Optical conductivity in commensurate spin-density-waves at quarter-filling

Yuh Tomio [1], Yoshikazu Suzumura

Department of Physics, Nagoya University, Nagoya 464-8602, Japan

Abstract

We examine the effects of the commensurability and charge ordering on the optical conductivity of spin-density-wave states using the extended Hubbard model with one-dimensional quarter-filled band. The conductivity obtained by both single particle and collective excitations is calculated within the random phase approximation. The mass enhancement due to inter-site repulsive interactions is estimated from the contribution of the collective mode.

Key words: optical conductivity; collective mode; spin-density-wave; charge ordering

1. Introduction

The collective mode describing the translational motion of the density wave is significant for the property associated with the low lying energy. A typical example is the dynamical behavior of the optical conductivity of organic conductor. [1,2].

For the incommensurate density wave, the optical conductivity exhibits the pronounced peak at zero frequency, which originates in the collective mode [3]. The optical conductivity for spin-density-wave (SDW) is determined only by the collective excitation since the effective mass associated with the dynamics of the density wave is the same as the band mass. The conductivity for charge-density-wave (CDW) is determined mainly by the single particle excitations due to a large effective mass coming from the coupling to phonon.

However, the property of the conductivity is still unclear for the commensurate SDW with a quarter-filled band and charge ordering, which has been found in the organic conductors [4]. In the present paper, we examine the conductivity and the effective mass for such a SDW state.

[1] Corresponding author. Fax: +81-52-789-2928; E-mail: tomio@edu2.phys.nagoya-u.ac.jp

2. Model and results

We consider a one-dimensional extended Hubbard model given by

$$H = -\sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} \left(t - (-1)^i t_{\rm d}\right) \left(C^\dagger_{i\sigma} C_{i+1,\sigma} + {\rm h.c.}\right) + \sum_i \left(U n_{i\uparrow} n_{i\downarrow} + V n_i n_{i+1} + V_2 n_i n_{i+2}\right) \quad , \qquad (1)$$

where $C^\dagger_{i\sigma}$ denotes a creation operator of an electron at the i-th site with spin σ. $n_i = n_{i\uparrow} + n_{i\downarrow}$ and $n_{i\sigma} = C^\dagger_{i\sigma} C_{i\sigma}$. The quantity t denotes the transfer energy and $t_{\rm d}$ corresponds to the dimerization. Quantities U, V and V_2 are the coupling constants for repulsive interactions of the on-site, the nearest-neighbor site and the next-nearest-neighbor site. We take t and the lattice constant as unity. By applying the mean-field theory to the Hamiltonian (1) at quarter-filling, the three kinds of ground states (I), (II) and (III) are obtained [5,6], i.e., (I) a pure $2k_{\rm F}$ SDW state, (II) a coexistent state of $2k_{\rm F}$ SDW and $4k_{\rm F}$ CDW for large V, and (III) a coexistent state of $2k_{\rm F}$ SDW, $2k_{\rm F}$ CDW and $4k_{\rm F}$ SDW for large V_2 where $k_{\rm F}(=\pi/4)$ the Fermi wave number.

The optical conductivity $\sigma(\omega)$ is obtained by calculating the current-current correlation function in a way

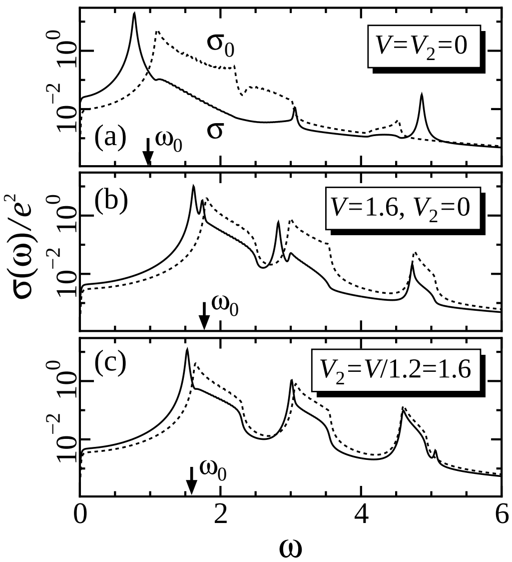

Fig. 1. The conductivity for $U = 4$, $t_\mathrm{d} = 0.1$ and $\eta = 0.02$ with the fixed (a) $V = V_2 = 0$ (state (I)), (b) $V = 1.6$ and $V_2 = 0$ (state (II)), and (c) $V_2 = V/1.2 = 1.6$ (state (III)).

similar to the incommensurate case [3], i.e., $\sigma(\omega) = \sigma_0(\omega)+\sigma_\mathrm{c}(\omega)$ with $\sigma_0(\omega) = \mathrm{Re}\{[\Pi^0_{jj}(\omega)-\Pi^0_{jj}(0)]/(\mathrm{i}\omega)\}$ and $\sigma_\mathrm{c}(\omega) = \mathrm{Re}\{\Pi^\mathrm{c}_{jj}(\omega)/(\mathrm{i}\omega)\}$ where $\Pi_{jj}(\omega) = N^{-1}\int_0^\beta \mathrm{d}\tau \, \langle T_\tau J(\tau)J(0)\rangle \, \mathrm{e}^{\mathrm{i}\omega_n\tau}|_{\mathrm{i}\omega_n\to\omega+\mathrm{i}\eta}$ and $J = \mathrm{i}e\sum_{i\sigma}(t-(-1)^i t_\mathrm{d})(C^\dagger_{i+1,\sigma}C_{i\sigma} - C^\dagger_{i\sigma}C_{i+1,\sigma})$. The conductivity σ_0 (σ_c) denotes the contribution of the single particle (collective) excitation [7].

In Fig. 1, the conductivity as a function of frequency ω is shown for $U = 4$ and $t_\mathrm{d} = 0.1$ with three choices of V and V_2. The three broad peaks of the conductivity σ_0 (dotted curve) correspond to the contribution from inter-band transitions [8], i.e., from the filled (lowest) band to upper three bands, where four bands originates in quarter-filling. We verified numerically two sum rules, $\int_0^\infty \mathrm{d}\omega \; \sigma_0(\omega) = -\pi e^2 \langle K\rangle_\mathrm{MF}/2$ and $\int_0^\infty \mathrm{d}\omega \; \sigma_\mathrm{c}(\omega) = 0$ where $\langle K\rangle_\mathrm{MF}$ is the average of the kinetic energy per site. The total conductivity σ (solid curve) exhibits three or four peaks at the frequencies corresponding to the spectrum of the collective mode where even the lowest spectrum has a gap due to the commensurability. The conductivity for $V = V_2 = 0$ (Fig. 1(a)) exhibits a main peak (i.e., first peak) around $\omega \simeq 0.85$ and the third peak with a finite weight around $\omega \simeq 4.9$. The second peak, which exists around $\omega \simeq 3.1$ in the absence of dimerization t_d [7], disappears due to $t_\mathrm{d} \neq 0$. The conductivity for large V and/or V_2 (Fig. 1(b) and (c)) is mainly determined by $\sigma_0(\omega)$. This indicates that the contribution from the collective mode is suppressed when the charge ordering appears. Such a fact is also understood by the result that the spectral weight of the collective mode decreases with increasing V or V_2 [9].

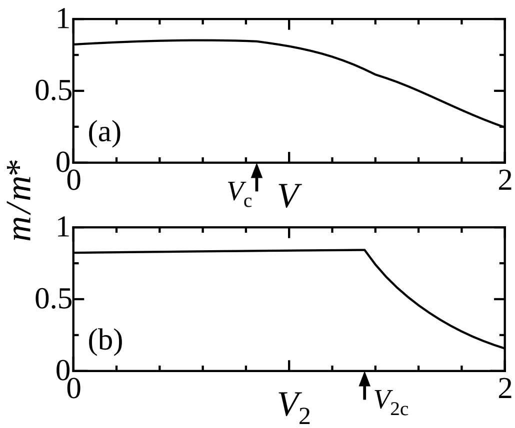

Fig. 2. (a) V dependence of m/m^* for $U = 4$, $t_\mathrm{d} = 0.1$ and $V_2 = 0$. The ground state is state (I) (state (II)) for $V < V_\mathrm{c} \simeq 0.85$ ($V > V_\mathrm{c}$). (b) V_2 dependence of m/m^* for $U = 4$, $t_\mathrm{d} = 0.1$ and $V = 1.2V_2$. The ground state is state (I) (state (III)) for $V_2 < V_{2\mathrm{c}} \simeq 1.35$ ($V_2 > V_{2\mathrm{c}}$).

Here we examine the effects of V and V_2 on the weight of the main peak of $\sigma(\omega)$. Since the finite imaginary part, η, is introduced in the present numerical calculation, we calculate the weight using a method given by $\int_0^{\omega_0} \mathrm{d}\omega \; \sigma_\mathrm{c}(\omega) \equiv \sqrt{2}\, e^2 m/m^*$ where m $(= \pi/(4\sqrt{2}))$ is the band mass and ω_0 shown by the arrow in Fig. 1 satisfies $\sigma_\mathrm{c}(\omega_0) = 0$. The quantity m^* corresponds to the effective mass for the collective mode with the first (lowest) pole. In the limit of the weak coupling, one obtains $m/m^* = 1$ showing that the conductivity is determined only by a collective mode with $\omega \to 0$. In Fig. 2, V or V_2 dependence of m/m^* is shown where $m/m^* < 1$ for $V = V_2 = 0$ due to the weight shifting to higher frequency as seen in Fig. 1(a). The rapid decrease of m/m^* is obtained when charge ordering appears for $V > V_\mathrm{c}$ and/or $V_2 > V_{2\mathrm{c}}$. For large V and V_2, the effective mass is enhanced since even the total weight of the collective modes decreases and that of higher frequency increases (Fig. 1(c)).

References

[1] D. Jérome, H. J. Schulz, Adv. Phys. **31** (1982) 299.

[2] D. Quinlivan, Y. Kim, K. Holczer, G. Grüner, Phys. Rev. Lett. **65** (1990) 1816.

[3] P. A. Lee, T. M. Rice, P. W. Anderson, Solid State Commun. **14** (1974) 703.

[4] J. P. Pouget, S. Ravy, Synth. Met. **85** (1997) 1523.

[5] N. Kobayashi, M. Ogata, K. Yonemitsu, J. Phys. Soc. Jpn. **67** (1998) 1098.

[6] Y. Tomio, Y. Suzumura, J. Phys. Soc. Jpn. **69** (2000) 796.

[7] Y. Tomio, Y. Suzumura, in preparation.

[8] H. Tajima, Solid State Commun. **113** (2000) 279.

[9] Y. Tomio, Y. Suzumura, J. Phys. Soc. Jpn. **70** (2001) 2884.