Competition of different types of electron-lattice coupling in 2D Peierls transition

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Abstract. The stability of the multimode Peierls (MMP) state, which has been predicted for the 2D square-lattice electron system with the Su-Schrieffer-Heeger (SSH) type electron-lattice \((e-l)\) coupling and with a half-filled electronic band, is discussed in the presence of a dilation-type e-l interaction. To understand the role of the latter interaction, the ground state for the model with only the latter interaction is numerically investigated for the 1D chain and the 2D square lattice. The results indicate that this interaction favors a phase separation into two regions, one with sites doubly occupied by electrons and the other with sites having no electron. Detailed numerical analyses show that the MMP state in the 2D system can survive even in the presence of the dilation-type interaction as long as its coupling strength is weak compared to that of the SSH-type interaction.

1. Introduction

The Peierls transition in a 1D electron-lattice \((e-l)\) system is a phenomenon in which a metal is changed into an insulator by the appearance of a lattice distortion with the wave number \(2k_F\), \(k_F\) being the Fermi wave number [1]. Since there is a nesting vector in a 2D square-lattice system with a half-filled electronic band, the realization of the Peierls transition in a 2D e-l system is conceivable as well as in a 1D e-l system. In fact, the Peierls transition in a 2D e-l system has been studied by many researchers [2], particularly in connection to the high \(T_c\) superconductors.

Recently, it has been shown that the Peierls distortion in a square-lattice 2D e-l system with a half-filled electronic band is essentially different from what is expected from the result in a 1D e-l system. The energetically most stable state in the 2D e-l system has been found to be what we call the multimode Peierls (MMP) state [3], where the Fourier components of the lattice distortion include not only the nesting vector mode but also other various modes with wave vectors parallel to the nesting vector. In these studies as well as in previous studies, the employed model was a 2D extension of the Su-Schrieffer-Heeger (SSH) model [4] where the e-l coupling is induced by the modification of the electronic transfer integral by lattice distortions. Although the model seems physically reasonable, no evidence of the MMP state has yet been observed experimentally. In this sense, it is quite important to check the stability of the MMP state against other perturbations. So far the effects of electron-electron interactions [5] and of the anisotropy [6] have been studied. It has been confirmed in these works that the MMP state...
can survive as the lowest energy state as long as the interaction parameters lie in a certain region.

In the present paper, we consider another type of e-l interaction in addition to the SSH type, and discuss the stability of the MMP state. As for the new interaction, we adopt the one induced by the local dilation, which is known as the deformation potential in 3D systems [7]. Although it is not clear whether such a dilation-type interaction exists in realistic 2D systems such as organic conductors, we employ this interaction, which has a completely different origin from the SSH type, in order to discuss the stability of the MMP state against perturbations.

2. Model and method
The model Hamiltonian involving both of the SSH-type and dilation-type e-l interactions is expressed in the following form,

\[ H = - \sum_{d,r} (t_0 - \alpha_{SSH} v^d_{r}) (c^+_{r+\vec{e}^d} c_r + \text{h.c.}) + \alpha_{dil} \sum_{d,r} (v^d_{r} + v^d_{r-\vec{e}^d}) c^+_{r} c_r + (K/2) \sum_{d,r} (v^d_{r})^2, \quad (1) \]

where the 1st term represents the electronic part of the standard SSH model, the 2nd the lattice version of dilation-type e-l interaction, \( \alpha \)'s meaning respective coupling constants, and the last the lattice elastic energy. We consider a square lattice with a lattice constant \( a \) (set to be unity in the following), and the lattice site is expressed by \( r = (i,j) \) (in 1D, \( r \) should be read as \( i \)), \( d \) indicating a direction, in a 1D system \( d = x \) and in a 2D system \( d = x \) or \( y \), \( t_0 \) the transfer integral for the equidistant (undeformed) lattice, \( e^d \) the unit vector in the direction \( d \). The lattice distortions \( \{v^d_{r}\} \) are related to the lattice displacements \( \{u^d_{r}\} \) as \( u^d_{r} = v^d_{r} + v^d_{r-\vec{e}^d} - v^d_{r}. \quad c^+_{r} \) and \( c_r \) are the creation and annihilation operators of an electron at the site \( r \), \( K \) the force constant of the lattice. As is well known, the strength of the e-l interaction is described by the dimensionless e-l coupling constants, \( \lambda_{SSH} \equiv \alpha_{SSH}^2 / K t_0 \) and \( \lambda_{dil} \equiv \alpha_{dil}^2 / K t_0 \). Since we are interested in bulk properties, the periodic boundary conditions are assumed. The ground state is numerically studied by minimizing the expectation value of \( H \) with respect to the lattice distortions, which results in a set of self-consistent equations for distortions; derivation of those equations is described in the literature [3], and is omitted here to save space.

3. Results
Let us first consider the role of the dilation-type interaction. The lowest energy state in the 1D system with \( \lambda_{SSH} = 0 \) and \( \lambda_{dil} \approx 0.8 \) is found to be of a phase separation type, where the system is divided into two regions, one with an almost uniform lattice contraction and the electronic density two per site and the other with an almost uniform lattice dilation and electronically empty sites. The Fourier analysis of the distortion pattern indicates that the distortion involves only the Fourier components with odd number times \( 2\pi/N \) \( (N \) the system size) and that the spectrum has a strong peak around the zero wave number. There is no \( 2k_F = (\pi) \) component, since \( 2k_F \) component has no contribution to the dilation-type coupling term in \( H \). The electronic energy spectrum splits into two bands with a gap around the original Fermi level, the upper band corresponding to those states mainly localized in the dilating region and the lower band to those mainly localized in the contracted region. Although the dilation and contraction push up the lattice energy, the electronic energy is largely lowered by the phase separation and by occupying the sites in the contracted region since the contraction increases the band width. Through calculations for different values of \( \lambda_{dil} \), it is found that the above-mentioned phase separation occurs only when \( \lambda_{dil} \) exceeds a certain critical value around 0.63, below which the lowest energy state of the system is the undistorted one. Transition between the undistorted and phase-separated states is of the 1st order.

The situation is essentially similar in the 2D system. In 2D, however, the phase separated state occurs even in the weak coupling case. Furthermore, the spatial structures of the contracted
and dilating regions are different between the weak and strong coupling cases. In the weak coupling case, there appear four phase boundary lines, two being parallel to horizontal axis and the other two to vertical axis, resulting in square shape of contracted and dilating regions. There appear only two phase boundary lines in the case of strong coupling; the direction of these lines is perpendicular to the nesting vector $Q = (\pi, \pi)$. As a result, the shape of the uniform phase regions becomes stripe-like. The weak and strong coupling cases are separated by a critical value of $\lambda_{\text{dil}}$ around 0.47 for $N \times N = 16 \times 16$. Details of the phase separated states in 2D case will be published elsewhere.

Next we consider a model involving both of the two types of e-l interactions. The numerical results for 1D systems are depicted in Fig. 1 as typical examples of the lattice distortion patterns for the cases with $\lambda_{\text{SSH}} = 0.3$ and with varying $\lambda_{\text{dil}}$ from 0.0 to 1.0, for $N = 128$. It is found that for smaller values of $\lambda_{\text{dil}}$ (0.0 to 0.2) the stable state is the normal Peierls state. When $\lambda_{\text{dil}}$ is increased, the system shows two-phase separation similarly as in the case without $\lambda_{\text{SSH}}$, although the ratio between the lengths of the contracted and dilating regions decreases with increasing $\lambda_{\text{dil}}$. Furthermore, due to the finite value of $\lambda_{\text{dil}}$, a kind of Peierls distortion appears in the contracted region. The length of the contracted region is longer than $N/2$ when $\lambda_{\text{SSH}} \neq 0$, resulting in partial filling of the lower band corresponding to the electronic states in the contracted region. The small ripples seen in Fig. 1 are thought to be the Peierls distortions due to this partially filled band. This situation can also be understood from the electronic energy spectrum.

By changing both coupling parameters, $\lambda_{\text{dil}}$ and $\lambda_{\text{SSH}}$, we obtain a phase diagram in the $\lambda_{\text{dil}}$-$\lambda_{\text{SSH}}$ plane. Data for $N = 128$ indicates that the critical value of $\lambda_{\text{dil}}$, above which the two-phase separated state is realized, is shifted to lower side by a finite $\lambda_{\text{SSH}}$, although the ground state is the normal Peierls state in the region $\lambda_{\text{dil}} < 0.25$. This would be interpreted as follows: When $\lambda_{\text{SSH}} = 0$, the energy gain due to the full occupation of the lower electronic band corresponding to those states in the contracted region overcomes the energy loss in the lattice system. In the presence of $\lambda_{\text{SSH}}$, the contracted region can be larger than $N/2$ leading to partial filling of the lower band, since the resulting Fermi level can be eliminated by the Peierls distortion due to a finite $\lambda_{\text{SSH}}$ and the widening of the contracted region can reduce the electronic energy; these two effects cooperatively enable the two-phase separation at smaller $\lambda_{\text{dil}}$.

The essential physics does not change also in 2D systems. When $\lambda_{\text{SSH}} \gg \lambda_{\text{dil}}$, we find that the MMP state induced by $\lambda_{\text{SSH}}$ is not affected by the dilatation coupling similarly as in the 1D case. On the other hand, when $\lambda_{\text{SSH}} \ll \lambda_{\text{dil}}$, the two-phase separation occurs although the areas of the contracted and dilating regions are not equal to each other; the former is larger than the latter, generally. As a result, the electronic filling of sites in the contracted region is not full, leading to the appearance of the Fermi line in the lower electronic band. Although it is not an easy task to construct the band structure in the 2D wave vector space, it will be easily understood that the new Fermi line in the presence of the two-phase separation is located near to the original Fermi line in the absence of lattice distortions.

From the data for various values of $\lambda_{\text{SSH}}$ and $\lambda_{\text{dil}}$, we can draw a phase diagram as in Fig. 2, where an example of the case with the system size $N \times N = 16 \times 16$ is depicted. The dark region represents the MMP state with no effect from the dilation-type coupling, and the less dark region indicates the two-phase separating state with an MMP-type modification. The transition between the MMP state and the two-phase separating state is of the first order. Here we have omitted the discussions about the boundary between different types of two-phase separation, since we are mainly interested in the stability of the 2D MMP state in this work.

From the above results, it may be concluded that the MMP state remains to be the lowest energy state as long as $\lambda_{\text{SSH}} \gg \lambda_{\text{dil}}$. 

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4. Summary

The present study has been started in order to check whether the MMP state, which has been found in recent theoretical investigations for a 2D e-l system with a half-filled electronic band, a square-lattice structure and the SSH-type e-l coupling, [3] can survive in the presence of an e-l coupling different from the SSH-type one. The results in this work indicate that the MMP state can be the lowest energy state in the 2D e-l system as long as the system parameters satisfy a certain condition which would not be unrealistic. In previous papers, we have studied the effects of the electron-electron (e-e) interaction and the anisotropy on the MMP state, and have found that the MMP state is the lowest energy state within a certain region of the parameter space. In this sense there remains a possibility to find the MMP state experimentally.

In the present work, we have concentrated to the lowest energy state and have not considered the finite temperature effect. It would be desirable to discuss the stable state and its properties at finite temperatures in order to make an explicit experimental proposal. Furthermore, we should know the combined effect of the e-e interaction, the anisotropy and different types of e-l interactions when we consider realistic materials. These problems are left for the future study.

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