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# Effect of frustration on optical conductivity in a two-dimensional triangular Hubbard model near half filling

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**Abstract**

We examine the regular part of optical conductivity in the strong-coupling limit of a hole-doped two-dimensional triangular Hubbard model near half filling. A numerically exact diagonalization method based on the Lanczos technique is employed for a 21-site triangular lattice. The regular part is calculated by averaging over various twisted boundary conditions to reduce finite-size effects. We find that the spectra show strong incoherent excitations extended to a higher energy region irrespective of the sign of the hopping amplitude. This is in contrast to the case of a square lattice without frustration. The results imply that geometrical frustration in strongly correlated electron systems influences incoherent charge dynamics.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

The interplay of geometrical frustration and strong electron correlation is one of the hot topics in the field of strongly correlated electron systems. The simplest example of such geometry is a triangular lattice in two dimensions (2D) [1]. In the triangular lattice, a three-sublattice coplanar-type antiferromagnetic (AF) order [2–4] at half filling under strong on-site Coulomb interaction is expected to be easily destroyed by carrier doping. In fact, it has been suggested that for the positive sign of hopping amplitude ($t > 0$) a resonant valance-bond state is favoured with hole doping [5] and $d + id$-wave superconductivity appears [6]. It was also suggested that three-sublattice magnetism is stable for a wide range of doping [7]. On the other hand, for $t < 0$ Nagaoka ferromagnetism emerges with doping [5–8]. These results indicate that geometrical frustration and strong correlation give rise to strong competition among many states.

The variety of the ground states in the triangular lattice may induce unconventional charge dynamics through coupling with frustrated magnetism. However, there are few theoretical studies about charge dynamics away from half filling, except for the Fermion-spin theory of

the $t$–$J$ model [9, 10]. Therefore, it is very important to investigate the effect of frustration on charge dynamics and to clarify the interplay of the charge and spin degrees of freedom in geometrically frustrated systems.

In this paper we perform an exact diagonalization study of the doping dependences of the optical conductivity for a 21-site triangular Hubbard cluster with large on-site Coulomb interaction. We introduce an averaging procedure over various twisted boundary conditions (BC) to reduce finite-size effects. We find that the regular part of the optical conductivity shows very strong incoherent excitations extended to a high-energy region of several times $t$. Such high-energy incoherent excitations are not seen in the square lattice. This implies that geometrical frustration causes unconventional charge dynamics.

The rest of this paper is organized as follows. We introduce an effective Hamiltonian of the Hubbard model in the strong-coupling limit, and show outlines of the procedure for choosing boundary conditions in the triangular lattice in section 2. Section 3 presents the doping dependence of the regular part of the optical conductivity. Comparison with that for the square lattice will be made. A summary is given in section 4.

## 2. Model and method

The Hubbard model with nearest-neighbour hopping $t$ and on-site Coulomb interaction $U$ is given by

$$H_{\rm Hub} = -t \sum_{\langle i,j\rangle,\sigma} \left( c^{\dagger}_{i,\sigma} c_{j,\sigma} + {\rm H.c.} \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \tag{1}$$

where $c_{i,\sigma}$ annihilates an electron with spin $\sigma$ at site $i$, and $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$, and the summation $\langle i, j\rangle$ runs over nearest-neighbour pairs. Being interested in the region of $U \gg t$, we take the strong-coupling limit of equation (1). The resulting Hamiltonian reads

$$H_{\rm SC} = H_{tJ} + H_{\rm 3S} \tag{2}$$

with

$$H_{tJ} = -t \sum_{\langle i,j\rangle,\sigma} \left( \tilde{c}^{\dagger}_{i,\sigma} \tilde{c}_{j,\sigma} + {\rm H.c.} \right) + J \sum_{\langle i,j\rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} \tilde{n}_i \tilde{n}_j \right), \tag{3}$$

and

$$H_{\rm 3S} = -\frac{J}{4} \sum_{\langle i,j,k\rangle,\sigma,\sigma'} \left(1 - n_{i,-\sigma}\right) c^{\dagger}_{i,\sigma} c_{j,\sigma} n_{j,-\sigma} \times n_{j,-\sigma'} c^{\dagger}_{j,\sigma'} c_{k,\sigma'} \left(1 - n_{k,-\sigma'}\right), \tag{4}$$

where $J = 4t^2/U$, $\tilde{c}_{i,\sigma} = c_{i,\sigma}(1 - n_{i,-\sigma})$, $\tilde{n}_i = \sum_{\sigma} \tilde{c}^{\dagger}_{i,\sigma} \tilde{c}_{i,\sigma}$, and $\langle i, j, k\rangle$ denotes a pair of three nearest-neighbour sites. We use $U/t = 20$, which is above a critical $U/t$ [11, 12] for the metal–insulator transition at half filling.

The exact diagonalization method based on the Lanczos algorithm is frequently applied to Hubbard-type models as an unbiased numerical method. In this study, we take a 21-site triangular lattice with the translation vectors $\mathbf{R}_a = 4\mathbf{u} + \mathbf{v}$ and $\mathbf{R}_b = -\mathbf{u} + 5\mathbf{v}$, where $\mathbf{u}$ and $\mathbf{v}$ are the vectors connecting nearest-neighbour sites given by $\mathbf{u} = \mathbf{x}$ and $\mathbf{v} = \frac{1}{2}\mathbf{x} + \frac{\sqrt{3}}{2}\mathbf{y}$ with the unit vector $\mathbf{x}$ ($\mathbf{y}$) in the $x$ ($y$) direction. The shape of the cluster and momenta defined under periodic BC are shown in figure 1.

In such a small cluster, we are not free from finite-size effects. In order to reduce the finite-size effects, we introduce various BC with a twist and average physical quantities over the twisted BC. This procedure has been applied for various quantities in $t$–$J$-type models [13–15]. The twist induces the condition that $c_{i+R_a,\sigma} = {\rm e}^{{\rm i}\phi_a} c_{i,\sigma}$ and $c_{i+R_b,\sigma} = {\rm e}^{{\rm i}\phi_b} c_{i,\sigma}$ with arbitrary

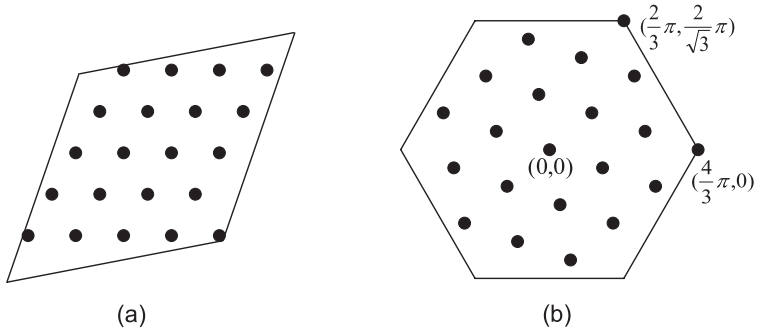


**Figure 1.** (a) The 21-site triangular lattice studied in this work. The filled circles denote lattice sites and the lines represent the translation vectors. (b) The first Brillouin zone of the triangular lattice. The filled circles denote momenta defined in the 21-site lattice with periodic boundary conditions. The distance between the nearest-neighbour sites is set to be unity.

phases $\phi_a$ and $\phi_b$. $\phi_{a(b)}$ is defined as $\phi_{a(b)} = \boldsymbol{\kappa} \cdot \mathbf{R}_{a(b)}$ with $\boldsymbol{\kappa} = \kappa_x \mathbf{x} + \kappa_y \mathbf{y}$. $\boldsymbol{\kappa}$ is taken within an area surrounded by four corners at $(\kappa_x, \kappa_y) = \pm\frac{\pi}{21}(4, \frac{6}{\sqrt{3}})$ and $\pm\frac{\pi}{21}(6, -4\sqrt{3})$. For the averaging procedure, we choose many $\boldsymbol{\kappa}$ with equal intervals of $\pi/40$ in the area for one-to four-hole cases. The total number of $\boldsymbol{\kappa}$ results in $N_\kappa = 353$. For a five-hole case, we take a smaller number $N_\kappa = 177$ because of time-consuming computations. This averaging procedure has been used for a triangular lattice for calculating the magnetic correlation function and the chemical potential as well as the optical conductivity [16].

The real part of the optical conductivity reads $\sigma(\omega) = 2\pi D\delta(\omega) + \sigma_{\rm reg}(\omega)$, where $D$ is the Drude weight and $\sigma_{\rm reg}(\omega)$ represents the regular part with finite $\omega$. Under the averaging procedure, $\sigma_{\rm reg}(\omega)$ is given by

$$\sigma_{\rm reg}(\omega) = \frac{1}{N_\kappa} \sum_{\boldsymbol{\kappa}} \frac{1}{N\omega} \,{\rm Im}\, \langle \Psi_0^{\boldsymbol{\kappa}} | \, j_x^{\boldsymbol{\kappa}} \frac{1}{\omega + E_0^{\boldsymbol{\kappa}} - H_{\rm SC} - {\rm i}\gamma} j_x^{\boldsymbol{\kappa}} \, | \Psi_0^{\boldsymbol{\kappa}} \rangle, \tag{5}$$

where $|\Psi_0^{\boldsymbol{\kappa}}\rangle$ represents the ground state with energy $E_0^{\boldsymbol{\kappa}}$ for a given $\boldsymbol{\kappa}$ and $H_{\rm SC}$ is the same as in equation (2) but under the twisted BC. The $x$ component of the current operator is given by $j_x = {\rm i}[H_{\rm SC}, \hat{x}]$, where $\hat{x}$ is the $x$ component of the total position operator. A standard continued-fraction expansion method based on the Lanczos algorithm is used to calculate the correlation function in equation (5) with the broadening factor $\gamma = 0.05|t|$.

## 3. Results and discussions

Figure 2 shows the doping dependence of $\sigma_{\rm reg}(\omega)$ for the 21-site triangular lattice with $t > 0$ and $t < 0$. We find that incoherent excitations are widely extended to a high-energy region up to several times $t$, irrespective of the sign of $t$. This is completely different from the Hubbard model in one dimension, where spin and charge are completely decoupled and incoherent weights are negligibly small [17]. Also such incoherent excitations are different from those of the square lattice. For comparison, $\sigma_{\rm reg}(\omega)$ in a 20-site square lattice is shown in figure 3. In the calculation, we take $N_\kappa = 320$ [14, 15]. The origin of the incoherent part in the square lattice is well understood based on the picture that magnetic polarons move in the system by inducing magnetic excitations scaled by the exchange interaction $J = 4t^2/U \sim 0.2t$. Therefore, the incoherent spectral weight shown in figure 3 is mainly located below $\omega \sim t$. Very incoherent $\sigma(\omega)$ up to several $t$ in the triangular lattices clearly indicates that such a magnetic-polaron picture cannot be applied.

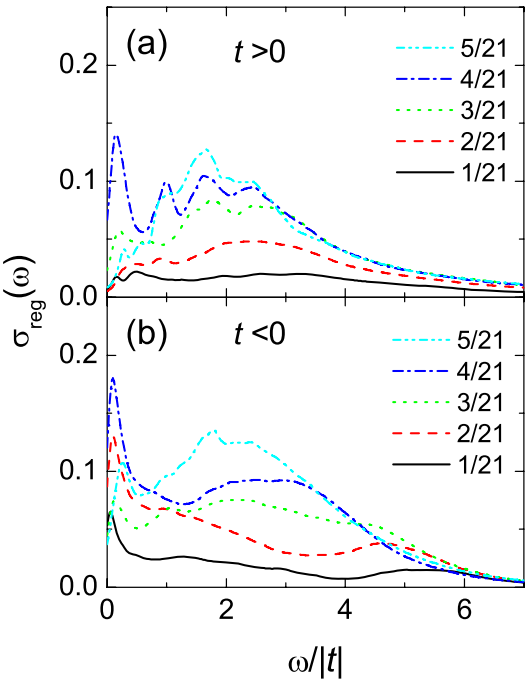


**Figure 2.** Regular part of the optical conductivity $\sigma_{\rm reg}(\omega)$ for various hole concentrations of the strong-coupling limit of the Hubbard model with $U/t = 20$. (a) $t > 0$ and (b) $t < 0$ for a 21-site triangular lattice. The numbers in the panels represent the hole concentration.

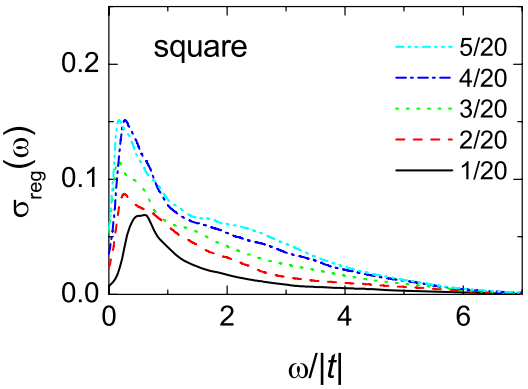


**Figure 3.** Regular part of the optical conductivity $\sigma_{\rm reg}(\omega)$ for various hole concentrations of the strong-coupling limit of a 20-site square Hubbard lattice with $U/t = 20$. The numbers in the panels represent the hole concentration.

An interesting feature of $\sigma(\omega)$ for both the $t > 0$ and $t < 0$ triangular lattices is that the incoherent spectral weight increases with increasing $\delta$ without changing its global energy distribution in the region of $t \lesssim \omega \lesssim 5t$. Furthermore, the spectral weight of the incoherent part is larger than that of the square lattice. This means that the motion of carriers is more incoherent than the square lattice. Enhanced incoherent structures have also been discussed in terms of the single-hole spectral function in triangular antiferromagnets [18] as well as in

kagome antiferromagnets [19]. Both quantities may have common origins. A possible origin is nontrivial phases from the spin degrees of freedom [20] with strong frustration. The phases may act as random fields on carriers and induce incoherent excitations. Obtaining analytical expressions for theses effects is a problem for the future. We note that such an enhanced incoherency might be a possible origin of the anomalous incoherent contribution of $\sigma(\omega)$ observed in a triangular compound $Na_{0.7}CoO_2$ [21].

## 4. Summary

In summary, we have performed an exact diagonalization study of the doping dependence of the regular part of the optical conductivity for a triangular Hubbard model. We find that the optical conductivity shows very strong incoherent excitations, which are absent in the square lattice. This implies that geometrical frustration influences the incoherent charge dynamics. Since the optical conductivity sees only the momentum-conserved charge excitation, it should be interesting to investigate momentum-dependent charge dynamics. This study is now in progress.

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