\[
\sigma(\omega) = \frac{\pi}{L} \sum_{i,j} |J_{i,j}|^2 \delta(E_j - E_i - \omega),
\]

where the current operator is defined by \( J_n = 2J_0(c_n^+c_{n+1} - h.c.) \), with a factor of 2 for spin, and \( J_0 = ev_F \), \( v_F = 2t_0a \). We take \( a = 1 \AA \) as the unit for length while energy is measured in eV.

We present the numerical results for the two types of random potential distributions, Eq. (2.3) and Eq. (2.4), in a series of plots and
discuss them separately in the following.

1. Disorder with rectangular distribution

We take $L = 128$ for the length of the system, and tested over 100 initial configurations of the lattice displacements. The number of systems used in the ensemble average is 40. We are particularly interested in how the energy gap and the averaged order parameter change with disorder strength. In this case we take $\alpha = 5.6$. $\Delta$ and the half energy gap $E_g$, both scaled by $\Delta_0$, is shown in Fig. 3 as a function of the scaled inverse scattering time $\Gamma/\Delta_0$, $\Gamma = \frac{W^2}{3\epsilon_0}$, and compared with the corresponding analytical results from perturbation method of Chapter III. We also plot in Fig. 4, form Eq. (3.26) and (3.27), the electron density of states in the Peierls gap region for several values of $W$ to show how the gap closes as the disorder is increased. For weak disorder, the numerical and analytical results tend to agree. As disorder increases, there are systematic deviations between them, especially when $\Gamma/\Delta_0 \sim 0.5$, corresponding to $W = 1.83$, where the perturbation theory predicts that the system has entered a gapless region where $\Delta$ drops rapidly, the numerical results indicate that both $\Delta$ and $E_g$ continue to be finite as we move to stronger disorder.

Fig. 5 to Fig. 7 describe the strong disorder regime, starting with $W = 2.0$, $\Gamma/\Delta_0 = 0.53$. These figures for different $W$ are arranged in a way so that each can be recognized and compared with each other. The electron density of states show typical band tails extending outward as $W$ increases. Note that the density of states for the pure system, Eq. (1.14), extends form 5.0 to 0.89 above and below the Fermi
level. The gap at the Fermi level, $E = 0$, closes very slowly, and even for very large $W \sim 4$, where the gap vanishes, there remains a large depression in the density of states. This behavior is related to the fact, which will be discussed later, that even for strong disorder, the lattice distortions remain finite, and while their mean-square value reduces, corresponding to smaller averaged elastic energy, there are large amplitude fluctuations at some places in the lattice (see Fig. 13).

The electronic states are localized over the entire energy range, as indicated by their effective sizes, $L_e$. Again, we see the typical behavior expected for the strong disordered systems. In the case of $W = 2.0$, the region where the gap stands, appear as the inner band edge, where the states are more localized since they are affected by the lattice displacements, in addition to the disorder. The energy scale of these states is roughly $2$. For stronger disorder, $W \geq 4$, where the Peierls gap is closed, these states have more or less the same $L_e$ as those in the band, which becomes more localized and is mainly determined by the disorder. To further look into the nature of the states, we show in Fig. 7 $\sigma(\omega)$ up to a proportional constant. Despite the fact that there is no gap for $W > 4$, the states around the Fermi level do not contribute to the conductivity, since they are strongly localized and almost do not overlap with other states of similar energies. In the cases of relatively small disorder in Fig. 7, $W = 4.0$ and $6.0$, with the exception of $W = 2.0$ due to the Peierls gap, the positions of the peaks can still be scaled to the same value, $\omega/\Gamma \sim 1$, a feature of weakly disordered system, despite the fact that for the latter, $\omega/\Gamma \sim 0.35$. This does not hold for larger $W$ cases. Moreover, in all cases, the large frequency region of $\sigma(\omega)$ do not follow the Drude tail,
\( \sigma(\omega) \propto [1 + (\omega/\Gamma)^2]^{-1} \), as for weak disorder.

It is of interest to see these features for different values of the electron-phonon coupling constant at fixed \( W \). These are shown in Fig. 8 to Fig. 11. It is clear that there is no gap when \( \Delta_0 = 0 \), as for the case \( \alpha = 2.0 \), \( \Delta_0 = 10^{-7} \), however, for \( \alpha = 4.0 \), \( \Delta_0 = 0.1 \), we see the large depression in the density of states at \( E = 0 \), a similar situation as in Fig. 5. In Fig. 8 we plot \( L_c \) as a function of \( \alpha \) for the localized states at different energies, which is read off from Fig. 10. The disorder in this case is very strong since \( L_c \) is close to 5 lattice spacings. For weaker disorder, where \( L_c \) is much larger, the effect of the electron-phonon interaction is to enhance the localization of the electron wave function. It appears that only the states near the band center, on the energy scale \( E \sim 2 \) as mentioned before, are affected by \( \alpha \). Moreover, the dependence is linear. We attempt to understand this behavior by inspecting the associated lattice distortions. It seems that even though all the occupied electronic states contribute to the lattice distortion and is in turn affected by it, those states outside the gap region are primarily determined by the disorder. These states, according to Eq. (2.8), induce local displacements of the lattice which should be of roughly the same magnitude for different \( \alpha \), and to certain extend, for different \( W \). We identify these as the fluctuations superimposed on the lattice dimerization in Fig. 13 (they are discernible even for \( W = 14.0 \) where dimerization is completely destroyed), and correspond largely to the flat part of the Fourier spectra in Fig. 12. These fluctuations act as off-diagonal disorder, modifying the electron hopping matrix element, on the states in the gap region which are much more affected by the lattice distortions. This off-diagonal disorder increases
linearly with $\alpha$. $\sigma(\omega)$ in Fig. 11 shows that as the Peierls gap opens up, its peak position is pushed to higher $\omega$ while its tail remains the same for the same $\mathcal{W}$. However, the edge of the sharp increase of the conductivity, corresponding to interband transition gradually disappear due to the change in the nature of the corresponding states as a result of stronger off-diagonal disorder as $\alpha$ increases.

We calculate the mean-square Fourier spectrum of the lattice distortion

$$F(q) = \left\langle \frac{1}{L} \sum_n \hat{u}_n e^{-iqn} \right\rangle_c. \quad (2.10)$$

In Fig. (12), we see that $F(q)$ is peaked at $q = 2k_F - \pi$, where the Peierls instability occurs, and are broadened by disorder. The area under $F(q)$ is proportional to the averaged elastic energy of the lattice which decreases but remains finite even after the Peierls gap has vanished. The localized electrons affect greatly the Peierls distortion by breaking the dimerization and sometimes altering the dimerized phase, as seen in Fig. 13. There are no mid-gap states responsible to the soliton excitations as in the pure system, due to the strong local distortions. Another feature we see in Fig. 13 is the large spikes which appear for $\mathcal{W} > 2$. We attribute these to the tendency of two nearby localized states, taking advantage of deep fluctuation of the disorder, to bond together by severely distorting the lattice around them, thus creating a large local hopping matrix element, a process analogous to the formation of bonding and anti-bonding states in covalent bonds. We expect that this phenomenon would be rarely seen in real materials even for strongly disordered system, since the presence of anharmonic forces may cost much more energy for such large distortions.
Fig. 3. The averaged order parameter and half energy gap as function of the inverse scattering time, numerical data are denoted by dots:

(a) averaged order parameter $\Delta/\Delta_0$ as a function of $\Gamma/\Delta_0$;

(b) half energy gap $E_g/\Delta_0$ as a function of $\Gamma/\Delta_0$
Fig. 4. The normalized electron density of states $N/N_0$ as a function of scaled energy $E/\Delta$, the curves are labeled with the values of the scaled inverse scattering time $\Gamma/\Delta$. 
Fig. 5. The electron density of states for the rectangular distribution of disorder at fixed electron-phonon coupling constant $\alpha = 5.6$, numbers in the figure indicate values of $W$. 
Fig. 6. The effective size of the electronic state \( L_e(E) \) for the rectangular distribution of disorder at fixed electron-phonon coupling constant \( \alpha = 5.6 \), numbers in the figure indicate values of \( W \).
Fig. 7. The frequency dependent conductivity $\sigma(\omega)$ for the rectangular distribution of disorder at fixed electron-phonon coupling constant $\alpha = 5.6$, numbers in the figure indicate values of $W$. 
The effective size of the electronic state $L_e$ as a function of the electron-phonon coupling constant $\alpha$ for the rectangular distribution of disorder at fixed $W = 6.0$, numbers in the figure indicate values of the electron energy.
Fig. 9. The electron density of states for the rectangular distribution of disorder at fixed $W = 6.0$, numbers in the figure indicate values of the electron-phonon coupling constant $\alpha$. 
Fig. 10. The effective size of the electronic state $L_e(E)$ for the rectangular distribution of disorder at fixed $W = 6.0$, numbers in the figure indicate values of the electron-phonon coupling constant $\alpha$. 
Fig. 11. The frequency dependent conductivity $\sigma(\omega)$ for the rectangular distribution of disorder at fixed $W = 6.0$, numbers in the figure indicate values of the electron-phonon coupling constant $\alpha$. 
Fig. 12. The mean-square Fourier spectrum of the lattice displacements $F(q)$ as a function of wave vector for the rectangular distribution of disorder:

(a) $F(q)$ for fixed electron-phonon coupling constant $\alpha = 5.6$, numbers in the figure indicate values of $W$;

(b) $F(q)$ for fixed $W = 6.0$, numbers in the figure indicate values of the electron-phonon coupling constant $\alpha$
Fig. 13. The lattice dimerization amplitude \((-1)^n \tilde{u}_n\) as a function of position for the rectangular distribution of disorder at fixed the value of the electron-phonon coupling constant \(\alpha = 5.6\) for the following values of \(W\): 

(a) \(W = 2.0\);

(b) \(W = 14.0\)
2. Disorder with binary distribution

We expect the binary disorder model to be more closely related to the experimental situation since the rapid deterioration of mechanical quality of the sample restricts the concentration of the doped impurities [11]. In generally, the impurity concentration, \( c \), of interest is less than 20%. Thus the disorder appears largely in the form of dilute random impurities, whose potential strength depends on the particular type of dopant. Thus situation is obviously different from that of the rectangular distribution of disorder. The energy minimization is done in the same way as for the rectangular distribution of disorder, however, due to the discrete nature of the binary disorder we found that the metastable states of the system differ much less in \( E_t \) and in the resulting electronic structure. Thus it is unnecessary to test different initial configurations of lattice displacements. As for the disorder average, we take into account the charge transfer from dopants to the chain as is commonly so in the experiments. Thus, the electron concentration is \( 1 + c \) for donor doping. Also, since the finite system that we use in the numerical study is of microscopic length, \( L = 100 \) sites, we simulate the fluctuation in the doping process by specifying a mean concentration \( c \) so that in the ensemble average of a quantity \( x \) over impurity positions, the number of impurities \( m \) is weighted according to a binary distribution function

\[
\sum_{m=0}^{L} \frac{L!}{m!(L-m)!} c^m (1-c)^{L-m} < x(m) >_c.
\]

The results are presented in Fig. 14 to Fig. 19, in a similar man-
ner as for the previous case, for two values of the impurity potential, namely, $W = -1.0 \sim \Delta_0$ and $W = -4.0 > \Delta_0$, since we found that the two regimes separated according to $\Delta_0$ have remarkable different features.

We compare the results for the density of states, $L_e$, and $\sigma(\omega)$ for different values of $c$ and $W$. The energy band is shifted towards negative energy by the amount $cW$, and the band edges broadened by the disorder, which in the larger $W$ case become a separate piece corresponding to the deeply trapped states. The bulk of the states stay in the band region of the pure system, and the band edge singularities remain in the electron density of states. While these states are almost extended for the smaller $W$ case, only the occupied states are so for the larger $W$ case. These seem to be the results of the collective effort of the occupied states to maintain their Bloch wave character and the band structure. Since the impurities are isolated in the lattice in most cases, the states below the Fermi level are able to keep their shapes by adjusting the phases of their wave functions, and by slightly shifting their energies, to minimize the effects of the impurity potentials and the associated local lattice distortions. This can be achieved most effectively by the states deep in the band, with their wave lengths shorter than the mean distance between the impurities, whereas those states with small wave vectors gradually become localized. Another signature for this collective action is the presence, despite the ensemble average, of intervals empty of states in the density of states in the weaker $W$ case. The large asymmetry in the sizes of states above and below the Fermi level, in the stronger $W$ case, reflects the fact that the states above the Fermi level, not participating
in the energy minimization process, are unable to make adjustment and are localized, more so for larger $W$. The extended nature of the band states, especially for small $W$, can also be seen from the short tails of $\sigma(\omega)$ (compare with the rectangular distribution of disorder), since small uncertainty in the Bloch wave vector restricts the photoexcitation process due to the wave vector conservation requirement.

We now turn to the gap region. The Peierls gap closes quickly due to the combined effects of impurity broadening and shifting of the electron concentration away from half-filling, which reduces the contribution of Umklapp processes to the electron-phonon interaction. The states inside the gap region of the pure system have distinct characters form the bulk of the other states. They are more localized and are very different in the two cases of small and large $W$. Studying their wave function together with the lattice distortions we can identify these states as a polaron states composed of electrons and lattice distortions localized at the impurity positions. The polaron states reduce locally the dimerization amplitude, and thus spread over the gap region for small $W \sim \Delta_0$, whereas in the larger $W$ case, they are more deeply trapped by the impurity potential as seen in Fig. 14 and Fig. 15, and most of them coalesce with the valence band. The prominent structure left in the density of states at gap center is due exclusively to the soliton states. We found these states exist in regions in the lattice that are free of impurities. Note that the coherent length for the soliton excitations is $\xi = 5.6$, corresponding to a width $\sim 11$ for the soliton state. For the impurity concentrations taken in these cases, such a distance between two impurities can always be found. In fact, due to microscopic fluctuations of the impurity concentration, the
soliton states can still survive at larger values of $c$. The soliton states exist as well in the smaller $W$ case, however, they are buried in the polaron band and have smaller weight.

Fig. 18 and Fig. 19 for $\sigma(\omega)$ show clearly the features we just discussed. In the small $W$ case, the single interband peak at $\omega \sim 1.8$ gradually diminishes as $c$ increases, and the transitions involving the polaron states dominate. In the larger $W$ case, the polaron states in the gap region are greatly depleted, leaving a large interband peak, together with a prominent peak with sharp edge positioned at $\omega = E_g = 0.9$, corresponding to the transitions between the gap center soliton states and the states near the band edges.

The dominant presence of the soliton states is in consistence with experimental results and support the soliton hopping conduction scenario [11]. Despite the fact that of all the states are localized in one-dimensional, the solitons are mobile charge carriers in the regions free of impurities, and can contribute to the conduction by hopping to the neighboring chains.
Fig. 14. The electron density of states for the binary distribution of disorder at fixed electron-phonon coupling constant $\alpha = 5.6$ and impurity potential strength $W = 1.0$, vertical line indicates the Fermi level, numbers in the figure indicate values of the mean impurity concentration $c$. 
Fig. 15. The electron density of states for the binary distribution of disorder at fixed electron-phonon coupling constant $\alpha = 5.6$ and impurity potential strength $W = 4.0$, vertical line indicates the Fermi level, numbers in the figure indicate values of the mean impurity concentration $c$. 
Fig. 16. The effective size of the electronic state for the binary distribution of disorder at fixed electron-phonon constant $\alpha = 5.6$ and impurity potential strength $W = 1.0$, vertical line indicates the Fermi level, numbers in the figure indicate values of the mean impurity concentration $c$. 
Fig. 17. The effective size of the electronic state for the binary distribution of disorder at fixed electron-phonon constant $\alpha = 5.6$ and impurity potential strength $W = 4.0$, vertical line indicates the Fermi level, numbers in the figure indicate values of the mean impurity concentration $c$. 
Fig. 18. The frequency dependent conductivity for the binary distribution of disorder at fixed electron-phonon coupling constant $\alpha = 5.6$ and impurity potential strength $W = 1.0$, numbers in the figure indicate values of the mean impurity concentration $c$. 
Fig. 19. The frequency dependent conductivity for the binary distribution of disorder at fixed electron-phonon coupling constant $\alpha = 5.6$ and impurity potential strength $W = 4.0$, numbers in the figure indicate values of the mean impurity concentration $c$. 
III. ANALYTICAL METHOD

A. Effective Hamiltonian for the Electron

We start with the one-dimensional Hamiltonian introduced in Chapter II, Eq. (2.1), which includes electron-phonon interaction and impurity scatterings. It can be written in Fourier space, 

\[ H = H_0 + H_{ep} + H_{imp} \]

\[ H_0 = \sum_k (-2t_0 \cos k) c_k^\dagger c_k + \sum_q \Omega(q)(B_q^\dagger B_q + \frac{1}{2}) \quad (3.1a) \]

\[ H_{ep} = \frac{1}{\sqrt{L}} \sum_{qk} g(k, q)(B_q + B_{-q}^\dagger) c_{k+q}^\dagger c_k \quad (3.1b) \]

\[ H_{imp} = \sum_{q \neq 0} V(q) \sum_k c_{k+q}^\dagger c_k \quad (3.1c) \]

where the bare phonon dispersion \( \Omega(q) = \sqrt{\frac{2K}{M}} (1 - \cos q)^{1/2} \), the electron-phonon coupling constant

\[ g(k, q) = \frac{2\alpha i}{\sqrt{2M\Omega(q)}} [\sin(k + q) - \sin k] \]

and \( V_q = L^{-1} \sum_n e^{-iqn} V_n \). The summation over \( k \) and \( q \) are restricted in the first Brillouin zone: \( k, q \in (-\pi, \pi] \). In \( H_{imp} \), the uniform component \( V(q = 0) \) is set to zero for convenience. We consider here disorder due to inherent structural defects or those introduced in the so-called isoelectronic doping processes in which the
number of electrons in the system is not changed, so that the system remain half-filled and the Fermi energy $\epsilon_F = 0$, at the band center.

As discussed in Chapter I, the Kohn effect and Peierls instability is manifested in the existence of finite mean-field amplitudes for the phonon field, $\langle B_q \rangle$. From the equation of motion for the phonon field,

$$i\frac{\partial}{\partial t} B_q(t) = [B_q(t), H]$$

$$= \sum_k g(k, -q)c_{k-q}^{\dagger}(t)c_k(t) + \Omega(q)B_q(t), \quad (3.2)$$

and a similar one for $B_q^{\dagger}(t)$, we obtain, in static mean-field approximation at $T = 0$,

$$\langle B_q \rangle = -\frac{1}{\Omega(q)} \sum_k g(k, -q)\langle c_{k-q}^{\dagger}c_k \rangle, \quad \langle B_q^{\dagger} \rangle = \langle B_{-q} \rangle,$$

and

$$H_{cp} = -\frac{2}{L} \sum_{q,k,k'} \frac{1}{\Omega(q)} g(k, q)g(k', -q)\langle c_{k-q}^{\dagger}c_{k'} \rangle c_{k+q}^{\dagger}c_k$$

$$= -\frac{g_0}{L} \sum_{q,k,k'} \cos(k + \frac{q}{2}) \cos(k' - \frac{q}{2})\langle c_{k-q}^{\dagger}c_{k'} \rangle c_{k+q}^{\dagger}c_k, \quad (3.3)$$

where the effective electron-phonon coupling constant $g_0 = 4\alpha^2/K$. In pure system, ignoring $H_{imp}$, the dominant amplitude $\langle c_{k-q}^{\dagger}c_k \rangle$ has $k = k_F$ and $q = 2k_F$, and is proportional to the order parameter $\Delta$. This results in an energy gap of size $E_g = 2\Delta$ at $E_F$, Eq. (1.12), and
a dimerized lattice with lattice displacement $u_0 = \frac{\Delta}{4a}$. In disordered systems, however, the impurity scatterings of electrons are reflected in the quantum expectation value $\langle c_{k-q}^\dagger c_k \rangle$ and the associated order parameter $\Delta(q)$, defined below, become random variables correlated with $V(q)$. Due to perfect nesting of Fermi surface in one-dimensional systems, both the forward (small momentum transfer) and the backward (large momentum transfer $\sim 2k_F$ across the Fermi surface) scattering processes of the electron by the disorder and the static order parameter fluctuation are important. In addition, in the half-filled case which we study, Umklapp processes have significant contributions, and the couplings between states at $k_F$ and $-k_F$ and those at $\pi - k_F$ and $-\pi + k_F$ are all important. To study adequately these effects, we introduce the two-component spinor fields for the electrons, in analogy to the Nambu notation in the theory of superconductivity [24] and in the problem of excitonic insulators [23],

$$\Psi_k \equiv \begin{pmatrix} c_{k+k_F} \\ -i c_{k-k_F} \end{pmatrix}, \quad \Psi_k^\dagger = (c_{k+k_F}^\dagger \quad i c_{k-k_F}^\dagger), \quad k \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right].$$

In doing so, we have separated the original electron fields $c_k$ corresponding to $k > 0$ and $k < 0$, into two branches [13,25], corresponding to $c_{k+k_F}$ and $c_{k-k_F}$, respectively, and at the same time reduced the Brillouin zone to $[-\frac{\pi}{2}, \frac{\pi}{2}]$. Such separation is convenient, as can be anticipated from the facts that the lattice dimerization produces effectively a two-band system.

The effective electron Hamiltonian in terms of $\Psi$ and $\Psi^\dagger$ is
\[ H_{\text{eff}} = \sum_k \epsilon(k) \Psi_k^\dagger \sigma_3 \Psi_k - \sum_{q,k} \Delta(q) \cos(k + \frac{q}{2}) \Psi_{k+q}^\dagger \sigma_1 \Psi_k + \sum_{q \neq 0, k} V(q) \Psi_{k+q}^\dagger \Psi_k - \sum_{q,k} V_b(q) \Psi_{k+q}^\dagger \sigma_2 \Psi_k , \] (3.5)

where \( k, q \in [-\frac{\pi}{2}, \frac{\pi}{2}] \), \( \sigma_i, i = 1, 2, 3 \), are the usual Pauli matrices, \( \epsilon(k) = 2t_0 \sin k \), \( V(q) \) and \( V_b(q) \equiv V(\pi + q \mod 2\pi) \) describe, respectively, the forward and backward scatterings. Note that now \( k_F = 0 \). Note also that the Umklapp terms are included when Eq. (3.5) is written in the above form. The important scattering processes now come from small \( q \) region, where electrons and holes with wave vectors \( k \) and \( k + q \) have similar energies. The function \( \Delta(q) \) is defined as

\[ \Delta(q) = \frac{g_0}{L} \sum_k \cos(k - \frac{\pi}{2})(\Psi_{k+1}^\dagger \sigma_1 \Psi_k) , \quad \Delta^*(q) = \Delta(-q) , \] (3.6)

which should in principle be determined self-consistently from the solutions of \( H_{\text{eff}} \). The order parameter after impurity average (denoted by \( \langle \cdots \rangle_c \)) is given by \( \Delta \equiv \langle \Delta(0) \rangle_c \). We have chosen the phase of the \( \Psi_k \) fields (see Eq. (3.4)) so that \( \Delta \) is real (Eq. (3.6)). In fact, it will be shown that \( \langle \Delta(q) \rangle_c = \Delta \delta_{q,0} \), since \( \Delta(q) \) is proportional to the Fourier components of the random lattice displacements such that \( \langle \Delta(q) \rangle_c = 0 \) for \( q \neq 0 \) due to phase cancellation. However, the fluctuation of \( \Delta(q) \), \( \langle |\Delta(q)|^2 \rangle_c \), will be finite.
B. Perturbation Method for Weak Disorder

We study the electronic properties described by $H_{eff}$ using perturbation method. The Green's function matrix is given in terms of $\Psi$ and $\Psi^{\dagger}$ in the Heisenberg representation:

$$G(p, p', t) = -i \langle T \Psi_{p}(t) \Psi_{p'}^{\dagger}(0) \rangle \ .$$

(3.7)

Using the commutation relations

$$\{\Psi_{k}, \Psi_{k'}^{\dagger}\} = 0, \quad \{\Psi_{k}, \Psi_{k'}^{\dagger}\} = \delta_{k,k'} \ ,$$

(3.8)

the equation of motion for $G(p, p', t)$ can be written down as

$$i \frac{\partial}{\partial t} G(p, p', t) = \delta_{p,p'} \delta(t) - i \langle T[\Psi_{p}(t) , H_{eff}] \Psi_{p'}^{\dagger}(0) \rangle \ ,$$

(3.9)

with

$$[\Psi_{p}, H_{eff}] = \sigma_{3} e_{p} \Psi_{p} - \sum_{q} \Delta(q) \cos(p - \frac{q}{2}) \sigma_{1} \Psi_{p-q}$$

$$+ \sum_{q \neq 0} V(q) \Psi_{0} \Psi_{p-q} - \sum_{q} V_{b}(q) \sigma_{2} \Psi_{p-q} \ .$$

(3.10)

Fourier transformation of Eq. (3.9) gives,

$$G(p, p', t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} G(p, p', \omega) \ ,$$
\[ G(p,p',\omega) = \delta_{p,p'} G_0(p,\omega) + G_0(p,\omega) \sum_q \{ V(q) - V_b(q) \sigma_2 \]
\[ + \Delta \cos p \sigma_1 - \Delta(q) \cos(p - \frac{q}{2}) \sigma_1 \} G(p,p',\omega), \tag{3.11} \]

where \( G_0^{-1}(p,\omega) = \omega - \epsilon_p \sigma_3 + \Delta \cos p \sigma_1 \). To obtain the averaged Green's function, we consider the random potentials with rectangular distribution (Eq. (2.3)),

\[ \langle V(q) \rangle_c = \langle V_b(q) \rangle_c = 0, \quad \langle V(q) V_b(q') \rangle_c = 0, \]
\[ \langle V(q) V(q') \rangle_c = \langle V_b(q) V_b(q') \rangle_c = \frac{W^2}{3L}. \tag{3.12} \]

\( \langle G(p,p',\omega) \rangle_c = \delta_{p,p'} G(p,\omega) \) can be obtained to any order of disorder by iterating Eq. (3.11). In the self-consistent Born approximation, \( G(p,\omega) \) is solved from the Dyson's equation

\[ G(p,\omega)^{-1} = G_0(p,\omega)^{-1} - \Sigma_0(\omega) - \Sigma_1(p,\omega), \tag{3.13} \]

where \( \Sigma_0(\omega) \), independent of \( p \), represents the contribution to the electron self-energy from \( V(q) \) and \( V_b(q) \), Fig. 1(c),

\[ \Sigma_0(\omega) = \frac{W^2}{3L} \sum_p [G(p,\omega) + \sigma_2 G(p,\omega) \sigma_2], \tag{3.14} \]

and \( \Sigma_1(p,\omega) \) comes from the correlations of \( \Delta(q) \) and the random potential \( \langle V(q) \Delta(q') \rangle_c \), \( \langle V_b(q) \Delta(q') \rangle_c \) and \( \langle \Delta(q) \Delta(q') \rangle_v \), Fig. 1(e) and Fig. 1(f). We study these correlations in Section D, where it is shown
there that their contributions to $\Sigma_1(p)$ in the lowest order in disorder are of the form

$$\langle V_b(q)\Delta(q') \rangle_c = 0, \quad \langle V(q)\Delta(q') \rangle_c = \frac{W^2}{3L} f(q)\delta_{q',-q},$$

$$\langle \Delta(q)\Delta(q') \rangle_c = \frac{W^2}{3L} f(q)\delta_{q',-q}, \quad (3.15)$$

where $f(q)$ is a real function, and $f(-q) = f(q)$, in consistence with Eq. (3.6). Thus we have

$$\Sigma_1(p,\omega) = \frac{W^2}{3L} \sum_{p'} \left\{ f^2(p-p') \cos^2 \left( \frac{p+p'}{2} \right) \sigma_1 G(p',\omega) \sigma_1 \right. \right.$$

$$+ \left. f(p-p') \cos \left( \frac{p+p'}{2} \right) \left[ \sigma_1 G(p',\omega) + G(p',\omega)\sigma_1 \right] \right\} \quad (3.16)$$

This form is much more complex than $\Sigma_0(\omega)$. Our problem of solving $G(p,\omega)$ is greatly simplified if we neglect $\Sigma_1$, as justified to some degree by the numerical results of Chapter II, where it is seen that $f(q)$ is smaller than unity and is sharply peaked at $q = 0$ (at $2k_F = \pi$ in Fig. 12) for small disorder while decreases for larger disorder. However, it remains finite in the region where the energy gap and $\Delta$ vanish and therefore is expected to have greater effect there. Furthermore, it constitutes a form of correlated disorder acting only on the electrons in the same chain, and thus is important in the problem of anisotropic properties in quasi-one-dimensional systems (see discussion in Chapter IV).

We are left with the problem of solving self-consistently the simplified Dyson's equation.
\[ G^{-1}(p, \omega) = G_0^{-1}(p, \omega) - \Sigma_0(\omega), \quad (3.17) \]

with \( \Delta \) determined from Eq. (3.6),

\[
\Delta = \frac{g_0}{L} \sum_p \cos p \langle \langle \Psi_p^+ \sigma_1 \Psi_p \rangle \rangle_c \\
= - \lim_{t \to 0^-} \frac{g_0}{L} \sum_p \cos p \text{Tr}[\sigma_1 \langle \langle T \Psi_p(t) \Psi_p^+(0) \rangle \rangle_c] \\
= \frac{g_0}{L} \sum_p \cos p \int \frac{d\omega}{2\pi i} e^{i\omega t} \text{Tr}[\sigma_1 G(p, \omega)]. \quad (3.18)
\]

Writing the Green's function matrix of Eq. (3.7) as

\[
G = \begin{pmatrix} G_b & F^* \\ F & G_a \end{pmatrix},
\]

Eq. (3.17) leads to

\[
\bar{G}_b(\omega) + \bar{G}_a(\omega) = 2\{\omega - \frac{W^3}{3} [\bar{G}_b(\omega) + \bar{G}_a(\omega)]\} \sum_p \frac{1}{C(p, \omega)},
\]

\[
[\bar{F}(\omega) - \bar{F}^*(\omega)] = 2 \frac{W^2}{3} [\bar{F}(\omega) - \bar{F}^*(\omega)] \sum_p \frac{1}{C(p, \omega)}, \quad (3.19)
\]

where

\[
C(p, \omega) = \{\omega - \frac{W^2}{3} [\bar{G}_b(\omega) + \bar{G}_a(\omega)]\}^2 - \epsilon^2(p) - \Delta^2 \cos^2 p \\
+ \left( \frac{W^2}{3} \right)^2 [\bar{F}(\omega) - \bar{F}^*(\omega)]^2,
\]
and

\[ G_b(\omega) = \frac{1}{L} \sum_p G_b(p, \omega), \text{ etc.} \]

The second equation in Eq. (3.19) for arbitrary \( \omega \) leads to \( \tilde{F}(\omega) = \tilde{F}^*(\omega) \), which is consistent, according to Eq. (3.18), with our choice of real \( \Delta \). Equation (3.17) reduced to \( \tilde{\omega} = \omega - \frac{W^2}{3} [\tilde{G}_b(\omega) + \tilde{G}_a(\omega)] \).

Evaluating \( \tilde{G}_b + \tilde{G}_a \),

\[ \tilde{G}_b(\omega) + \tilde{G}_a(\omega) = 2\tilde{\omega} \frac{1}{L} \sum_p \frac{1}{\tilde{\omega}^2 - \epsilon^2(p) - \Delta^2 \cos^2 p} \]

\[ = -\tilde{\omega} N_0 \int_{-\infty}^{+\infty} d\epsilon \frac{1}{\eta^2 \epsilon^2 + \Delta^2 - \tilde{\omega}^2} \]

\[ = \frac{\pi N_0}{\eta} \frac{i\tilde{\omega}}{(\tilde{\omega}^2 - \Delta^2)^{1/2}} \]

where \( \eta^2 = 1 - \frac{\Delta^2}{4t_0^2} \), \( N_o = \frac{1}{\pi t_0} \) is the electron density of states at Fermi energy when there is no interaction. Finally, the Dyson's equation is written as

\[ \tilde{\omega} = \omega + i \frac{\Gamma}{\eta} \frac{\tilde{\omega}}{(\tilde{\omega}^2 - \Delta^2)^{1/2}} \]  \hspace{1cm} (3.20)

The inverse impurity scattering time \( \Gamma = \frac{W^2}{3} \pi N_0 \) and the corresponding mean free path \( l_0 = v_F/\Gamma = 6t_0^2/W^2 \). The complex function \( \tilde{\omega}(\omega) \) is single-valued if we introduce a branch cut along the real axis in the \( \omega \)-plane and require \( \text{Re} (\tilde{\omega}^2 - \Delta^2)^{1/2} > 0 \). The Green's function is then defined on the complex \( \omega \)-plane

\[ G(p, \omega) = \frac{\tilde{\omega} + \epsilon(p)\sigma_3 - \Delta \cos p\sigma_1}{\tilde{\omega}^2 - \eta^2 \epsilon^2(p) - \Delta^2}, \]  \hspace{1cm} (3.21)
which has the same analytic properties as the usual temperature Green's function, Eq. (1.2), \( G(p, i\omega_n) \), \( \omega_n = (2n + 1)\pi/T \), \( n \) integer, analytically continued to complex \( \omega \)-plane. Namely, \( G(p, \omega) \) is analytic in the \( \omega \)-plane except a branch cut along the real axis, and \( \text{Im} \ G(p, \omega) \) changes sign when the cut is crossed. These properties can be expressed by the following equations [26, 27],

\[
\tilde{\omega}(\omega^*) = \tilde{\omega}^*(\omega), \quad [\tilde{\omega}^2(\omega^*) - \Delta^2]^{1/2} = -\{[\tilde{\omega}^2(\omega) - \Delta^2]^{1/2}\}^* . \tag{3.22}
\]

C. Results and Discussions

We should point out that the fact that our basic result of Section B is expressed in terms of a single equation, Eq. (3.20), is particular to the model Hamiltonian that we study, Eq. (3.5), and to the momentum independence of the quantities in Eq. (3.12), which is a good approximation in many disordered systems. In the formally analogous theories of the magnetic impurities in superconductor alloy [20,21,22] and of impurities in excitonic insulator [23], there is another equation arising from the off-diagonal elements of the Green's function matrix, originating from a similar equation as the second one in Eq. (3.19). The absence of this equation in our problem is attributed to the fact that the contributions to the inverse scattering time from the forward and the backward impurity scatterings have the same magnitude, which doubles the effect of the disorder that each process contributes individually. In more general cases, such as when the energy band is not half-filling, or when there is angle dependence in the impurity scattering potential, the results will appear in the same form as
obtained here, but the effective $\Gamma$ will have different meaning.

In the following, we calculate explicitly the averaged order parameter and the electron density of states, from which the energy gap is also obtained. Since $\Delta$ is much smaller than the band width $2t_0$, we take $\eta = 1$ in what follows.

1. **Averaged order parameter**

From Eq. (3.18), we obtain, after the momentum integration, the equation determining $\Delta$ is,

$$1 = \frac{g_0}{2\eta} \int_C d\omega \frac{1}{(\tilde{\omega}^2 - \Delta^2)^{1/2}}, \quad (3.23)$$

where the contour of integration follows the real $\omega$-axis below for $\omega < 0$ and above for $\omega > 0$. The integral can be performed by first deforming contour $C$ to follow the imaginary axis in the $\omega$-plane, then making the following substitution and using Eq. (3.23)

$$\omega = iy, \quad \tilde{\omega} = ix, \quad y = x \left[1 - \frac{\Gamma}{(x^2 + \Delta^2)^{1/2}}\right]. \quad (3.24)$$

Substracting the resulting equation by its corresponding form in the limit $\Gamma = 0$, $\Delta \to \Delta_0$ given by Eq. (1.13), we obtain

$$\ln \frac{\Delta}{\Delta_0} = \int_{x_0}^{\infty} \frac{dx}{(x^2 + \Delta^2)^{1/2}} \left[1 - \frac{\Gamma}{(x^2 + \Delta^2)^{3/2}}\right] - \int_0^{\infty} \frac{dx}{(x^2 + \Delta^2)^{1/2}},$$

where $x_0$ is obtained from Eq. (3.24)
Finally, we have

\[
\ln \frac{\Delta}{\Delta_0} = -\frac{\pi}{4} \frac{\Gamma}{\Delta}, \quad \Gamma \leq \Delta
\]

\[
= \frac{1}{2\Gamma} (\Gamma^2 - \Delta^2)^{1/2} - \ln \frac{\Gamma + (\Gamma^2 - \Delta^2)^{1/2}}{\Delta}
\]

\[
- \frac{\Gamma}{2\Delta} \arctan \frac{\Delta}{(\Gamma^2 - \Delta^2)^{1/2}}, \quad \Gamma > \Delta .
\]  

(3.25)

This result is plotted in Fig. 3. The critical value \( \Gamma_c = 2\Delta_0 \) where \( \Delta = 0 \) corresponds to \( W_c = 1.827 \).

2. Energy gap and density of states

The electron density of states as a function of energy is defined by

\[
N(\omega) = -\frac{1}{\pi} \sum_p \text{Im} \text{Tr} G(p, \omega + i0)
\]

\[
= N_0 \text{Im} \left[ \frac{\tilde{\omega}}{(\Delta^2 - \tilde{\omega}^2)} \right]_{\omega+i0}
\]

\[
= \frac{N_0}{\Gamma} \text{Im} \tilde{\omega}(\omega + i0) .
\]  

(3.26)

In the case of zero disorder, \( \Gamma = 0 \),
\[
\frac{N_0(\omega)}{N_0} = 0, \quad \omega \leq \Delta_0 \\
= \frac{|\omega|}{(\omega^2 - \Delta^2)^{1/2}}, \quad \omega > \Delta_0. \quad (3.27)
\]

This expression coincides with that of the pristine dimerized system if the outer band edge is ignored, i.e. \(|\omega| < 2t_0\).

For finite \(\Gamma\), it is easy to see from Eq. (3.20) that when \(0 < \Gamma < \Delta\), \(\tilde{\omega}\) is real for \(\omega < E_g\), with the half energy gap \(E_g = (\Delta^{2/3} - \Gamma^{2/3})^{3/2}\). When \(\Gamma > \Delta\), or \(\Gamma < \Delta\) but \(\omega > E_g\), there is a finite density of states which is obtained by solving simultaneously Eq. (3.25) and Eq. (3.20).

The value of \(\Gamma\) where \(E_g = 0\) gives the second critical disorder, \(\Gamma_c'\), which is smaller by a finite amount than the first critical value, in fact, from Eq. (3.25), \(\Gamma_c' = 2\exp(-\frac{\pi}{4})\Gamma_c\), or \(W_c' = 1.744\). This indicates that there exists a gapless region near the critical disorder.

These results, valid in the weak disorder regime, are plotted in Fig. 3 and Fig. 4, and compared with the numerical data, as discussed in Section B. of Chapter II.

D. Fluctuations of the Order Parameter

In this section, we study the correlation between \(\Delta(q)\) and the random potential in the self-consistent Born approximation. From Eq. (3.6), it follows

\[
\Delta(q) = \frac{g_0}{L} \sum_p \cos \left( p - \frac{q}{2} \right) \int \frac{d\omega}{2\pi i} e^{i\omega q + \text{Tr} [\sigma_1 G(p, p - q, \omega)]}. \quad (3.23)
\]
Using Eq. (3.11) up to $\langle V^2 \rangle_c$, we have

$$\langle \Delta(q) \rangle_c = \Delta \delta_{q,0} ,$$

where we have replaced $G(p, \omega)$ by the full Green's function and $\Delta$ is given by Eq. (3.18), and

$$\langle V(q)\Delta(q') \rangle_c = \frac{W^2}{3L} \frac{g_0 \Pi_1(q)}{1 + g_0 \Pi_2(q)} \delta_{q',-q} , \quad (3.24a)$$

$$\langle V_0(q)\Delta(q') \rangle_c = -\frac{W^2}{3L} \frac{g_0 \Pi_3(q)}{1 + g_0 \Pi_2(q)} \delta_{q',-q} , \quad (3.24b)$$

$$\langle \Delta(q)\Delta(q') \rangle_c = \frac{W^2}{3L} \frac{g_0 \Pi_1^2(q) + \Pi_3^2(q)}{[1 + g_0 \Pi_2(q)]^2} \delta_{q',-q} . \quad (3.24c)$$

The electron polarizations have the following expressions:

$$\Pi_1(q) = \frac{1}{L} \sum_p \cos(p - \frac{q}{2}) \int \frac{d\omega}{2\pi i} e^{i\omega_0 + \text{Tr}[\sigma_1 G(p, \omega)G(p - q, \omega)]} , \quad (3.25a)$$

$$\Pi_2(q) = \frac{1}{L} \sum_p \cos^2(p - \frac{q}{2}) \int \frac{d\omega}{2\pi i} e^{i\omega_0 + \text{Tr}[\sigma_1 G(p, \omega)\sigma_1 G(p - q, \omega)]} , \quad (3.25b)$$

$$\Pi_3(q) = \frac{1}{L} \sum_p \cos(p - \frac{q}{2}) \int \frac{d\omega}{2\pi i} e^{i\omega_0 + \text{Tr}[\sigma_1 G(p, \omega)\sigma_2 G(p - q, \omega)]} . \quad (3.25c)$$

Using $G(p, \omega)$ given in Eq. (3.21) we see that the integrand in Eq. (3.25c) is almost an odd function of $\epsilon(p)$ for small $q$, and as a result of summation over $p$, can be neglected. Thus Eq. (3.24) reduces to Eq. (3.15) with
This result, derived from the self-consistent Born approximation, can be understood basically in terms of the linear response theory. If we introduce a lattice distortion field for the disordered Peierls state

\[ b(q) \equiv \frac{1}{\sqrt{L}} \sum_p \cos \left( p - \frac{q}{2} \right) \Psi_{p-q}^+ \sigma_1 \Psi_p , \]  

(3.27)

then its mean-field contribution to \( H_{\text{eff}} \) in Eq. (3.5) can be written as

\[ -g_0 \sum_q \langle b(q) \rangle * b(q) , \]

which leads to an effective potential field acted on \( b(q) \), \( V_{\text{eff}}(q) = -g_0 \langle b(q) \rangle \), so that the response of \( \langle b(q) \rangle \) to \( V_{\text{eff}}(q) \) is \( \langle \sigma(q) \rangle = \Pi_2(q) V_{\text{eff}}(q) \). In addition, in the presence of disorder, the response of \( \langle b(q) \rangle \) to the impurity potential through its coupling to the density fluctuations induced by \( V(q) \), \( \langle b(q) \rangle = g_0 \Pi_1(q) V(q) \). Then, in the linear response theory, we have

\[ \langle b(q) \rangle = g_0 \Pi_1(q) V(q) + \Pi_2(q) V_{\text{eff}}(q) , \]

or

\[ \langle b(q) \rangle = V(q) \frac{g_0 \Pi_1(q)}{1 + g_0 \Pi_2(q)} , \]

which immediately leads to Eq. (3.24) and Eq. (3.25).

For the linear response theory to be valid, it is essential that the state be stable to the impurity perturbation potential. Thus, we must calculate \( f(q) \) in terms of the Green's functions which already include the Peierls distortion. In fact, the Kohn anomaly is a result of the spontaneous response of the electron gas by coupling to the phonons.
When calculated using the bare electron propagators, \( 1 + g_0 \Pi_2(0) = 0 \) is identified to the condition for the Kohn anomaly, Eq. (1.3), and \( f(q \to 0) \) diverges.

A more formal way to understand \( f(q) \) is suggested in the Feynman diagrams in Figs. 1(d), 1(e) and 1(f). In this case, we consider the dynamical phonon propagator matrix \( D(q, \omega) \) which in the presence of disorder acquires a static contribution to its self-energy coupled to \( V(q) \) through the electron polarization \( \Pi_1(q) \), Fig. 1(d). This contribution is static because there is no energy transfer through \( V(q) \). Note that this type of phonon self-energy, in the form of a tadpole diagram analogous to the Hatree term, vanishes in the ordered system, since there it describes, in contrast to the dynamical exchange term in Fig. 1(b), the exchange of a \( q = 0 \) phonon or the uniform translation of the lattice. Including these static contributions in the electron self-energy in Fig. 1(a) with the renormalized phonon propagator which contains in the distorted Peierls state its own self-energy \( \Pi_2(q, \omega) \), we obtain, respectively, the terms in \( \Sigma_1(p, \omega) \), Eq. (3.16) and Figs. 1(e) and 1(f), with the corresponding \( f(q) \).

The function \( f(q) \) is related to the mean-square Fourier spectrum of the lattice displacements in Eq. (2.10) through Eq. (3.24). We are interested in describing the lattice distortion by a self-consistent perturbation method, especially in the vicinity of the Peierls instability, since for weak disorder it is strongly peaked at \( 2k_F \). Preliminary calculations show that \( f(q) \) has a Lorentzian shape in \( q \) for small \( q \), its width dependent upon \( \Delta \) and \( W \). From this information, the next step is to calculate \( \Sigma_1 \) and thus to study the electronic states in the presence of both the disorder and the induced lattice distortion.
IV. CONCLUSIONS AND FUTURE PERSPECTIVES

To summarize, our numerical results suggest that localization of the electrons affects the distorted Peierls state to a much greater degree than expected from the perturbation point of view, even when the "pair-breaking" effects of the impurities are included, as we did in Chapter III. The two types of disorder, corresponding to the rectangular distribution and the binary distribution, result in remarkable differences in the electronic structure and the lattice distortion of the system. In the latter case, the electronic states in the energy band are much more extended, while localized polaron states form around the largely isolated impurities by reducing locally the lattice dimerization amplitude. The polaron states may overlap in space and shift their energies. As a result, these states fill up the Peierls gap, in much the same way as impurity band forms in the energy gap in disordered semiconductors, and the Peierls distortion is destroyed. In addition, there are soliton states, as the elementary excitations of the pure system, in the regions of the lattice that are free of impurities. In the case of rectangular distribution of disorder, the impurity potential fluctuates everywhere in the system, and the coupling between the localized states and the lattice distortion is more complicated. At the same time as the localized states around the Peierls gap move into the gap region with increasing disorder, these states affect one another through the lattice distortion they induce, most notably by forming bonding and antibonding pairs. This happens on a energy scale larger than the gap in the pure system, which is the energy region where Bloch states are affected by the electron-phonon in-
teraction. The lattice displacements induced by these localized states act as correlated off-diagonal disorder which in turn affects the electron states, resulting in a depression in the electron density of states and altering the nature of these states, as reflected in frequency dependent conductivity. These states are different from those far away from the Fermi level which are mostly affected only by the disorder. Our understanding of them is preliminary and only qualitative. To better understand them, we believe one should start from the weak disorder regime, and study the correction to the electron self-energy, $\Sigma_1$ in Eq. (3.16). The numerical results indicate that the function $f(q)$ is strongly peaked at the Fermi level for weak disorder (Fig. 12). Thus we can approximate $\Sigma_1(p)$ by $\Sigma_1(p_F)$. Our interest here is to see whether this correction will improve the agreement between the analytic and numerical results shown in Fig. 3. To study the localization of these states, one has to calculate the averaged two-particle Green's function, from which the frequency dependent conductivity and the localization length are obtained. The back scattering correction mentioned in Section B of Chapter II is crucial here, and is more difficult to handle than in the case without the Peierls distortion. Work on this problem is in progress.

The experimental situation is much more complex, partly due to the presence of other interaction effects such as the Coulomb correlation and the interchain interaction, and there exist a number of contesting theories. In polyacetylene, experimentally the electrical conductivity can be varied on doping systematically and reversibly over 13 orders of magnitude [11], indicating a insulator-metal transition. Although our results cannot explain this transition, they are
nonetheless consistent with the experimental observation that as the conductivity arises, the electron spin susceptibility is reduced and has the Curie type temperature dependence, before its sharp rise to the value typical of the metallic Pauli susceptibility. This suggests that before the system finally enters the metallic state with increasing doping, spinless charged solitons form and their population grow, as supported by our results of increasing density of soliton states in Chapter II for the binary distribution of the disorder (Fig. 15 and Fig. 19). When the interchain hopping is taken into consideration, the charged solitons may hop to the neighboring chains, according to the soliton hopping theory [11], and become charge carriers in the electrical conduction processes. However, the complicating factor in this case is that the doping processes are reversible, indicating that the impurities are not substitutional in nature and can rearrange themselves, in response to the electrons in the chains and to each other, or even form a ordered phase as evidenced in some experiments. More recently, it was reported that the dopant ions become disordered when the doping concentration exceeds $\sim 12\%$ [27], while the conductivity remains its high value. Our objective here is to at least understand the effects of impurities and the electronic structure when the system is disordered. Even if all the states are localized, a insulator-metal transition may take place when the interchain electron hopping is included and the system effectively becomes three-dimensional.

Based on the analytical method in Chapter III, it is interesting to generalize it to study the disordered Peierls system in quasi-one-dimensional system. The Hamiltonian in Eq. (3.1) can be modified to include the hopping of the electrons between neighboring chains,
described by the transverse hopping matrix element $t_1 \ll t_0$. The phonon term and the electron-phonon interaction remain in the same chain, while the disorder can be conveniently taken as isotropic in the three-dimensional space. In the perturbation approach, the electron-phonon interaction in mean-field theory behave like a correlated disorder, described by the function $f(q)$ in Eq. (3.26), acting only on the electrons in the same chain. Then, for the electrons, the problem reduces to the one of quasi-one-dimensional system in the presence of anisotropic and correlated disorder. It has been shown in recent studies [28], that the mobility edge in a three-dimensional tight-binding system with anisotropic disorder depends on the degree of the anisotropy, which can not be described by the one-parameter scaling theory [1]. In our case, this anisotropic disorder arises naturally from the electron-phonon interaction, and it can be controlled by adjusting the coupling constant, $\alpha$. 
V. REFERENCES


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