Optical conductivity of geometrical frustrated electronic systems

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Abstract. We study optical conductivity of the one-band Hubbard model on a two-dimensional isotropic triangular lattice at half filling by using the cellular dynamical mean field theory and particularly investigate its behavior near the critical end point of the first order Mott transition. In the metallic phase, the enhancement of effective mass and the significant frequency dependence of scattering rate is identified near the Mott transition. From the results in the insulating state near the Mott transition, we find that the frequency dependence of optical conductivity decays quite smoothly toward zero frequency and exhibits a power-law-like behavior in an intermediate frequency region. We also study optical conductivity of the Hubbard model on a kagomé lattice near the critical end point of the Mott transition. It shows a larger incoherent peak both in the metallic and insulating phases and a stronger frequency dependence of effective mass and scattering rate.

1. Introduction
Transport properties are one of the central topics in strong correlated electronic systems. As a typical example, the measurement of optical conductivity provides us useful information on charge dynamics, in particular, effective mass, scattering process and electric structure. As for geometrically frustrated systems, it is interesting to investigate how spin frustration influences charge dynamics. This is the issue of this paper and we study optical conductivity of geometrical frustrated electronic systems. The organic compound $\kappa$-(ET)$_2$Cu$_2$(CN)$_3$ has a structure of the two-dimensional (2D) isotropic triangular lattice of dimer pairs with a half-filled conduction band. At ambient pressure, the compound is a Mott insulator and a transition to metal has been observed under pressure [1]. In the insulating phase, the system exhibits a spin liquid behavior, which shows no magnetic long-range order [2, 3, 4]. In a recent work, interesting behaviors of optical conductivity have been observed in this insulating state, such as the smooth decay of the spectra toward zero frequency at low temperatures [5]. In contrast, the anisotropic triangular lattice organic compound $\kappa$-(ET)$_2$Cu[N(CN)$_2$]Cl exhibits an antiferromagnetic order and a clear gap in the optical conductivity [6]. Another example is the spinel compound LiV$_2$O$_4$. It exhibits heavy fermion behaviors, showing large Sommerfeld coefficient of specific heat and temperature square coefficient of resistivity. Optical conductivity shows a Drude peak at low temperatures, indicating the formation of coherent quasiparticles [7]. The spectra gradually decays towards high frequencies unlike a simple Drude formula.

In this paper, we study transport properties in strongly correlated electronic systems on the isotropic triangular lattice. We focus on optical conductivity near the critical end point of the
2. Model and Method
We consider the one-band Hubbard model on a two-dimensional isotropic triangular lattice at half filling

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i c^\dagger_{i\uparrow} c_{i\uparrow}, \]

where \( t \) is nearest-neighbor hopping amplitude, \( U \) is on-site Coulomb repulsion and \( \mu \) is chemical potential. \( c^\dagger_{i\sigma}(c_{i\sigma}) \) is an electron creation (annihilation) operator at site \( i \) with spin \( \sigma \) and \( n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} \). To take into account strong electronic correlations and geometrical frustration, we use the cellular dynamical mean field theory (CDMFT) [10], employing a triangular three-site cluster to calculate various dynamical correlation functions at finite temperatures as shown in Fig. 1. We numerically obtain the electron Green’s function by using the continuous-time Monte Carlo method based on the strong coupling expansion [11]. We first confirm the finite temperature Mott transition with varying \( U \) and then calculate optical conductivity.

Optical conductivity \( \sigma(\omega) \) is defined by the Kubo formula and is described as

\[ \sigma(\omega) = -ie^2 \lim_{q \to 0} \frac{\chi(q, \omega) - \chi(q, 0)}{\omega}, \]

where \( \chi(q, \omega) \) denotes the current-current correlation functions and \( e \) is the elementary charge. In our calculation, we do not consider vertex corrections in \( \chi(q, \omega) \) and calculate

\[ \chi(q = 0, i\omega_n) = -\frac{2T}{N} \sum_k \sum_{i\omega} v(k)^2 G(k, i\omega) G(k, i\omega + i\omega_n), \]

where \( v(k) = 2t\{\sin(k_x) + \sin(k_x/2)\cos(\sqrt{3}k_y/2)\} \) is the \( x \)-component of velocity in the case of the isotropic triangular lattice. \( G(k, i\omega_n) \) is the electron Green’s function with the Matsubara frequencies \( i\omega_n \) and wave vector \( k \), \( T \) is a temperature and \( N \) is the total number of sites. From \( \chi(0, i\omega_n) \), we calculate the real part of \( \sigma(\omega) \) by analytic continuation \( i\omega_n \to \omega + i\delta \) by using the maximum entropy algorithm [12].
3. Results

We first identify the location where the first order Mott transition takes place in the parameter space of temperature $T$ and Coulomb repulsion $U$. Figures 2 (a) and (b) present $U$-dependence of double occupancy $D = \langle n_i^+ n_i \rangle$ and density of state $A(\omega) = -(1/\pi N) \sum_k \text{Im} G(k, \omega + i0)$ at $T/t = 0.08$. At $U/t = 7.5$, $A(\omega)$ shows the formation of coherent quasiparticles around $\omega = 0$ and thus, the system is metallic. At $U/t = 10.5$, these quasiparticles disappear and there emerges a gap around $\omega = 0$ and the system is in the insulating phase. Near $U_c/t = 9.4$, $D$ jumps and the first order Mott transition takes place. Repeating calculations for various $T$, we obtain the $U$-$T$ phase diagram shown in Fig. 2 (c).

Let us start with investigation of optical conductivity $\sigma(\omega)$. We concentrate on $\sigma(\omega)$ near $T_c/t \sim 0.09$, which corresponds to the critical end point of the line of the first order Mott transition. For simple metals at low temperatures, it is well known that the frequency dependence of $\sigma(\omega)$ is described by a simple Drude formula $\sigma(\omega) = \omega_p^2/[4\pi(-i\omega + 1/\tau)]$, where $\omega_p$ is plasma frequency and $1/\tau$ is scattering rate. On the other hands, the simple Drude formula does not work in Mott insulators, since a Drude peak around $\omega = 0$ disappears and an incoherent broad peak appears near $\omega \sim U$. Figure 3 (a) shows the real part of $\sigma(\omega)$ at $T/t = 0.08$ with varying $U$. The first order Mott transition takes place at $U_c/t = 9.4$. For $U \leq U_c$, a Drude peak is identified, indicating the formation of coherent quasiparticles. As $U$ increases, the spectral weight at low frequencies is depressed at low frequencies and an incoherent peak around $\omega = 5$ evolves significantly. Moreover, $\omega$-dependence of $\sigma(\omega)$ is not described by a simple Drude formula. From these results, it is expected that these characteristics are attributed to a renormalization of the scattering rate $1/\tau(\omega)$ and the effective mass $m^*(\omega)$ due to strong electronic correlations and the effects of the frustration. In order to clarify the charge dynamics in the metallic state, we analyze the frequency dependence of $\sigma(\omega)$ by using an extended Drude formula:

$$\sigma(\omega) = \frac{\omega_p^2}{4\pi} \left( \frac{1}{m_0} + \frac{1}{\tau(\omega)} \right).$$

}\]
where $m_b$ is the unrenormalized band mass. $\omega_0^2$ is estimated from the integration of $\text{Re}[\sigma(\omega)]$. From the results of $1/\tau(\omega)$, rather unexpectedly, we find a suppression in $1/\tau(\omega)$ with increasing $U$. On the other hands, $m^*(\omega)/m_b$ exhibits an enhancement with increasing $U$. From these results, we also estimated the mean free path $l(\omega) = p_F\tau(\omega)/m^*(\omega)$, where $p_F$ is Fermi momentum. We have found that $l(\omega)$ decreases at low frequencies with increasing $U$ as expected. To discuss the low-frequency behavior, we analyze the most characteristic value, namely, the static limit $\omega = 0$, of $1/\tau(\omega)$ and $m^*(\omega)$. Near the Mott transition, it is expected that $1/\tau(0)$ or $m^*(0)$ increase with increasing $U$. Their $U$-dependence is plotted in Fig. 3 (b). While $1/\tau(0)$ shows little change with $U$, $m^*(0)$ shows a noticeable increase with increasing $U$. From these results, we find that the increase of mass is more related to the Mott transition rather than scattering rate.

For $U > U_c$, the system is insulating and, correspondingly, $\sigma(\omega)$ exhibits two features. First, as shown in Fig. 3 (a), a Drude peak disappears and $\sigma(\omega)$ shows a large incoherent peak around $\omega \sim U - 2.5t$. This value $2.5t$ is the renormalization of the energy difference between the lower and upper Hubbard bands due to charge fluctuation. This comes from the kinetic energy of a pair of doublon and holon. We numerically estimated this renormalization from the peak position of the incoherent part of $\sigma(\omega)$. Secondly, it is also interesting that the $\omega$-dependence of $\sigma(\omega)$ decays quite slowly toward $\omega = 0$. For this behavior, we have found that $\sigma(\omega)$ follows a power-law-like behavior in an intermediate frequency region near the Mott transition.

Finally, we also investigate $\sigma(\omega)$ of another frustrated system, the Hubbard model on a kagomé lattice, and compare $\sigma(\omega)$ of the two models near the critical end point of the first order Mott transition. To make fair comparison between the two models, we normalized $\omega$ by the effective bandwidth $W$ of the dimension of energy. We use $W = \langle (\omega - \langle \omega \rangle)^2 \rangle^{1/2}$ calculated from density of state $A(\omega)$. For the isotropic triangular lattice, the critical end point is near $T/t = 0.08$ ($U_c/t \sim 9.4$) and $W/t = 7.6034$ at $U/t = 9.4$, $W/t = 5.6249$ at $U/t = 9.5$. For the kagomé lattice, the critical end point is near $T/t = 0.07$ ($U_c/t \sim 8$) and $W/t = 7.6438$ at $U/t = 8$, $W/t = 5.9929$ at $U/t = 8.1$. As for $\sigma(\omega)$, the Kubo formula shows that it has the
Figure 4. Real part of optical conductivity $\sigma(\omega)$ in the metallic phase (a) and in the insulating phase (b) near the Mott transition for the isotropic triangular lattice ($U_c/t \sim 9.4$ at $T/t = 0.08$) and kagomé lattice ($U_c/t \sim 8$ at $T/t = 0.07$). $W$ is the effective band width $W = \langle (\omega - \langle \omega \rangle)^2 \rangle^{1/2}$ calculated from density of state $A(\omega)$.

dimension zero in our units, and therefore we do not need to renormalize $\sigma(\omega)$ for comparison. Figure 4 shows $\sigma(\omega)$ as a function of dimensionless frequency $\omega/W$ near the critical end point of the first order Mott transition of the two models. As shown in Figs. 4 (a) and (b), an incoherent peak of $\sigma(\omega)$ emerges clearly both in the metallic and insulating phases. From the results of an extend Drude analysis in the metallic phase, we find that $1/\tau(\omega)$ and $m^*(\omega)$ in the kagomé case show the larger $\omega$-dependence than in the isotropic triangular one corresponding to sharper incoherent peak. In the insulating phase, we find similar power-law-like behaviors of $\sigma(\omega)$ of the kagomé lattice in an intermediate frequency region. The detailed analysis of $\sigma(\omega)$ is in progress and will be published elsewhere.

4. Summary
In this paper, we have studied optical conductivity of the one-band Hubbard model on a two-dimensional isotropic triangular lattice at half filling by using the cellular dynamical mean field theory. We calculate optical conductivity near the critical end point of the first order Mott transition. In the metallic phase, an extend Drude analysis indicates the enhancement of the mass and the significant frequency dependence of the scattering rate with increasing Coulomb repulsion. In the insulating phase near the Mott transition, we have found that the frequency dependence of optical conductivity decays quite smoothly toward zero frequency and exhibits a power-law-like behavior in an intermediate frequency region. Optical conductivity of the Hubbard model on a kagomé lattice near the critical end point of the Mott transition also shows similar behaviors. We have also found the larger incoherent peak both in the metallic and insulating phases and stronger frequency dependence of effective mass and scattering rate.

In future publication, we will take into account vertex corrections in current-current correlation function and discuss their effects as well as detailed analysis of these frustrated lattice systems.

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