Multi-Modes Phonon Softening in Two-Dimensional Electron-Lattice System

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Phonon dispersion in a two-dimensional electron-lattice system described by a two-dimensional square-lattice version of Su-Schrieffer-Heeger’s model and having the half-filled electronic band is studied theoretically at temperatures higher than the mean field critical temperature of the Peierls transition. When the temperature is lowered from the higher region down to the critical one, softening of multi phonon modes which have wave vectors equal to the nesting vector $Q = (\pi/a, \pi/a)$ with $a$ the lattice constant or parallel to $Q$ is observed. Although both of the transverse and longitudinal modes are softened at the critical temperature in the case of the wave vector equal to $Q$, only the transverse modes are softened for other wave vectors parallel to $Q$. This behavior is consistent with the Peierls distortions at lower temperatures.

KEYWORDS: two-dimensional electron-lattice system, phonon softening, Peierls transition, longitudinal mode, transverse mode, linear mode analysis, SSH model

1. Introduction

The Peierls transition\(^7\) which is caused by the competition between the energy loss due to lattice distortions and the gain due to the formation of a gap at the Fermi level in the electronic energy spectrum is one of peculiar properties of one-dimensional electron-lattice systems. It is also well known that this transition can occur even in higher dimensions if the structure of the Fermi surface allows strong nesting by a single nesting vector. A two-dimensional square lattice system with a half-filled electronic band described by a tight-binding model is a typical example where the Fermi surface (more properly Fermi line) can be completely nested by the wave vector $Q = (\pi/a, \pi/a)$ with $a$ the lattice constant. Early studies on the issue of two-dimensional Peierls transition in the half-filled systems suggested that the lowest energy phase would be the state with lattice distortions whose Fourier components involved only $Q$-modes.\(^7\) The relation between the electron-electron interactions and the two-dimensional Peierls instability has been discussed rather intensively in connection to the mechanism of high $T_c$ superconductivity.\(^7,\) Nevertheless the investigation of the true ground state of the pure electron-lattice system without electron interactions was not clearly understood until recently. In recent works by Hamano and one of the present authors,\(^7,\) it has been shown that the lowest energy state of a two-dimensional electron-lattice system described by a two-dimensional version of Su, Schrieffer and Heeger’s (SSH) model

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Hamiltonian\(^7\) involves not only the distortions with \(Q\)-vector but also those with various wave vectors parallel to \(Q\), the latter contributing to the formation of the electronic energy gap through a second order process (see Fig. ??), and that there are an infinite number of non-equivalent lattice distortion patterns which indicates an infinite degeneracy of the lowest energy states. It has also been argued\(^7\) that those behaviors are maintained at finite temperatures and that the amplitudes of lattice distortions with different wave vectors, all being parallel to \(Q\), vanish all together at a critical temperature.

![Fig. 1. The situation of the Fermi-line nesting in the half-filled two-dimensional square-lattice system. The thick-line square represents the Fermi line, and a solid line is the nesting vector connecting two different parts of the Fermi line. The dotted lines describe the nesting due to the second order perturbation, where two different parts of the Fermi line are connected through a second order process.](image)

It is also known\(^7\) that the Peierls transition in one-dimensional systems is accompanied by the softening of the \(2k_F\) phonon mode at the transition temperature, where \(k_F\) represents the Fermi wave number and \(2k_F\) corresponds to \(Q\) in the two-dimensional square lattice systems with a half-filled electronic band. As has been clarified by previous papers, phonon modes relevant to the Peierls transition in the two-dimensional square lattice system described by the SSH model involve not only the \(Q\) modes but also many other modes with wave vectors parallel to \(Q\). Furthermore, as discussed in refs. ? and ?, the lowest energy states are not unique. In this sense it will be worthwhile to investigate the phonon dispersion at finite temperatures in this two-dimensional system. Even at temperatures higher than the transition temperature, we may expect a phonon softening phenomenon which is much different from that in one-dimension. In the present paper, we consider the phonon dispersion of the two-dimensional square lattice system with a half-filled electronic band only in the temperature region higher than the critical one, and study which types of phonon modes are softened when the temperature approaches the critical one from above. The dispersion at lower temperatures cannot be treated in a simple way because of the degeneracy of the lowest energy states, and therefore it will be discussed in a forthcoming separate paper.

Since the formation of the energy gap at the Fermi level leads a metallic system into an insulator, it is quite important to understand the mechanism of the Peierls transition. The present
work will shed light on the understanding of the Peierls instability in two-dimensional electron-phonon systems.

The paper is organized as follows; in the following section the model for and the method of the calculation are described. In Sec. 3, the results of the calculations are shown. The last section is devoted to summary and discussion.

2. Model and Formulation

In the following calculations we use a two-dimensional version of the SSH model\(^7\) which was originally introduced in the studies of one-dimensional electron-lattice systems and where the electron-lattice coupling is introduced through the dependence of the electronic nearest-neighbor transfer integral on the hopping distance. Since we are treating a two-dimensional square lattice, the explicit form of the model Hamiltonian is written as follows,

\[
H = -\sum_{i,j,s} \left\{ [t_0 - \alpha (u_x(i+1,j) - u_x(i,j))] \\
\times \left( c_{i+1,j,s}^\dagger c_{i,j,s} + c_{i,j,s}^\dagger c_{i+1,j,s} \right) \\
+ [t_0 - \alpha (u_y(i, j+1) - u_y(i,j))] \\
\times \left( c_{i,j+1,s}^\dagger c_{i,j,s} + c_{i,j,s}^\dagger c_{i,j+1,s} \right) \right\} \\
+ \frac{K}{2} \sum_{i,j} \left[ (u_x(i+1,j) - u_x(i,j))^2 \right. \\
\left. + (u_y(i, j+1) - u_y(i,j))^2 \right] \\
+ \frac{M}{2} \sum_{i,j} \left[ (\dot{u}_x(i,j))^2 + (\dot{u}_y(i,j))^2 \right],
\]

where the field operators \(c_{i,j,s}\) and \(c_{i,j,s}^\dagger\) annihilate and create an electron with spin \(s\) at the site \((i, j)\), respectively, and \(t_0\) is the transfer integral for the equidistant lattice, \(\alpha\) the electron-lattice coupling constant, \(u(i,j)\) the lattice displacement vector whose \(x\)- and \(y\)-components are denoted as \(u_x(i,j)\) and \(u_y(i,j)\), respectively, \(K\) the force constant describing ionic coupling strength in the lattice system, \(M\) the mass of an ion unit at a site. Throughout this paper, we assume the periodic boundary conditions (PBC) for both directions.

The equations of motion for the lattice system can be derived on the assumption that the ionic mass \(M\) is much larger than the effective mass of an electron and by introducing the Born-Oppenheimer approximation\(^7\) in the case of the \(x\)-components of the displacement vectors, they are explicitly written as follows,

\[
M\ddot{u}_x(i,j) = \alpha \sum_{s} \left( (c_{i+1,j,s}^\dagger c_{i,j,s} + c_{i,j,s}^\dagger c_{i+1,j,s} \right)
\]
\[-\langle c_{i,j,s}^\dagger c_{i-1,j,s}^\dagger + c_{i-1,j,s}^\dagger c_{i,j,s} \rangle \]
\[+ K (u_x(i+1,j) - 2u_x(i,j) + u_x(i-1,j)), \] (2)

and similar expressions for the \(y\) components can be written down, which will be omitted here because they can be easily speculated from the above ones. Assuming the electronic system is in the equilibrium state for the given lattice configuration at any moment, the above equations of motion can be rewritten as follows,

\[M \ddot{u}_x(i,j) = 2\alpha \sum_\nu f(\varepsilon_\nu) \left( \phi_\nu(i+1,j) \phi_\nu(i,j) - \phi_\nu(i,j) \phi_\nu(i-1,j) \right) + K (u_x(i+1,j) - 2u_x(i,j) + u_x(i-1,j)), \] (3)

where \(f(\varepsilon_\nu)\) represents the Fermi distribution function for the eigenenergy \(\varepsilon_\nu\) corresponding to the single particle eigenstate \(\phi_\nu\), which is obtained by solving the eigenvalue problem for a given configuration of the lattice displacements \(\{u(i,j)\}\). Because of the electron-hole symmetry of the present system, the electronic chemical potential is fixed to be zero at any temperature. Again the equations for the \(y\)-component are omitted.

The stable static lattice displacements \(\{u^0(i,j)\}\) are obtained by solving a set of self-consistent equations which are nothing but those given by setting the right-hand side of eq. (3) to be zero. The linear modes around this static solution, i.e. the phonon modes, can be calculated by linearizing the equations of motion for \(u_x(i,j)\) and \(u_y(i,j)\) with respect to the deviations from the static configurations. In deriving equations for the linear modes, we should take into account the effects of those deviations on the electronic eigenfunctions:

\[u(i,j,t) = u^0(i,j) + \delta u(i,j,t) \] (4)
\[\phi_\nu(i,j;t) = \phi^0_\nu(i,j) + \delta \phi_\nu(i,j;t), \] (5)

where we have introduced the time variable \(t\) explicitly and the electronic eigenfunctions corresponding to the static displacements are denoted as \(\phi^0_\nu(i,j)\). The time dependence of the electronic wave functions is implicit one through the slow time dependence of the lattice displacements. The deviations of the wave functions \(\delta \phi_\nu(i,j;t)\) are calculated within the first order perturbation theory in the form,

\[\delta \phi_\nu(i,j;t) = \sum_{\mu(\neq \nu)} \frac{\phi^0_\mu(i,j)}{\varepsilon_\nu - \varepsilon_\mu} V_{\nu\mu}, \] (6)
with
\[
V_{\nu\mu} = 2\alpha \sum_{n,m} \left[ \left( \delta u_x(n+1, m, t) - \delta u_x(n, m, t) \right) \times \left( \phi_\mu^0(n+1, m) \phi_\nu^0(n, m) \right) + \left( \delta u_y(n+1, m, t) - \delta u_y(n, m, t) \right) \times \left( \phi_\mu^0(n, m+1) \phi_\nu^0(n, m) \right) \right].
\]  
(7)

In order to determine the normal modes, we postulate that the time dependence of the deviations of the lattice displacements is given by
\[
\delta \mathbf{u}(i, j, t) = (\delta u_x(i, j, t), \delta u_y(i, j, t)) = \phi(i, j; \omega) e^{i \omega t}.
\]  
(8)

Then the equation for \( \delta \mathbf{u}(i, j; \omega) \) can be expressed in the following form,
\[
M \omega^2 \delta \mathbf{u}(i, j; \omega) = \sum_{m,n} W(i, j; m, n) \delta \mathbf{u}(m, n; \omega),
\]  
(9)

where the 2\( \times \)2 matrices \( W(i, j; m, n) \) are defined as follows,
\[
W_{a,b}(r; R) = 2\alpha^2 \sum_{\mu} \sum_{\nu(\neq \nu)} \frac{f(\varepsilon_\nu)}{\varepsilon_\nu - \varepsilon_\mu} \times \left[ \phi_\mu^0(r) \left( \phi_\nu^0(r + e_a) - \phi_\nu^0(r - e_a) \right) \right. \\
+ \phi_\nu^0(r) \left( \phi_\mu^0(r + e_a) - \phi_\mu^0(r - e_a) \right) \left. \right] \times \left[ \phi_\mu^0(R) \left( \phi_\nu^0(R + e_b) - \phi_\nu^0(R - e_b) \right) \right. \\
+ \phi_\nu^0(R) \left( \phi_\mu^0(R + e_b) - \phi_\mu^0(R - e_b) \right) \right] + K \delta_{a,b} \left( - \delta_{r+e_a,R} + 2\delta_{r,R} - \delta_{r-e_a,R} \right).
\]  
(10)

Here \( a \) and \( b \) stand for \( x \) or \( y \), and for simplicity we expressed the lattice sites as \( r[i,j] \) and \( R[m,n] \) and introduced unit vectors \( e_x = (1, 0) \) and \( e_y = (0, 1) \). The eigenfrequency \( \omega \) and the corresponding eigenfunction \( \delta \mathbf{u}(r; \omega) \) for the normal modes are determined by solving the eigenvalue problem eq. (??).

The above-mentioned formulation can be used at any temperature irrespective of the presence or absence of finite static lattice distortions. In the present paper we consider only the high temperature region where there is no static lattice distortion. In this situation, the normal modes equations
can be reduced into a much simpler form. If there is no distortion, the electronic eigenenergies and eigenfunctions are given by those of the plane waves;

\[
\varepsilon_k = -2t_0[\cos(k_x) + \cos(k_y)],
\]

\[
\phi^0_k(r) = \frac{1}{L} e^{ik \cdot r},
\]

where \( k = (k_x, k_y) \) is the wave vector characterizing the electronic eigenstate, and the system size is assumed to be \( L \times L \). We use a length unit where the lattice constant is equal to unity. It can be easily confirmed that the phonon normal modes are also expressed in the plane wave form in the present situation, i.e.

\[
\delta u(r, \omega) = g(q, \omega) e^{iq \cdot r}. 
\]

Thus the linear modes equations are rewritten in the following form,

\[
\omega^2 g(q, \omega) = U(q) g(q, \omega),
\]

where the elements of the \( 2 \times 2 \) matrix \( U(q) \) are given by

\[
U_{a,b}(q) = \frac{4\alpha^2}{ML^2} \sum_k \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q}}
\]

\[
\times \left[ \sin(k_a + q_a) - \sin k_a \right] \left[ \sin(k_b + q_b) - \sin k_b \right]
\]

\[
+ \frac{K}{M} (1 - \cos q_a) \delta_{a,b}.
\]

Here again \( a \) and \( b \) stand for \( x \) or \( y \). It is easily confirmed that \( U(q) \) is a symmetric matrix. The eigenfrequency \( \omega \) does not appear in the matrix \( U(q) \) because of the Born-Oppenheimer approximation. It is straightforward to calculate the eigenvalues and eigenvectors from eq. (13). The results are discussed in the following section. It should be noted that the calculation of the phonon dispersion in the low temperature region, where distortions involving various wave numbers parallel to the nesting vector \( Q \) are appearing, is not so simple as in the present situation without any static distortion.

3. Results of Calculations

As stated in the previous section, the frequencies of the phonon modes in the temperature region higher than the Peierls transition temperature \( T_c \) are obtained from the eigenvalue problem for a \( 2 \times 2 \) matrix \( U \), the elements of which depend only on the wave vector \( q \) and the temperature included in the electronic distribution function (Fermi distribution). The result is written as

\[
\omega^2 = \frac{1}{2} \left\{ U_{x,x} + U_{y,y} \pm \sqrt{(U_{x,x} - U_{y,y})^2 + 4U_{x,y}^2} \right\}
\]

When \( q_x = q_y = 0 \), all the elements of the matrix \( U \) vanishes irrespective of the temperature and consequently we have two degenerate uniform modes with zero frequency; they correspond
to the long-wave-length limit of two acoustic modes. For general values of \(q_x\) and \(q_y\), the matrix elements are calculated only numerically.

As has been shown in the previous works,\(^7\)\(^,\)\(^7\) the phonon modes relevant to the Peierls transition are those with wave vectors parallel to \(Q\) including \(Q\) itself. Therefore, let us first discuss the temperature dependence of several phonon frequencies for the case with \(q_x = q_y = q\). In this case, the phonon modes are longitudinal (\(g(q) \parallel q\), i.e. \(g_x = g_y\)) or transverse (\(g(q) \perp q\), i.e. \(g_x = -g_y\)).\(^7\) In Fig. 2 the eigenvalue \(\omega^2\) is plotted as a function of the temperature \(T\) for the transverse (a) and longitudinal (b) modes with \(q = \pi\) (solid curve), \(\pi/2\) (dashed curve) and \(\pi/4\) (dotted curve). The product of the temperature \(T\) and the Boltzmann constant is scaled by \(t_0\) and \(\omega^2\) by \(K/M\). The dimensionless coupling constant \(\lambda \equiv \alpha^2/t_0K\) is assumed to be 0.32 throughout the paper. In evaluating the \(k\)-sums included in the definition of the matrix elements \(U_{a,b}\), we have set the system size \(L\) to be 64; this choice of the system size is to get a clear presentation of the wave vector dependence of the dispersion (see Fig. 2). It has been confirmed that the results shown in Fig. 2 do not change even if larger values of \(L\) are used.

![Fig. 2. The temperature dependence of the eigenvalue \(\omega^2\) for transverse (a) and longitudinal (b) modes with fixed values of the wave number \(q (= q_x = q_y)\); the values of \(q\) are given in the graph. In the inset of (a) all eigenvalues for the transverse modes with \(q_x = q_y = q\) (including \(q = \pi\)) scaled by corresponding values for free phonons \(\omega_0^2(q)\) are plotted; they fall into a single curve. The temperature \((k_B T)\) with \(k_B\) the Boltzmann constant) is scaled by \(t_0\) and \(\omega^2\) by \(K/M\). The dimensionless coupling constant is \(\lambda = 0.32\) and the system size \(L\) is chosen to be 64.](image-url)

In Fig. 2(a), there are three examples of temperature dependence of the eigenfrequencies for the transverse modes with wavevectors \(q_x = q_y = q\) are plotted, it should be noted that all the eigenvalues cross 0 at the same temperature \((k_B T_c \simeq 0.35)\). We have numerically confirmed that the eigenvalues \(\omega^2(q, T)\) for the transverse modes with \(q_x = q_y = q\) scaled by \(\omega_0^2 (= (K/M)(1 - \cos q))\) the square frequency of the corresponding free phonon depend on the temperature \(T\) but not on \(q\) as shown in the inset of Fig. 2(a). It will be clear that all the frequencies of the transverse modes with wavevectors \(Q\) and the parallel to it vanish at the same temperature. This is consistent with the structure of the lower temperature Peierls phase.\(^7\)\(^,\)\(^7\)\(^,\)\(^7\) The critical temperature \(T_c\) is the same with that estimated from the vanishing of the order parameters in the low temperature regime.\(^3\)
In the case of the longitudinal modes, only the mode with the nesting vector (i.e. \( q = \pi \)) vanishes at the critical temperature as seen in Fig. ??(b). When the temperature is reduced below the critical temperature, the values of \( \omega^2 \) for all the modes in Fig. ??(a) and that for the nesting vector mode in Fig. ??(b) become negative, indicating these modes are unstable in the lower temperature regime and suggesting a phase transition.

In order to see the softening of the phonon modes with wave vectors parallel to the nesting vector at the critical temperature, we have calculated the wave vector dependence of the phonon dispersion at \( T_c \). The results are summarized in Fig. ??, where in (a) the dispersion of the lower branch [see eq. (??)] which corresponds to the transverse modes for some special directions of the wave vector is shown and in (b) the upper branch connected to the longitudinal modes for some special directions.

For the sake of simplicity we call the lower branch [Fig. ??(a)] the transverse modes and the upper branch [Fig. ??(b)] the longitudinal modes. In the case of the transverse modes, all those with wave vectors parallel to the nesting vector \( Q \), including the \( Q \)-mode itself, are found to have zero frequency at the critical temperature, while in the case of the longitudinal modes, only the frequency of the \( Q \)-mode vanishes at the critical temperature.

4. **Summary and Discussion**

In the present work, the temperature dependence of the phonon dispersion in the high temperature regime (i.e. at temperatures higher than the Peierls transition temperature) has been studied for a two-dimensional electron-lattice system with a half-filled electronic band, which is described by the SSH-type model extended to the case of a two-dimensional square lattice. In this system, it was shown in the previous papers\(^7\),\(^8\),\(^9\) that the lowest energy state in the low temperature regime is the Peierls state with multi-modes distortions where the Fourier components of the distortions involve not only the nesting vector modes but also many other modes having wave vectors parallel to the nesting vector \( Q = (\pi, \pi) \). In accordance with this low temperature behavior of the system, we have found the softening of phonon modes with wave vectors \( Q \) and with those parallel to it as the temperature is lowered from the high temperature region towards the critical temperature. As for the polarization of the softened modes, both of the longitudinal and transverse modes are softened in the case of the \( Q \)-vector, while only the transverse mode has zero frequency in the case of wave vectors parallel to but not equal to \( Q \) at the critical temperature.

Although the zero temperature ground state of the system has an infinite number of degeneracy,\(^7\) depending on different amplitude distributions of the Fourier components of the static Peierls distortions, we have confirmed that the polarization of distortion components corresponding to non-\( Q \)-modes (i.e. those with wave vectors parallel but not equal to \( Q \)) is transverse and that the polarization of the \( Q \)-mode is longitudinal, in all cases. This fact is maintained even at
finite temperatures (below the critical temperature). In spite of the softening of the transverse $Q$-mode, there is no transverse component of the $Q$-mode in the ground state Peierls distortions. On the other hand, the asymmetrically dimerized Peierls state, which was suggested by Tang and Hirsch\(^2\)) but has a higher energy than the multi-modes Peierls state,\(^3\)) involves the longitudinal and transverse components of the $Q$-mode with an equal amplitude in the Fourier expansion of the distortions.

Similarly, although all the transverse modes with wave vectors parallel to $Q$ are softened, not all the components appear in the Fourier expansion of the multi-modes Peierls distortions. The simplest pattern in the degenerate ground states will be the one consisting of the longitudinal $Q$-mode and the transverse $Q/2$-mode.\(^3\)) These facts indicate that, when many phonon modes are softened, it is not necessary for all the modes to show condensation in order to realize the lowest energy Peierls state. At the moment, there is no guiding principle to determine which of the infinitely degenerate low temperature states is chosen when the temperature is lowered from the higher region across the critical temperature.

It will also be worthwhile to study the phonon dispersion in the Peierls distorted phase, which is to be treated in the future work. Furthermore the effect of electron-electron interactions should be considered in order to discuss the Peierls transition in real systems, which is left for future studies.

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1) R.E. Peierls: *Quantum theory of Solids* (Clarendon Press, Oxford, 1955).
2) S.Tang and J.E.Hirsh: Phys. Rev. B 37 (1988) 9546.
3) K. Machida and M. Kato: Phys. Rev. B36 (1987) 854.
4) R.T. Scalettar, N.E. Bickers, and D.J. Scalapino: Phys. Rev. B40 (1989) 197.
5) S. Mazumdar: Phys. Rev. B39 (1989) 12324.
6) S. Tang and J.E. Hirsch: Phys. Rev. B39 (1989) 12327.
7) Y.Ono and T.Hamano: J. Phys. Soc. Jpn. 69(2000) 1769.
8) T.Hamano and Y.Ono: J. Phys. Soc. Jpn. 70 (2001) 1849.
9) T.Hamano and Y.Ono: unpublished.
10) W. P. Su, J. R. Schrieffer, and A. J. Heeger: Phys. Rev. Lett. 42 (1979) 1698, Phys. Rev. B22 (1980) 2099.
11) H.J. Schulz: Phys. Rev. B18 (1978) 5756.
12) M. Born and J.R. Oppenheimer: Ann. Phys. 84 (1927) 457.
13) A.Terai and Y.Ono: J. Phys. Soc. Jpn. 55 (1986) 213, and references therein.
14) N.W. Ashcroft and N.D. Mermin: *Solid State Physics* (Holt, Rinehart and Winston, 1976).
Fig. 3. Phonon dispersions at $T_c$. (a) the dispersion related to “transverse” modes and (b) that related to “longitudinal” modes. The eigenvalue $\omega^2$ is scaled by $K/M$. The dimensionless coupling constant $\lambda$ is 0.32, the system size $L$ being 64.