Photo-induced metallic states in a Mott insulator are studied for the half-filled, one-dimensional Hubbard model with the time-dependent density matrix renormalization group. An irradiation of strong AC fields is found to create, in the nonequilibrium steady state, a linear dispersion in the optical spectrum (current-current correlation) reminiscent of the Tomonaga-Luttinger liquid for the doped Mott insulator in equilibrium. The spin spectrum in nonequilibrium retains the de Cloizeaux-Pearson mode with the spin velocity differing from the charge velocity. The mechanism of the photocarrier-doping, along with the renormalization in the charge velocity, is analyzed in terms of an effective Dirac model.

PACS numbers: 71.10.Fd, 71.30.+h, 72.20.Ht, 72.40.+w

Introduction — Doped one-dimensional (1d) Mott insulators are fascinating due to a special metallic state known as the Tomonaga-Luttinger (TL) liquid, where excitations have collective nature as distinct from the conventional Fermi liquid. Specifically, the charge velocity becomes renormalized due to the electron-electron interaction, so that the charge excitation propagates with a velocity different from that of spin excitations—a hallmark of the “spin-charge separation”. Experimentally, TL liquids have been observed in quantum wires and carbon nanotubes.

Now, there is another way of making a Mott insulator metallic, which is entirely different from the chemical doping. Namely, photo-doping is now being highlighted as a way to control the carrier density in 1d correlated systems. Pump-probe experiments have shown that strong electric fields can turn Mott insulating crystals into metals. Theoretically, TL liquids have been observed in quantum wires and carbon nanotubes.

Nonequilibrium steady state — We consider a Mott insulator in strong AC electric fields in the half-filled, 1d Hubbard model with the Hamiltonian given, in standard notation, by $H(t) = H_0 + H_F(t)$, where $H_0 = -t_{\text{hop}} \sum_{i, \sigma} (c_{i+1, \sigma}^\dagger c_{i, \sigma} + \text{h.c.}) + U \sum_i n_{i, \uparrow} n_{i, \downarrow}$, and $H_F(t) = F(t) \sin(\Omega t) \sum_i n_i (n_{i, \uparrow} = c_{i, \uparrow}^\dagger c_{i, \uparrow}, n_i = n_{i, \uparrow} + n_{i, \downarrow})$. Here $F$ and $\Omega$ are, respectively, the strength and frequency of the external electric field, which is switched on at $t = 0$ (hence the insertion of a step function). In the calculation we take the length of the system $L = 80$, a time step $\Delta t = 0.04$, and the DMRG Hilbert space size of $m = 140$, in natural units. After obtaining the groundstate $|\Psi_0\rangle$ of $H(t < 0)$ with the finite-system DMRG algorithm, we let the system evolve according to the time-dependent Hamiltonian $H(t)$ with the td-DMRG[12] to obtain the wave function $|\Psi(t)\rangle = U(t; 0)|\Psi_0\rangle$, with the time-evolution operator $U(t; t') = e^{-i \int_0^t H(s) ds}$ (T: the time-ordering).

For $t > 0$, the system relaxes into a nonequilibrium steady state, where we can define the photo-doping rate as $x_{\text{ph}}(t) = \frac{1}{T} \sum_{m} \langle \Psi(t)| n_{i, \uparrow} n_{i, \downarrow} |\Psi(t)\rangle - \langle \Psi_0| n_{i, \uparrow} n_{i, \downarrow} |\Psi_0\rangle$ which is the increment in the double occupancy. We also monitor the total energy, $E_{\text{avg}}(t) = \text{avg}(\Psi(t)| H(t) |\Psi(t)\rangle$.

In these expressions, we eliminate the $T_{\text{period}} = 2\pi/\Omega$ oscillation by taking the average over each period, as denoted by “$\text{avg}$”. The time profiles of the photo-doping rate and the total energy in Fig(1) are similar, which
indicates that the energy absorbed from the AC field is used to excite electron-hole pairs, i.e., photo-doping. The system relaxes to a steady state until the situation where pair production rate = annihilation (stimulated emission) rate is achieved.

The doping rate depends both on the frequency $\Omega$ and the strength $F$ of the electric field. When $\Omega$ is greater than the Mott gap $\Delta$, excitations occur via one-photon absorptions. Even when $\Omega < \Delta$, multi-photon processes can excite the system above the gap for sufficiently strong fields, where the process becomes resonant when $m\Omega = \Delta$ with $m$ being an integer. The extreme case is the DC limit $\Omega \to 0$, where many-body Landau-Zener tunneling across the Mott gap induces metallization [13, 14, 17].

**Correlation functions** — To characterize the 1d many-body system we calculate the correlation functions after a steady state is attained,

$$\chi_{AB}(t, T_1; i, j) = \langle \Psi(t)|A_i U(t, T_1) B_j |\Psi(T_1)\rangle,$$

where $A, B$ are operators, e.g., the current $J_i = -i t_{\text{hop}} \sum_\sigma (c_i^{\sigma\dagger} c_{i+1}^{\sigma} - \text{h.c.})$, or the spin $s_i = \frac{1}{2} \sum_{\alpha \beta} \sigma_{\alpha\beta} c_i^{\alpha\dagger} c_{i\beta}$, and $T_1$ is the time around which the steady state is reached (and the curves in Fig. 1 flatten; typically $T_1 = 50$, 100 depending on the field strength). Physically, $\chi_{JJ}$ represents the probing process in standard pump-probe experiments, where a photon in the probe light generates a local electron-hole pair at position $j$. To focus on the interplay between the charge and spin degrees of freedom, we can compare in Fig. 2 the current correlation function with the behaviors of spin and charge. For the spin we define the local spin energy, $\varepsilon_i^{\text{spin}}(t) = \langle \Psi(t)| s_i |\Psi(t)\rangle$, which measures the exchange energy (normalized by the exchange coupling $J_{\text{exch}} = 4t_{\text{hop}}^2 / U$). For the charge we examine the double occupancy defined by $n_i^d(t) = \langle \Psi(t)| n_i n_i |\Psi(t)\rangle$. Here $|\Psi(t)\rangle = U(t, T_1) J_j |\Psi(T_1)\rangle$ is the state where a perturbation ($J_j$) is added at site $j$ on the steady, nonequilibrium state. The behavior of the three quantities shows that the temporal evolution after the probe-excitation on $j$ at $t = T_1$ propagates in two processes. The first is diffusion of the doublon-hole pair, which is followed by the relaxation process. The relaxation is seen as a decay of the current correlation, which is seen to be accompanied by a disturbance in the spin structure (as marked with a red broken line in the figure). This indicates that the spin and charge degrees of freedom become coupled more strongly, where spins act as a kind of energy reservoir for charges. Spin-charge coupling already exists in equilibrium for higher-energy states [21] which is natural since charge excitations act as boundary conditions to spins with spin vanishing at doubly occupied or empty sites. The decay of the current correlation, already present for zero AC electric field ($F = 0$), becomes faster in finite fields, which implies that the spin-charge coupling becomes stronger, due to higher-energy states become involved. However, in the field range studied here, the coupling is not strong enough to destroy the spin-charge separation picture [10], i.e., the spin and charge degrees of freedoms still have independent dispersions, as discussed below.

**Collective excitations in nonequilibrium** — So what is the nature of the photo-induced carriers? We can obtain the excitation spectrum as the Fourier transform of the
following the equilibrium case, the optical spectrum for the front reaches the sample boundary. We call the quantity, where 

\[ \chi \]

is a zero-gap, linear dispersion, finding here, is that, while we have an optical gap (= \( U/t \)) for zero field (left), and for a finite field \( F = 0.4 \) (right) with \( U/t_{\text{hop}} = 8.0 \), \( \Omega/t_{\text{hop}} = 8.0 \). (b) Color-coded spin spectrum \( \chi_{ss}(q, \omega) \) in the half-filled Hubbard model with \( U/t_{\text{hop}} = 8.0 \) for zero AC field (left), or for a finite AC field \( F/t_{\text{hop}} = 0.4 \) (right). The white dashed lines are the des Cloizeaux-Pearson mode. (c) The AF peak \( \chi_{ss}(q, \omega) = 0 \) vs \( q \) are also displayed for various field strengths.

by Luther, Emery, and by Giamarchi to study linear-responses in the presence of a charge gap. In this approach we start from the 1+1 dimensional massive Thirring model. The charge degrees of freedom is represented by two spinless fermions \( \Psi = (\psi_1(x), \psi_2(x)) \), where \( \psi_1, \psi_2 \) represent left mover and right mover, respectively, and the Hamiltonian reads

\[ H_{\text{MT}}(t) = v_c \int dx \left[ \Psi^\dagger(x)(-i\nabla_x(t))\sigma_3 + \frac{\Delta}{2}\sigma_1 \right] \psi(x) + H_I(3) \]

where \( \sigma_i \) are Pauli matrices, \( v_c \) the renormalized charge velocity, and \( \Delta \) the Umklapp-scattering coupling constant, an descendant of the original Mott gap at half filling. This model is dual to the sine-Gordon model, where the size of the interaction term \( H_I = g \int dx [\Psi^\dagger(t)\Psi^2 - (\Psi^\dagger(t)\Psi)^2] \) translates to the sine-Gordon coupling through a duality relation. However, in the following we make a further simplification, namely, we neglect the self-interaction \( H_I \). This by no means implies a neglect of the original electron-electron interaction, but amounts to neglect self-energy corrections to quasi-particle life time, etc. We employ this approximation to focus on the effect of the charge gap, which primarily appears from the first term in eqn. 3.

The AC electric field is taken as the coupling, \( \nabla_x(t) = \partial_x + iA_1(t) \), in the above, with \( A_1(t) = (F/\Omega)\sin \Omega t \). We then obtain the nonlinear, nonequilibrium evolution of the state in this model. After a Fourier transform, the equation of motion becomes

\[ i\hbar \frac{d}{dt} \Psi_k(t)) = [v_c(k + (F/\Omega)\sin \Omega t)\sigma_3 + \frac{\Delta}{2}\sigma_1] \Psi_k(t)) \]

Here we adopt the Floquet method for treating systems in AC fields (see e.g., 28), i.e., we seek a solution of the form

\[ u_\alpha(k; t) = \sum_m e^{-i\epsilon_m(k)t - im\Omega t} \rho_\alpha^m(k) \]

where \( m \) is the
In this model is \[29\] the Floquet quasi-energy \(\varepsilon_\alpha(q)\), where the red lines represent occupied states, green lines unoccupied states. (c) A schematic level repulsion.

The optical spectrum, Fig.5(a), shows that a metallic, linear-dispersion mode emerges in the gap in the presence of an AC field. The result does resemble the present model result for the doped 1d Mott insulator. The origin of the gapless excitation in nonequilibrium can be traced back, in the present massive Thirring + Floquet analysis, to the quasi-energy level scheme in Fig. 3(b). In the absence of AC fields, the Dirac model has two branches with the lower band completely filled. As we turn on the AC field, we have a series of replicas (i.e., Floquet modes equally spaced by \(\Omega\) for each of the electron and hole branches. Physically, these modes correspond to \(m\)-photon absorbed states. As in standard quantum mechanics, level repulsion takes place when two modes cross with each other with nonzero matrix element between them. In our model, the most important feature is the level repulsion between an occupied Floquet mode (red in Fig.3(b)) and an unoccupied one (green). As shown in the blowup (Fig.3(c)), gapless excitations then emerge across the occupied and unoccupied states, which should contribute to the optical spectrum when we evaluate eqn.(4). Specifically, the linear dispersion of the photo-induced state is \(u_\omega \sim v_\sigma|q|\), where the renormalized velocity \(v_\sigma\), a parameter independent of the spin velocity, is conceived to have a value that depends on the detail of the irradiation.

Another interesting point is when the photon energy \(\Omega\) is below the gap \(\Delta\). In this situation, multi-photon processes with \(m \geq 2\) are necessary to excite the system. We can indeed show that, when the condition \(\Omega \sim \Delta/m\) is met, the excitation becomes resonant and carriers are injected efficiently, which will be described elsewhere.

In conclusion, we have shown that a Mott insulator irritated by strong AC electric fields has a collective mode which is reminiscent of the Tomonaga-Luttinger liquid in equilibrium. While spins and charges are coupled in the relaxation process, the collective modes have different spin and charge velocities. Emergence of the linear collective mode is also supported by an effective Dirac model. We have greatly benefited from discussions with Naoto Tsuji on the Floquet method. TO acknowledges Keiji Saito and Keiichiro Nasu for valuable discussions. This work has been supported in part by a Grant-in-Aid for Scientific Research on a Priority Area “Anomalous quantum materials” from the Japanese Ministry of Education.

[1] M. Imada et al., Rev. Mod. Phys. 70, 1039 (1998).
[2] See, e.g., H. J. Schulz in Correlated electron systems, ed. by V. J. Emery, World Scientific (1992).
[3] H. Ishii et al., Nature 423, 540 (2003).
[4] G. Yu et al., Phys. Rev. Lett. 67, 2581 (1991).
[5] S. Iwai et al., Phys. Rev. Lett. 91, 057401 (2003).
[6] H. Okamoto et al., Phys. Rev. Lett. 98, 037401 (2007).
[7] A. Takahashi et al., Phys. Rev. Lett. 89, 206402 (2002).
[8] H. Matsueda et al., Phys. Rev. B 70, 033102 (2004).
[9] N. Maeshima and K. Yonemitsu, J. Phys. Soc. Jpn. 74, 671 (2005).
[10] A. Takahashi, H. Itoh, and M. Aihara, Phys. Rev. B 77, 205105 (2008).
[11] N. Nagaosa and T. Ogawa, Solid State Comm. 88, 295 (1993).
[12] M. A. Cazalilla and J. B. Marston, Phys. Rev. Lett. 88, 256403 (2002), S. R. White and A. E. Feiguin, Phys. Rev. Lett. 93, 076401 (2004), A. J. Daley, et al., J. Stat. Mech.: Theor. Exp. (2004)P04005.
[13] T. Oka and H. Aoki, Phys. Rev. Lett. 95, 137601 (2005).
[14] T. Oka and H. Aoki, in Quantum and Semi-classical Percolation & Breakdown, (Lecture Notes in Physics,
Springer-Verlag), to appear (arXiv0803.0422).
[15] J. Schwinger, Phys. Rev. 82, 664 (1951).
[16] Y. Kluger et al., Phys. Rev. Lett. 67, 2427 (1991); Phys. Rev. D 45, 4659 (1992).
[17] T. Oka et al., Phys. Rev. Lett. 91, 66406 (2003).
[18] S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
[19] T. Oka, and H. Aoki, in preparation.
[20] For the Heisenberg model $\varepsilon_{\text{spin}}(t) \simeq -0.443$, as shown by H. A. Bethe, Z. Physik 71, 205 (1931); L. Hulthén, Ark. Mat. Astron. Fys. A 26, 1 (1938).
[21] The way in which spin and charge are coupled in the excited states of 1d Hubbard model has been analysed in, e.g., K. Kusakabe and H. Aoki, Phys. Rev. B 44, 7863 (1991).
[22] F. Woynarovich, J. Phys. C 16, 5293 (1983).
[23] M. Mori and H. Fukuyama, J. Phys. Soc. Jpn. 65, 3604 (1996).
[24] A. Luther and V. J. Emery, Phys. Rev. Lett. 33, 589 (1974).
[25] V. J. Emery, Phys. Rev. Lett. 65, 1076 (1990).
[26] T. Giamarchi, Phys. Rev. B 44, 2905 (1991).
[27] S. R. Coleman, Ann. Phys. 101, 239 (1976).
[28] P. Hänggi in Quantum Transport and Dissipation ed. by T. Dittrich et al. (WILEY-VCH, 1988).
[29] T. Oka and H. Aoki, arXiv:0807.3767.