Two-Dimensional Peierls Transition with Multimode Lattice Distortions

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Usual Peierls transition involves only the lattice distortion with a wave vector causing a nesting of the Fermi surface. In the case of a two-dimensional square lattice system with a half-filled electronic band, the Fermi surface (or line) takes a square form in the first Brillouin zone of the electronic momentum space, and the strong nesting is realized by a vector $\boldsymbol{Q} = (\pi, \pi)$ [1], where and hereafter we assume the lattice constant is unity. In recent studies [2, 3] we have found unusual Peierls distortions at absolute zero of temperature for a two-dimensional square lattice system described by a two-dimensional version of Su, Schrieffer, and Heeger's model [4] with a half-filled electronic band; the distortions include Fourier components not only with the nesting vector $\boldsymbol{Q}$ but also with wave vectors parallel to $\boldsymbol{Q}$ [2], and furthermore there are many nonequivalent patterns of spatial variation of the distortions, which gives the same lowest energy [3]. Since the wave vectors different from $\boldsymbol{Q}$ cannot connect directly different parts of the Fermi line, this multimode Peierls phase involves necessarily the second order process with respect to the electron-lattice coupling. As far as the authors know, the Peierls transition including second order process has not been reported so far.

In the present work, we discuss the above-mentioned two-dimensional Peierls phase at finite temperatures. The model Hamiltonian is given by

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

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. Since se are interested in static distortions, the kinetic energy term for the lattice system is neglected here. At a finite temperature T, the values of the static distortions are determined by minimizing the free energy of the system,

$$F = 2\sum_{\nu}\ln[1 + \exp(-\varepsilon_\nu/k_{\mathrm{B}}T)] + E_{\mathrm{lat}}, \tag{2}$$

where ε_ν represents an electronic eigenenergy for a single electron eigenstate in the presence of lattice distortions, and E_{lat} the lattice energy. Here it should be noted that the electronic chemical potential for the half-filled case is maintained to be zero even at finite temperatures because of the electron-hole symmetry of the model. On the assumption that the Fourier

components of the distortions include only the wave vector $\boldsymbol{Q}$ and those parallel to it, the self-consistent equations for the Fourier components of distortions are very much simplified as discussed in the calculations at absolute zero of temperature [2]. The coupled self-consistent equations are solved numerically by iteration. In the iterative calculation we have to set up initial values. This choice of initial values fix one of many degenerate lowest energy states. In Fig. 1, we show the temperature dependence of the Fourier components of the distortions minimizing the free energy of the system in the case where only $\boldsymbol{Q}$- and $\boldsymbol{Q}/2$-components are existing, i.e. where the distortions are expressed in the form,

$$\boldsymbol{u}(i,j) = \begin{pmatrix} X_{\boldsymbol{Q}} \\ Y_{\boldsymbol{Q}} \end{pmatrix} (-1)^{i+j} + \begin{pmatrix} X_{\boldsymbol{Q}/2} \\ Y_{\boldsymbol{Q}/2} \end{pmatrix} \exp\left(\mathrm{i}\frac{\pi}{2}(i+j)\right) + \text{c.c.} \tag{3}$$

The dimensionless coupling constant $\lambda(\equiv \alpha^2/Kt_0)$ is assumed to be 0.6 in obtaining the data for Fig. 1.

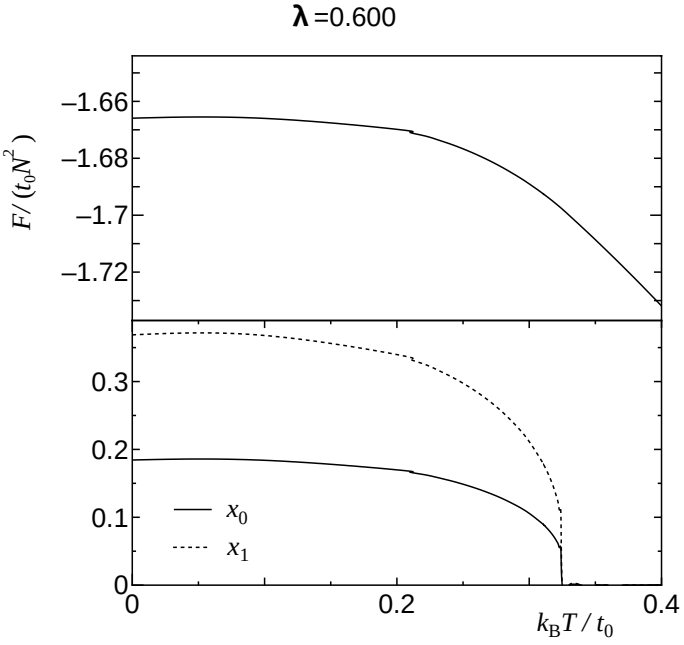

Fig. 1: The temperature dependence of the order parameters $x_0 = X_{\boldsymbol{Q}}$ and $x_1 = 2|X_{\boldsymbol{Q}/2}|$ in the case with $\lambda = 0.6$. The free energy is also plotted as a function of the temperature. The latter is a continuous function even at the critical temperature $T_{\mathrm{c}} \simeq 0.325t_0/k_{\mathrm{B}}T$. The system size is assumed to be $N \times N$ with $N = 32$.

Both order parameters are found to vanish at the same temperature ($k_{\mathrm{B}}T_{\mathrm{c}} \simeq 0.325t_0$), while the free energy of the system is continuous at that temperature. We have confirmed that the critical temperature is the same for other patterns where two or more other modes are present in addition to the $\boldsymbol{Q}$ mode and that all the order parameters vanish at the same critical temperature. Furthermore the simple Peierls phase with distortions involving only the $\boldsymbol{Q}$ mode [1] is found to have a larger free energy throughout all the temperature region, and the temperature at which the order parameter vanishes is lower than the critical temperature of the multimode Peierls phase discussed above.

References

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