Dynamic Exponent of $t$-$J$ and $t$-$J$-$W$ Model

Hirokazu Tsunetsugu and Masatoshi Imada

Institute of Applied Physics, University of Tsukuba, Tsukuba 305-8573
1 Institute for Solid State Physics, University of Tokyo, Tokyo 106-8666

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Drude weight of optical conductivity is calculated at zero temperature by exact diagonalization for the two-dimensional $t$-$J$ model with the two-particle term, $W$. For the ordinary $t$-$J$ model with $W=0$, the scaling of the Drude weight $D \propto \delta^z$ for small doping concentration $\delta$ is obtained, which indicates anomalous dynamic exponent $z=4$ of the Mott transition. When $W$ is switched on, the dynamic exponent recovers its conventional value $z=2$. This corresponds to an incoherent-to-coherent transition associated with the switching of the two-particle transfer.

KEYWORDS: strongly correlated electrons, optical conductivity, Drude weight, Mott transition

High-$T_c$ superconductors (HTSC) are a typical example of strongly correlated electron systems, and show many unusual physical properties which challenge the picture of the standard Fermi liquid theory. In particular, transport properties are among the most peculiar ones. Electric resistivity exhibits a linear temperature dependence $\rho(T) \sim T$ near the optimal doping, and the frequency dependence of optical conductivity is long-tailed, $\sigma(\omega) \sim \omega^{-1}$. These are not compatible with the standard Fermi liquid theory, which predicts $\rho(T) \sim T^2$ and $\sigma(\omega) \sim \omega^{-2}$, and indicate that electric transport in HTSC is anomalously incoherent. Similar incoherent transport properties have also been observed in many other strongly correlated systems including a number of transition-metal oxides and organic conductors and therefore it may be natural to ascribe the incoherent character to strong correlation effects.

Concerning the mechanism of high-$T_c$ superconductivity, many experiments indicate that the strong electron-electron correlation may play an essential role, and various theoretical approaches have been proposed with emphasizing different aspects of the correlation effects. As discussed above, incoherent motion of electrons is a notable ingredient of the strong correlation effects, and one possible scenario is that the incoherence in the normal phase may drive the superconductivity so that the system can acquire an additional energy due to coherent motion which is recovered in the superconducting phase.

This idea has recently been explored in terms of the quantum criticality of the Mott transition, where singularity of two quantities has been numerically investigated. One is the doping dependence of compressibility $\kappa$ and the other is the localization length of the single-electron Green’s function, $\xi$, with varying chemical potential in the insulator phase. Both results support the scaling hypothesis of the Mott transition with dynamic exponent $z=4$, larger than the conventional value $z=2$. If this is the case, carrier transport is expected to be largely incoherent. However, this has not been examined directly. It is imperative, for the direct experimental relevance of the above idea, to clarify the incoherence of transport properties. Moreover the singular behavior of compressibility could allow an alternative interpretation, the spin density wave (SDW) or equivalently the nested Fermi surface.

In this paper, we investigate coherence of electronic transport in strongly correlated electron systems by numerical calculations for the $t$-$J$ model. First, we calculate the doping dependence of the Drude weight at zero temperature. The result shows the failure of the SDW picture and supports the scaling theory. We also determine the dynamic exponent $z$ to quantify how coherence is suppressed on approaching the Mott transition. It turns out that the spatial dimensionality is crucial and the two-dimensional (2D) $t$-$J$ model is much more incoherent than the 1D case. Secondly, we explore whether the incoherent nature in the 2D system could be changed to evolve coherence by including additional electron-electron interactions. Recently, Assaad et al. found an insulator-superconductor transition in the 2D half-filled $t$-$U$-$W$ model, i.e., the Hubbard model with additional two-electron processes. Supplementing the $t$-$J$ model with a similar term, we calculate the Drude weight and determine $z$ to see if coherence changes.

The Hamiltonian to investigate is the 2D $t$-$J$ model and its variant generalized by including the square of local kinetic energy. For later convenience, we include an Aharonov-Bohm (AB) flux, $\phi$, and then the Hamiltonian using standard notation is given as

$$\mathcal{H} = \mathcal{H}_{tJ} + \mathcal{H}_W,$$

$$\mathcal{H}_{tJ} = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P} (\chi_{i,j} \sigma c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) \mathcal{P} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

$$\mathcal{H}_W = -W \sum_j \mathcal{P} \left( \sum_{\delta, \sigma} (\chi_{j,\delta} + \sigma c_{j,\sigma}^\dagger c_{j,\delta \sigma} + \text{H.c.}) \right)^2 \mathcal{P}. \quad (3)$$

Here $\mathcal{P}$ is the Gutzwiller projection operator excluding double occupancy at every site, and the sum $\sum_{\delta}$ should be taken over nearest-neighbor sites. The phase factor

$$\chi_{i,j} = t_1 e^{i\phi} (c_{i\sigma}^\dagger - U c_{i\sigma}^\dagger),$$

$$t_1 = -W \sum_{\delta, \sigma} (\chi_{j,\delta} + \sigma c_{j,\sigma}^\dagger c_{j,\delta \sigma} + \text{H.c.})$$

is the single-electron Green’s function with varying local chemical potential $\mu$.
For the latter step, we have used the Lanczos method and then employed the first relation in eq. (8). The energy along the first obtained the ground state of \( H \) or if long-range electron hoppings are introduced. It is noted that if \( \sigma = 0 \), \( D_{\mu} = D \), and \( \langle -F_{\mu\nu}\rangle = \langle -F \rangle \delta_{\mu\nu} \).

First we show the results for the 4\times4-site t-J model (i.e., \( W = 0 \)) at various \( J/t \)’s. The Drude weight \( D \) and the total weight \( \langle -F \rangle \) are plotted as a function of electron density \( n_e \equiv N_e/V \) in Fig. 1(a). The total weight \( \langle -F \rangle \) has a maximum at \( n_e \approx 0.5 \), and it is nearly symmetric around it. In contrast, the Drude weight is considerably reduced from \( \langle -F \rangle \) in the region of \( n_e > 0.5 \). Similar calculations were performed for a 2D t-J model by Dagotto et al.\(^{10}\) to study the dependence on hole doping \( \delta = 1 - n_e \), and they concluded \( D \sim \delta \) as \( \delta \to 0 \).

We have reexamined the doping dependence and found a different scaling. To this end, it is convenient to calculate first the \( \delta \)-dependence of the ratio of \( D \) to \( \langle -F \rangle \) and then transform the result to that of \( D \). Fig. 1(b) shows \( D/\langle -F \rangle \) calculated from the data in Fig. 1(a), as a function of electron density. It is clear that this ratio becomes smaller with decreasing hole doping, indicating \( D/\langle -F \rangle \sim \delta \) as \( \delta \to 0 \). The kinetic energy \( \langle -F \rangle \) contains not only the coherent part of electron motion but also the incoherent part. Therefore it is natural that \( \langle -F \rangle \sim \delta \), and the data shown in Fig. 1(a) confirms this scaling. Combining these \( \delta \)-dependencies, we obtain \( D \sim \delta^2 \).

The result for the 1D t-J model is very different from the 2D case.\(^{11}\) We plot in Fig. 2 the electron-density dependence of \( D \) and \( \langle -F \rangle \) for various system sizes at \( J/t = 0.3 \). Difference between the two weights, i.e. the integrated weight of \( \sigma_{\mu\nu}^{reg}(\omega) \), is nearly zero at this scale. Therefore, not only \( \langle -F \rangle \sim \delta \), but also \( D \sim \delta \) as \( \delta \to 0 \) in the 1D case. This result is consistent with the Luttinger liquid theory.\(^{12}\) It predicts \( D = 2w_vK_c \), where \( w_v \) is the charge velocity and asymptotically \( w_v \sim \delta \). \( K_c \) is the Tomonaga-Luttinger liquid parameter, and \( K_c \approx 2/3 \) in the strong correlation limit, leading to \( D \sim \delta \).

The different \( \delta \)-dependence of \( D \) between 1D and 2D cases results in different values of the dynamic exponent \( z \). The dynamic exponent \( z \) is defined by the divergence of correlation time \( \tau \) and correlation length \( \xi \) on approaching the critical point \( \xi \sim \xi^z \). Scaling theory for the Mott transition by Imada\(^{5}\) predicts \( D \sim \delta^{1+z(2-z)/d} \), where \( d \) is the spatial dimension. As shown above, \( D \sim \delta^2 \) and \( \delta^1 \) for 2D and 1D t-J model, respectively, and this implies \( z = 4 \) for the 2D and \( z = 2 \) for the 1D cases. The dynamic exponent is a measure for characterizing the coherence of the system: the larger it is, the faster the coherent part of conductivity vanishes at the Mott transition, indicating that the system is more incoherent. Thus, coherence is very sensitive to the spatial dimensionality of the system, and the 2D t-J model is more incoherent than the 1D model.

The present result for \( z \) is consistent with other numerical studies, if one is based on the scaling theory. One is the compressibility of the 2D Hubbard model,\(^{13}\) where \( \kappa \sim \delta^{-1} \) near half filling. A similar behavior was again. The result agrees well with the value calculated via the second relation in eq. (8), and the relative error is typically as small as \( 10^{-6} \). The lattice used in this work is a 4\times4-site cluster with periodic boundary conditions in both directions, \( \phi=(0,0) \) and the total wave number \( \mathbf{K} = (0,0) \), unless explicitly mentioned. Due to the symmetry of the cluster, the conductivity is isotropic: \( \sigma_{\mu\nu} = \sigma, D_{\mu} = D, \) and \( \langle -F_{\mu\nu} \rangle = \langle -F \rangle \delta_{\mu\nu} \).

is given by \( \chi_{\mu,j} \equiv \exp[-i\phi \cdot (r_i - r_j)/a\phi_0] \), where \( \phi_0 \) is flux quantum divided by \( 2\pi \), \( a \) is the lattice constant, and we shall set \( a = 1, \hbar = 1 \), and the velocity of light \( c = 1 \) throughout this paper. It should be noted that \( \phi \) is constant, corresponding to a pure gauge, and therefore the magnetic field is zero everywhere.

One may derive the main part of the \( W \)-term by expanding the square of the Hubbard Hamiltonian, and then \( W \propto t^2/U \) with \( U \) being the on-site Coulomb repulsion. It is also useful to rewrite the \( W \)-term by expanding the square in eq. (3) taking account of the projection operators. The result is

\[
\mathcal{H}_W = W \sum_{j,\sigma\sigma'} \mathcal{P}(2c_j^\dagger c_{j\sigma'} - \delta_{\sigma\sigma'})
\]

\[
\times [\chi_{j+\delta\delta'} c_{j+\delta\sigma'} + \chi_{j+\delta\delta'} c_{j+\delta\sigma}] \mathcal{P}
\]

\[
+ 8W \sum_{(i,j)} (S_i \cdot S_j + \frac{1}{4}n_in_j) - 2\zeta N_e W,
\]

where \( \zeta \) is the number of nearest-neighbor sites \( (\zeta = 4 \) for a square lattice) and \( N_e \) is the number of electrons. We note that as shown in eq. (4), the \( W \)-term contains so-called three-site terms\(^{14}\) and also renormalizes the value of \( J \) in \( H_{ij} \).

Optical conductivity at \( T=0 \) may be defined via the Kubo formula as

\[
\sigma_{\mu\nu}(\omega) = \frac{i\epsilon^2}{V} \omega 
\]

\[
\sum_{\alpha \neq 0} \langle \alpha | J^\mu_\alpha(0) | \alpha \rangle^2 \left\{ \frac{2(E_\alpha - E_0)}{(E_\alpha - E_0)^2 - (\omega + i\eta)^2} \right\}.
\]

where \( -\epsilon \) is the electron charge, \( \mu \) denotes the spatial index, \( V \) is the number of sites, and \( \eta \) is an adiabatic constant. \( |\alpha\rangle \)’s are eigenstates of the Hamiltonian with eigenenergy \( E_\alpha \), where \( |0\rangle \) denotes the ground state, and

\[
J^\mu_\alpha = \frac{1}{\epsilon} \frac{\partial \mathcal{H}}{\partial \phi_\mu}, \quad F^\mu_{\mu\nu} = -\frac{1}{\epsilon} \frac{\partial^2 \mathcal{H}}{\partial \phi_\mu \partial \phi_\nu}.
\]

We may separate the Drude part from the formula (5) and the remaining is the regular part:

\[
\sigma_{\mu\nu}(\omega) = \frac{i\epsilon^2}{V} D\delta(\omega) + \sigma_{\mu\nu}^{reg}(\omega).
\]

The Drude weight is simply given by

\[
D_{\mu} = \langle -F_{\mu\nu} \rangle - 2 \sum_{\alpha \neq 0} \langle \alpha | J^\mu_\alpha(0) | \alpha \rangle^2 
\]

\[
\frac{1}{E_\alpha - E_0} = \frac{1}{\epsilon^2} \frac{\partial^2 E_\alpha(\phi)}{\partial \phi_\mu^2}.
\]

In addition to the Drude weight, another important quantity is the total weight of the optical conductivity. It is straightforward to rewrite the Kubo formula (5) and obtain the following sum rule\(^{15}\)

\[
\int_{-\infty}^{\infty} \sigma_{\mu\nu}(\omega) d\omega = \frac{\pi \epsilon^2}{V} (\langle -F_{\mu\nu} \rangle).
\]

It is noted that if \( W = 0 \), \( \langle F_{\mu\nu} \rangle \) reduces to the kinetic energy along the \( \mu \)-direction, while it does not if \( W \neq 0 \) or if long-range electron hoppings are introduced.

To calculate the Drude weight numerically, we have first obtained the ground state of \( \mathcal{H} \) by the Lanczos method, and then employed the first relation in eq. (8). For the latter step, we have used the Lanczos method again. The result agrees well with the value calculated via the second relation in eq. (8), and the relative error is typically as small as \( 10^{-6} \). The lattice used in this work is a 4\times4-site cluster with periodic boundary conditions in both directions, \( \phi=(0,0) \) and the total wave number \( \mathbf{K} = (0,0) \), unless explicitly mentioned. Due to the symmetry of the cluster, the conductivity is isotropic: \( \sigma_{\mu\nu} = \sigma, D_{\mu} = D, \) and \( \langle -F_{\mu\nu} \rangle = \langle -F \rangle \delta_{\mu\nu} \).
also found for the 2D $t$-$J$ model by Kohno.\cite{8} According to the scaling theory, these results indicate $z=4$ and agree with the present study. Another support is the chemical-potential dependence of the localization length $\xi_d$. It is found that $\xi_d \sim |\mu - \mu_c|^{-\nu}$ for $\nu=\frac{3}{2}$, and combining with the relation $\xi_z\sim1$, this also gives $z=4$. An alternative explanation for the $\delta$-dependence of $\kappa$ may be given by the SDW picture, which gives the energy $E(\delta) \sim \Delta \delta + A \delta^3$ in the 2D case, with $\Delta$ being the momentum-independent quasiparticle gap. This implies $\kappa = [(1-\delta^2)E'(\delta)]^{-1} \sim \delta^{-1}$, consistent with the numerical results. In the SDW picture, however, the kinetic energy is carried by coherent quasiparticles, and therefore both the Drude weight and total weight should have a $\delta^z$-term, which is not the case as shown in Fig. 1.

Next, we study the stability of the incoherent phase with $z=4$ found for the 2D $t$-$J$ model and study what kind of extra processes could drive the evolution of the coherence. A similar idea has been explored by Assaad et al.\cite{11} for the 2D Hubbard model at zero temperature, where $H_W$ of eq. (4) without the projection operator $P$ was introduced.

We show the result for the 2D $t$-$J$-$W$ model in Fig. 3(a). The electron-density dependence of the Drude weight and total weight is plotted for $J/t=0.3$ and various values of $W$. For $N_e=14$ and 12, the ground state is obtained for the AB flux $\phi=\pi$, and this point will be discussed later. With increasing $W$, the Drude weight and the total weight both increase. This is because the W-term introduces additional processes of transfer involving eight second-neighbor sites, which yields a gain of the corresponding energy described in eq. (4).

An important effect of the W-term is that it affects the ratio $D/(-F)$ noticeably as shown in Fig. 3(b). In particular, the ratio increases drastically near half-filling, and seemingly converges to a finite value as $\delta \to 0$. This is in contrast to the case for $W=0$, where the ratio vanishes linearly with $\delta$. If this is the case, it means that the scaling of the Drude weight is now $D \sim \delta^z$ as in the 1D $t$-$J$ model, distinct from $D \sim \delta^2$ at $W=0$. Therefore, the dynamic exponent is correspondingly modified to $z=2$, the conventional value as in uncorrelated electron systems, and we can infer that the system is stabilized by gaining an energy of coherent motion driven by the W-term. A similar change in $z$ has also been observed for the 2D $t$-$U$-$W$ model\cite{12} where the exponent for the single-electron localization length changes from $\nu=\frac{3}{2}$ to $\frac{1}{2}$.

It is interesting that the Drude weight calculated at $\phi=(0,0)$ is negative at $N_e=14$ for $W/t \geq 0.3$. This means that a finite AB flux is induced spontaneously. To see this in more detail, we have calculated the $\phi$-dependence of the lowest eigenenergy for all the sixteen wave vectors $K$. For the system size of 4x4 sites, the system with $\phi=\pi$, $\phi=\pi$ (p,q: integer and, $\phi$ is in units of $\phi_0$) has the same energy spectrum as that with $\phi=0$. Thereafter it is sufficient to vary $\phi$ in a triangular region defined by the three points, $(0,0)$, $(\frac{\pi}{2}, \frac{\pi}{2})$, and $(\frac{\pi}{2}, -\frac{\pi}{2})$. We have kept track of the lowest eigenenergy for all the $K$'s along the edges of the triangular $\phi$-region, and the result is shown in Fig. 4. The eigenstates have the lowest energy at $\phi=(\frac{\pi}{4}, \frac{\pi}{4})$ and $K=(-\frac{\pi}{4}, -\frac{\pi}{4})$, when $W/t \geq 0.05$. A finite AB flux is also found for $N_e=12$ when $W/t \geq 0.1$, and the value is again $\phi=(\frac{\pi}{4}, \frac{\pi}{4})$, but now at $K=(\pi, \pi)$. This spontaneous AB flux may be an evidence of enhancement of $d_{x^2-y^2}$-wave superconducting correlation due to the $W$-term. Actually, such a superconducting phase has been observed in the $t$-$U$-$W$ model\cite{8, 11}. Recall that the finite flux shifts one-particle momentum as $k \rightarrow k-\phi$, and no electrons then have the renormalized momentum $k'=(\pm \frac{\pi}{2}, \pm \frac{\pi}{2})$. Therefore all electrons on the tight-binding “Fermi surface” can utilize a pairing potential with $d_{x^2-y^2}$ symmetry. This also suggests the importance of strong momentum dependence of charge excitations, and that incoherence around $(\pm \pi,0)$ and $(0, \pm \pi)$ rather than $(\pm \frac{\pi}{2}, \pm \frac{\pi}{2})$ is responsible for the retrieval of the coherence and the pairing. We will discuss this point in more detail elsewhere.

In this paper, we have numerically studied coherence character in transport properties of strongly correlated electron systems. We have calculated the doping dependence of the Drude and total weights of optical conductivity for the 2D and 1D $t$-$J$ model at zero temperature. The result shows different scalings near half filling, $D \sim \delta^2$ and $\delta^z$ for the 2D and 1D case, respectively. The dynamic exponent of the Mott transition as $\delta \to 0$ is determined as $z=4$ for the 2D case while $z=2$ for the 1D case. Incoherent transport properties in the 2D system may be attributed to this anomalous dynamic exponent. We have also examined the effects of the extra electron-electron interaction, $H_W$, in two dimensions. It turns out that the dynamic exponent changes to $z=2$ and coherence is retrieved.

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Fig. 1. (a) Drude and total weights of the optical conductivity of the 2D $t$-$J$ model with $4 \times 4$ sites at $T=0$. (b) The ratio of the two weights $D/(\langle F \rangle)$.

Fig. 2. Drude and total weights of the optical conductivity of the 1D $t$-$J$ model at $T=0$ for $J/t=0.3$.

Fig. 3. (a) Drude and total weights of the optical conductivity of the 2D $t$-$J$-$W$ model with $4 \times 4$ sites at $T=0$ for $J/t=0.3$. $D$: open symbols, and $(\langle F \rangle)$: solid symbols. For $n_e=\frac{14}{16}$ and $\frac{12}{16}$, the ground state is calculated at $\phi=(\frac{\pi}{4}, \frac{\pi}{4})$. (b) The ratio of the two weights $D/(\langle F \rangle)$. (c) The $W$-dependence of the ratio $D/(\langle F \rangle)$ for $n_e=\frac{14}{16}$ at $J/t=0.3$.

Fig. 4. The AB-flux dependence of the lowest eigenenergy for all wave vectors for the 2D $t$-$J$-$W$ model, 14 electrons in $4 \times 4$ sites, and $J/t=0.3$, $W/t=1.0$. 
\[ <F>, D \text{ (per site)} \]

(a)  

(b)
\[ <F>, D \text{ (per site)} \]

\[ \text{D (10 sites)} \]
\[ \text{D (9 sites)} \]
\[ \text{D (8 sites)} \]
\[ \langle -F \rangle, D \text{ (per site)} \]

(a) (b)

(a) \[ W/t = 0.5 \quad 0.3 \quad 0.1 \quad 0.05 \quad 0.0 \]

(b) \[ W/t = 0.5 \quad \triangle W/t = 0.3 \quad \square W/t = 0.1 \quad \bigcirc W/t = 0.05 \quad \times W/t = 0.0 \]
$\phi = (\phi_x, \phi_y)$

$E/t$ vs. $\phi = (\phi_x, \phi_y)$

Axes:
- $E/t$ from $-156$ to $-144$
- $\phi = (\phi_x, \phi_y)$ from $(\pi/4, \pi/4)$ to $(\pi/4, \pi/4)$