Photo-induced metallic liquid in a one-dimensional Mott insulator in AC fields

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Abstract.
    We theoretically study the properties of the photo-carriers created in a one-dimensional Mott insulator subject to strong AC electric fields. The time-dependent density matrix renormalization group method is used to calculate the nonlinear optical conductivity, for which a metallic, gapless mode is found to emerge. The mode has linear dispersion with a charge velocity that differs from the free electron velocity, which indicates that the photo-doped carriers behave collectively as in the Tomonaga-Luttinger liquid.

1. Introduction

The collective nature of carriers introduced, or doped, into one-dimensional (1D) Mott insulators[1] is fascinating as a dramatic many-body effect. The special metallic state in doped Mott insulators has been analyzed as the Tomonaga-Luttinger (TL) liquid which has features distinct from the conventional Fermi liquid (see e.g., [2]). In the TL liquid the charge velocity becomes renormalized due to the electron-electron interaction, so that the charge excitation propagates with a velocity different from that of the spin excitation, which is the well-known "spin-charge separation" taking place in 1D many-body systems.

    Experimental realization of TL liquids, however, is not so easy. This is because we have to find appropriate donors or acceptors for chemical doping for 1D materials. Now, there is an entirely different way of doping the system — photo-doping, which is now being highlighted as a way to control the carrier density in 1D correlated systems [3, 4, 5, 6, 7]. Pump-probe experiments have shown that strong electric fields may turn Mott insulating crystals metallic [3, 4, 5]. Conceptually distinct from the chemical doping, photo-doping puts the system out of equilibrium, where two types of carriers, holes and electrons (=doubly occupied sites), coexist because they are pair-produced. Since the TL liquid has been proposed as an equilibrium effective theory for a single carrier species, we *a priori* do not know how the photo-induced metallic state should behave. This has motivated us to perform a detailed numerical study of the photo-induced metallic state in 1D Mott insulators in strong AC electric fields with the time-dependent density matrix renormalization group (td-DMRG) [8]. In this article, we give further examples of the non-equilibrium optical spectrum.

2. Non-equilibrium steady state

Here, we study the effect of strong AC electric fields on a Mott insulator with the 1D Hubbard model in external electric fields. The Hamiltonian is given by

$$H(t) = H_0 + H_{\mathrm{F}}(t), \tag{1}$$

$$H_0 = -t_{\mathrm{hop}} \sum_{i\sigma} \left(c_{i+1\sigma}^{\dagger} c_{i\sigma} + \mathrm{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

$$H_{\mathrm{F}}(t) = F\theta(t)\sin(\Omega t)\sum_i i n_i, \tag{3}$$

where t_{hop} is the hopping integral (which is taken to be the unit of energy hereafter), U the on-site repulsion, $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, $n_i = n_{i\uparrow} + n_{i\downarrow}$ and F denotes the strength and Ω the frequency of the electric field. We concentrate here on the half-filled case where the groundstate is a Mott insulator.

The procedure of the calculation is as follows:

step 1. We obtain the groundstate $|\Psi_0\rangle$ of $H(t < 0)$ with the finite-system DMRG algorithm [9].

step 2. Next, we let the system evolve according to the time-dependent Hamiltonian $H(t)$ for a finite electric field. We denote the wave function $|\Psi(t)\rangle = U(t;0)|\Psi_0\rangle$, with the time-evolution operator $U(t;t') = \hat{T}e^{-i\int_{t'}^{t} H(s)ds}$ ($\hat{T}$: the time-ordering). The time-evolution is calculated with td-DMRG[10, 11, 12] until $t = T_1$ at which a non-equilibrium steady state is reached. The typical value of T_1 is $50 - 100$ depending on the strength of the field.

step 3. We then calculate the current-current correlation function χ_{JJ} that 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. So the correlation function reads

$$\chi_{JJ}(t, T_1; i, j) = \langle \Psi(t)|J_i U(t, T_1) J_j|\Psi(T_1)\rangle, \tag{4}$$

with $J_i = -it_{\mathrm{hop}} \sum_{\sigma}(c_{i+1\sigma}^{\dagger} c_{i\sigma} - \mathrm{h.c.})$.

step 4. We can finally make a Fourier transform,

$$\mathrm{Im}\chi_{JJ}(q, \omega) = \tag{5}$$
$$\mathrm{Im} \int_{T_1}^{T_1+T_2} dt \sum_j e^{i\omega(t-T_1)-iq(j-j_c)} \mathrm{Im}\chi_{JJ}(t, T_1; j, j_c),$$

to obtain the optical spectrum. The time used to perform the transformation is $T_2 = 15$.

3. Results

If we look at the result for the spectrum $\mathrm{Im}\chi_{JJ}(q, \omega)$ in Fig. 1, an excitation gap $\Delta/t_{\mathrm{hop}} \sim 4.7$ for the Mott insulator is seen in (a) for zero electric field. In finite electric fields in (b,c), we find an emergence of metallic states with a linear dispersion (V-shaped structures) starting from $q = 0$, $\omega = 0$. The charge velocity – the slope of the dispersion – is different from the free-electron velocity, which indicates that a renormalization due to interaction makes the photo-carriers behave collectively as in the Tomonaga-Luttinger liquid [8]. An interesting feature is that the dispersion has double branches. The effect of interaction between the electron and hole modes may be the origin of the splitting, and further study should be done.

Fig. 1 (b) depicts the result for a photon energy exceeding the Mott gap, while (c) the result for a photon energy smaller than the gap. In the latter, the spectrum acquires another feature,
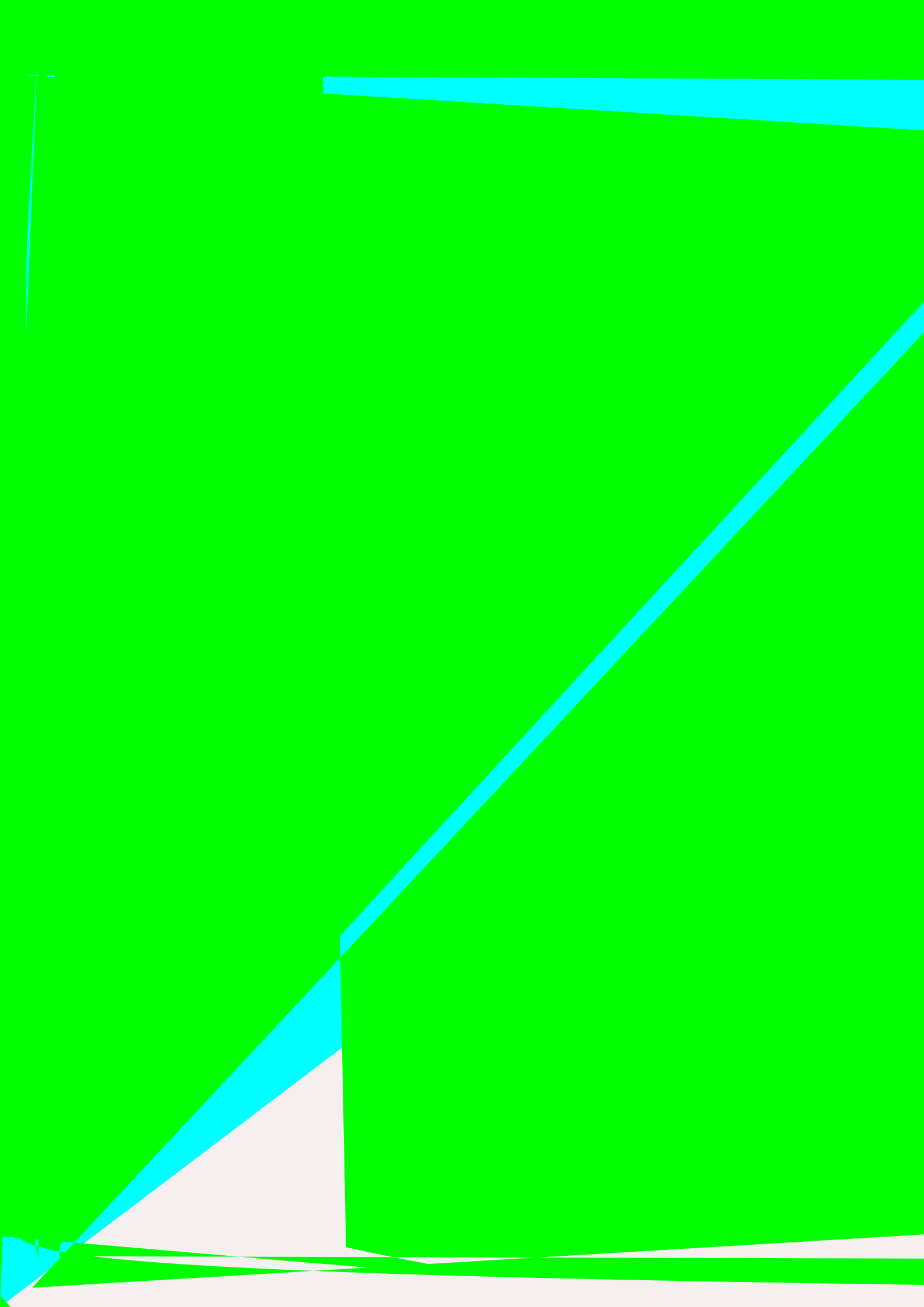
4. Conclusion

We have studied the optical spectrum of the metallic state photo-induced by continuous AC fields in one dimensional Mott insulators. The metallic state has a linear dispersion reminiscent of the Tomonaga-Luttinger liquid, with the charge velocity renormalized by interaction. We also found that the original Mott gap becomes larger in finite fields, as distinct from the case of band insulators.

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