Effect of charge ordering on spin Peierls state in low dimensional electron systems

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Abstract

A competition of the spin Peierls state and the charge ordering is examined using a Peierls- Hubbard model with a quarter-filled band, dimerization and the nearest-neighbor repulsive interaction (V), which is treated by the renormalization group method and the bosonization. When the charge ordering appears with increasing V, it is found that the spin Peierls state is strongly reduced indicating a crossover to spin density wave. We discuss the relevance to the spin Peierls state in organic conductors.

Key words: spin Peierls state; charge ordering; quarter-filling

1. Introduction

Spin Peierls (SP) state in which both a spin singlet state and an alternation of the lattice occur due to the coupling to phonon, has been studied extensively in spin systems. However the electron system is convenient for the study of the case where the charge gap is large but finite compared with the spin gap. In organic conductors which present the SP state[1], the carrier is quarter-filled but is regarded as effectively half-filled due to the dimerization. When the effective pressure is applied to the conductor[1,2], charge ordering appears and the SP state is reduced leading to spin density wave state. Based on the previous work at half-filling[3], such a competition is investigated by considering an electron system in the presence of the inter-site repulsive interaction, which induces the charge ordering.

2. Formulation

We consider a Peierls-Hubbard model with a quarter-filled band, dimerization (x_d) and the repulsive interactions (U and V), given by

$$H = -\sum_{j,\sigma}\{t-(-1)^j x_d - t_d\cos\frac{\pi}{2}j\}(c^\dagger_{j,\sigma}c_{j+1,\sigma}+h.c.) + U\sum_j n_{j,\uparrow}n_{j,\downarrow} + V\sum_j n_j n_{j+1} + \sum_j \frac{2}{\pi\lambda v_{\rm F}}t_d^2 \ , (1)$$

where $n_{j,\sigma}{=}c^\dagger_{j,\sigma}c_{j,\sigma}$ and $n_j{=}n_{j,\uparrow}+n_{j,\downarrow}$. The operator $c^\dagger_{j,\sigma}$ creates an electron at the site j and with spin σ. Quantities λ and $v_{\rm F}$ denote coupling to lattice and Fermi velocity, respectively. The bond alternation ,t_d, is determined so as to minimize Eq. (1), $t_d/\lambda = -(\pi v_{\rm F}/4N)\sum_{j,\sigma}\left\langle \cos(\pi j/2)(c^\dagger_{j,\sigma}c_{j+1,\sigma}+h.c.)\right\rangle$, where r.h.s. is an average of the order parameter for SP state and is calculated from the long range behavior of the correlation function of the order parameter [3] .

We take t and lattice constant as unity. The calculation is performed using the renormalization group (RG) equations based on the bosonization in a way similar to the previous calculation [3]. By changing a cutoff $\alpha(=1.9a/\pi)$ as $\alpha\to\alpha(1+dl)$, we derive the RG equations for $K_\rho = (1/(1+\tilde U + 4\tilde V))^{1/2}$, $K_\sigma = (1/(1-\tilde U))^{1/2} \simeq 1+G_\sigma$, $y_{1/4} = A^4(a/2\alpha)^2\tilde U^2(\tilde U - 4\tilde V)$, $y_{1/2} = 2(x_d/t)\tilde U/\{1+(x_d/t)^2\}$, $y_\sigma = \tilde U$, $y_d = 4\alpha t_d/v_{\rm F}$, $v_{\rm F} = \sqrt{2}ta\{1-(x_d/t)^2\}/(1+(x_d/t)^2)^{1/2}$, $\tilde U = Ua/(\pi v_{\rm F})$,

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$\tilde{V} = Va/(\pi v_{\rm F})$, where $A = (1-(x_d/t)^2)/(1+(x_d/t)^2)$. Quantities y_σ, $y_{1/2}$, $y_{1/4}$ and y_d are coefficients of the non-linear term in the scheme of bosonization where $y_{1/4}$ and $y_{1/2}$ correspond to the commensurability energy for the quarter-filling and the half-filling respectively and y_d denotes the amplitude for the SP state. RG equations are given by

$$\frac{d}{dl} y_{1/4}(l) = [\,2 - 8K_\rho(l)\,]\, y_{1/4}(l) + \frac{1}{4}\, y_{1/2}^2(l) \ ,$$

$$\frac{d}{dl} y_{1/2}(l) = [\,2 - 2K_\rho(l)\,]\, y_{1/2}(l) + \frac{1}{2}\, y_{1/4}(l)\, y_{1/2}(l) + \frac{1}{8}\, y_d^2(l) \ , \qquad (2)$$

and $dK_\rho(l)/dl = -2y_{1/4}^2(l)K_\rho^2(l) - y_{1/2}^2(l)K_\rho^2(l)/2 - y_d^2(l)K_\rho^2(l)/16$, $dG_\sigma(l)/dl = -y_\sigma^2(l) - y_d^2(l)/8$, $dy_\sigma(l)/dl = -G_\sigma(l)y_\sigma(l) - y_d^2(l)/8$, $dy_d(l)/dl = [3/2 - K_\rho(l)/2 - G_\sigma(l)/4]y_d(l) + y_{1/2}(l)y_d(l)/2 - y_\sigma(l)y_d(l)/2$.

3. Spin Peierls state vs. charge ordering

The SP state is obtained for $t_d \neq 0$. The interplay of U-term and x_d-term produces $y_{1/2}$, i.e, Umklapp scattering as 1/2-filling, which is compatible with SP state. The V-term is incompatible with SP state, since it induces the charge ordering as seen from $y_{1/4} < 0$ for large V. The RG equations for $y_{1/4}$ and $y_{1/2}$ indicates such a competition.

Solutions of RG equations as the function of l are divided into two cases. For small V (case (i)), $y_{1/2}(l)$ increases to infinity and $y_{1/4}(l)$ increases to $+\infty$ regardless the sign of $y_{1/4}(0)$. For V larger than a critical value V_c (case (ii)), $y_{1/4}(l)$ decreases to $-\infty$ and $y_{1/2}(l)$ is reduced to zero indicating a competition between $y_{1/4}(l)$ and $y_{1/2}(l)$. In the case (ii), the charge ordering appears with the gap induced by the commensurability of quarter-filling. The V dependence of t_d is shown in Fig. 1. The case $V < V_c$ leads to SP state with a small dip of t_d while t_d undergoes rapid decrease for $V > V_c$. One obtains $V_c \simeq 2.9(3.1)$ for $x_d = 0.2(0.4)$. In Fig. 2, V dependence of charge gap (Δ_ρ) and spin gap (Δ_σ) are shown. For $V < V_c$, Δ_ρ decreases slowly and takes a sharp cusp at $V = V_c$ and increases rapidly for $V > V_c$. On the other hand, Δ_σ becomes negligibly small for $V > V_c$ indicating a crossover from the SP state to the spin density wave state, which may be obtained in the limit of small λ.

Based on Figs. 1 and 2, we comment on the experiment on organic conductor DCNQI salts with a quarter-filled band [1]. The salt (DMe-DCNQI)$_2$Ag corresponding to low pressures undergoes dimerizarion at $\sim$ 100K and SP transition at $\sim$ 80 K , while the salt (DI-DCNQI)$_2$Ag corresponding to high pressures undergoes charge ordering at $\sim$ 220K and antiferromagnetic ordering at $\sim$ 5.5 K. Thus, the state at low temperatures could be explained in terms of the present model by noting that the (effective) pressure increases V.

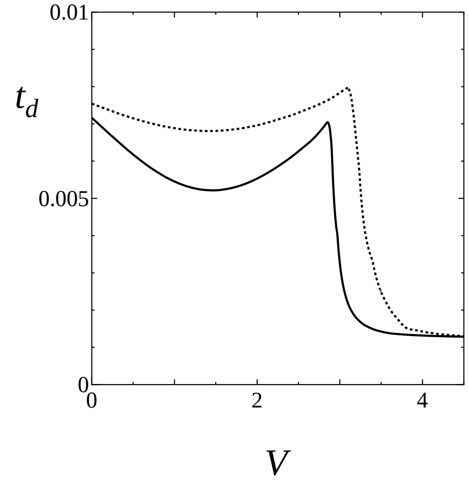

Fig. 1. The V-dependence of t_d with $U = 6$ and $\lambda = 0.2$ for $x_d = 0.1$(solid curve) and $x_d = 0.2$ (dotted curve).

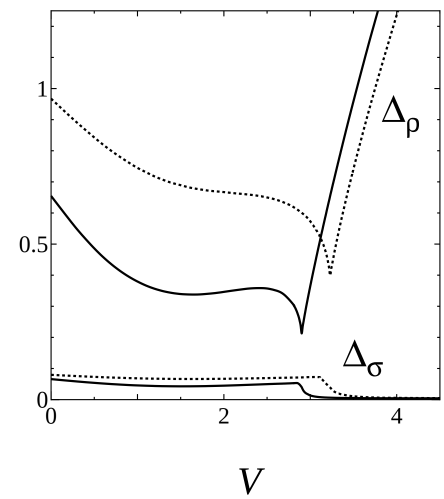

Fig. 2. The V-dependence of charge gap (Δ_ρ) and spin gap (Δ_σ) with $U = 6$ and $\lambda = 0.2$ for $x_d = 0.1$ (solid curve) and $x_d = 0.2$ (dotted curve).

References

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