Phonon Dispersion Relations in Two-Dimensional Electron-Lattice Systems at Non-Zero Temperature

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In one-dimensional electron-lattice systems with a half-filled electronic band it is well-known that the lowest energy state of the system has the Peierls distortion with a wave number π, the lattice constant is unity, and that the system behaves as an insulator. In recent studies [1,2], it is reported that the Peierls distortions in a two-dimensional square lattice system described by the SSH (Su-Schrieffer-Heeger) model have different properties from those in the well-known one-dimensional case; in this two-dimensional case the Peierls distortions are composed of Fourier components with various wave vectors parallel to $\boldsymbol{Q} = (\pi, \pi)$ including $\boldsymbol{Q}$ itself (we call this state Multi-Mode Peierls State: MMPS). The known properties of this MMPS are summarized as follows; (1) there are an infinite number of degenerate ground states at absolute zero of temperature, which have non-equivalent different patterns of lattice distortions and the same electronic energy structure, (2) the Fourier components of lattice distortions concerning the MMPS vanish all together at a critical temperature $T_{\rm c}$, and (3) The infinite degeneracy of the lowest energy states survives at finite temperatures lower than $T_{\rm c}$ [3]. In order to understand the mechanism of the Peierls transition in this two-dimensional system, it will be useful to study the phonon dispersion relations at finite temperatures taking account of the effect of the electron-lattice interaction.

In this work, we discuss phonon dispersion relations at non-zero temperatures, and particularly study the softening of multi-phonon-mode related to the Peierls distortions. The details of the formulation used here are described in [4]. The model Hamiltonian treated in this work is given by

$$
\begin{aligned}
H \;=\; & -\sum_{i,j,s}\Big\{[t_0 - \alpha(u_x(i+1,j) - u_x(i,j))]\left(c^{\dagger}_{i+1,j,s}c_{i,j,s} + c^{\dagger}_{i,j,s}c_{i+1,j,s}\right) \\
& +[t_0 - \alpha(u_y(i,j+1) - u_y(i,j))]\left(c^{\dagger}_{i,j+1,s}c_{i,j,s} + c^{\dagger}_{i,j,s}c_{i,j+1,s}\right)\Big\} \\
& +\frac{K}{2}\sum_{i,j}\left[(u_x(i+1,j) - u_x(i,j))^2 + (u_y(i,j+1) - u_y(i,j))^2\right],
\end{aligned}
\tag{1}
$$

where the field operators $c_{i,j,s}$ and $c^{\dagger}_{i,j,s}$ 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, α the electron-lattice coupling constant, $\boldsymbol{u}(i,j) = (u_x(i,j), u_y(i,j))$ the lattice displacement vector, K the force constant describing ionic coupling strength in the lattice system. The periodic boundary conditions (PBC) are assumed for both directions. The phonon normal modes are obtained through a standard linear mode analysis. In the temperature region higher than $T_{\rm c}$, the system has no lattice distortion, and therefore the electronic eigenfunctions in the absence of phonon excitations are described by simple plane waves, $\phi^0_{\boldsymbol{k}}(\boldsymbol{r}) = L^{-1}{\rm e}^{{\rm i}\boldsymbol{k}\cdot\boldsymbol{r}}$, where L is the system size and $\boldsymbol{r}$ stands for a site (i,j). As a consequence the phonon normal modes are expressed in the form of plane waves, $\delta\boldsymbol{u}(\boldsymbol{r},t) = \mathcal{G}(\boldsymbol{q},\omega){\rm e}^{{\rm i}(\boldsymbol{q}\cdot\boldsymbol{r}-\omega t)}$, with $\boldsymbol{q}$ represents a wave vector of a phonon mode and ω the corresponding eigenfrequency. The linear mode equations in the temperature region higher than T_c are given in the following form,

$$\omega^2 \mathcal{G}(\mathbf{q},\omega) = \mathcal{U}(\mathbf{q})\mathcal{G}(\mathbf{q},\omega), \tag{2}$$

where

$$\begin{aligned} \mathcal{U}_{x,y}(\mathbf{q}) &= \frac{4\alpha^2}{ML}\sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k+q}})}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}}} \Big(\sin(k_x+q_x) - \sin k_x\Big)\Big(\sin(k_y+q_y) - \sin k_y\Big) \\ &+ \frac{K}{M}(1-\cos q_x)\delta_{x,y}. \end{aligned} \tag{3}$$

Here $f(\epsilon_{\mathbf{k}})$ is Fermi distribution function for eigenenegy $\epsilon_{\mathbf{k}}$, which is given by $\epsilon_{\mathbf{k}} = -2t_0(\cos(k_x) + \cos(k_y))$. The above equation is easily solved and we find softening of transverse phonon modes with various wave vectors parallel to $\boldsymbol{Q}$ when the temperature is lowered (see Fig. 1).

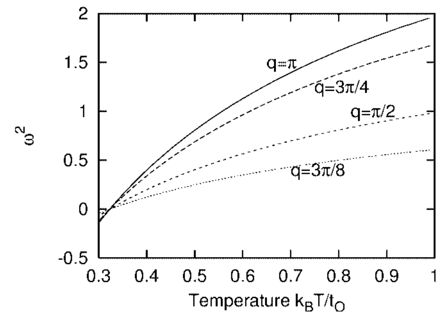

Fig. 1: The temperature dependence of square eigenfrequency ω^2 which belong to *transverse* modes where wave vectors indicated by $q_x = q_y = q$. The temperature is scaled by t_0 and ω^2 by K/M.The dimensionless coupling constant is $\lambda = \alpha^2/Kt_0 = 0.6$ and the system size L is chosen to be 64

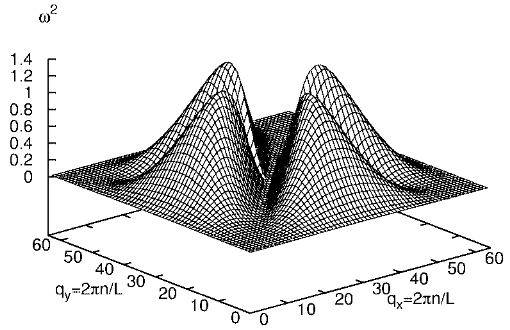

Fig. 2: Whole picture of phonon dispersion relations at critical temperature $T_c \sim 0.33t_0/k_B$. Only transeverse modes are plotted, and the condition for calculations are the same as above.

Figure 1 indicates that all eigenfrequencies connected to MMPS cross 0 at the same temperature $T_c \simeq 0.33t_0/k_B$. The negative values for ω^2 mean that those modes are unstable. In the case of longitudinal modes we find that only the $\boldsymbol{Q}$-mode shows a softening at T_c. In Fig. 2, the whole dispersion relation for the transverse modes at T_c is depicted, which clearly shows that all the transverse modes with wave vectors parallel to $\boldsymbol{Q}$ are equal to zero. These behavior is confirmed to be consistent with the structure of the Peierls distortion below T_c. Although the treatment of the phonon modes in the temperature region lower than T_c is a bit more complicated because of the presence of static Peierls distortions, similar analysis can be performed.

References

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[4] S.Chiba and Y.Ono: unpublished