An Effective Model for the One-Dimensional Extended Hubbard Model Applicable to Linear Optical Spectrum Calculations in Large Systems: A New Approach Based on Many-Body Wannier Functions

We have developed a charge model as an effective model of the one-dimensional extended Hubbard model based on the spin-charge separation. The charge model includes the effect of charge fluctuations and is applicable to the photoexcitation of one-dimensional Mott insulators. It is numerically shown that the charge model reproduces the optical conductivity spectra calculated by the original model quantitatively. In order to calculate a larger system to compare with experimental results, we also developed a method of many-body Wannier functions (MBWFs). We succeeded in obtaining the optical conductivity spectrum for a large enough system by using the MBWFs constructed from the photoexcited states of the charge model.

Materials that have strong electron-electron interaction energy are called strongly correlated systems. These systems show various fascinating properties such as high-temperature superconductivity and have attracted many researchers in condensed matter physics for a long time.

Recent progress in laser technology has made it possible to observe ultrafast electronic response in strongly correlated systems, and it is now expected to be possible to control their optical properties on an ultrafast timescale (10^{-15} ~ 10^{-12} sec). To this end, a theoretical understanding of the experimental results is indispensable.

It is widely accepted that low-energy phenomena in strongly correlated systems can be described well by the extended Hubbard model. Two parameters are specified for the target system in this model: U/T and V/T, where U is the on-site Coulomb interaction energy, V is the nearest-neighbor site Coulomb interaction energy, and T is the transfer energy between nearest-neighbor sites. When U/T is greater than about 5, many-body effects play essential roles. Generally, the number of basis states to describe a many-body wave function increases exponentially with respect to the system size N. Thus, even in one-dimensional systems, it is difficult to solve the model for large enough system sizes (N ~ 100) that can compare with experimental results due to the computational cost. The density matrix renormalization group (DMRG) is the only method of obtaining quantitative results for large one-dimensional systems. However, the DMRG method cannot provide wave functions directly, which prevents us from understanding photoexcitation processes. It is still a challenging problem to understand the photoexcited states of strongly correlated systems even in one-dimensional systems.

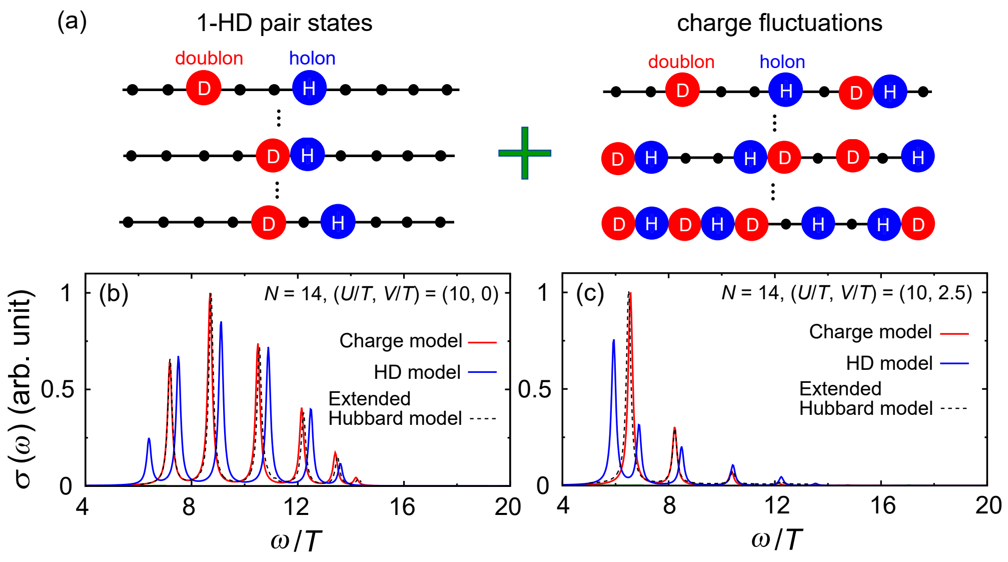

Figure 1: (a) Schematics of charge fluctuations in the charge model. Comparison of the optical conductivity spectra σ(ω) of the extended Hubbard model, the charge model and the HD model for (b) (U/T, V/T) = (10, 0) and (c) (U/T, V/T) = (10, 2.5). The system size N = 14. Reprinted figures with permission from [2] Copyright (2019) by the American Physical Society.

Photoexcitation in a Mott insulator generates pairs of a holon (H; +) and a doublon (D; –) as charge carriers.

As is well known, the separation of spin and charge degrees of freedom (spin-charge separation) holds well in a one-dimensional Mott insulator [1, 2]. For a large U/T limit, the holon-doublon (HD) model [3] based on the spin-charge separation is proposed. In this model, a spin degree of freedom is not considered and only the 1-HD pair states are considered. However, for the realistic U/T region, *charge fluctuations*, which arise from multi-HD pair states and are not included in the HD model at all, become important.

In this study, we developed an effective model of the one-dimensional extended Hubbard model, named the *charge model* [4]. The spin-charge separation holds and the charge fluctuations are fully included in the charge model as schematically shown in Fig. 1(a).

In Fig. 1, optical conductivity spectra calculated by the extended Hubbard model, the charge model and the holon-doublon model for N = 14, for which the numerically exact solutions are available, are compared. We chose the parameters for typical strongly correlated systems: (b) (U/T, V/T) = (10, 0) and (c) (U/T, V/T) = (10, 2.5). The charge model quantitatively reproduces the extended Hubbard model, while the holon-doublon model does not. This result shows that the charge fluctuations play an essential role in this case.

Although the charge model can greatly reduce the number of basis states, the maximum size is limited to 40, which is not enough to compare with experimental results.

We have developed a method to construct localized many-body basis states, *many-body Wannier functions* (MBWFs), for further extension of the size [4]. Unlike the commonly used one-body Wannier functions, MBWFs include the correlation effects. Many-body Wannier functions can be constructed by unitary transformation of the photoexcited states of a small system calculated from the charge model. Once MBWFs are obtained, we can easily extend the system size by extrapolating the Hamiltonian matrix elements because of the localized nature of MBWFs.

In Fig. 2, a numerical demonstration of the method of MBWFs is shown. We first calculated the dominant excited states of the charge model for (U/T, V/T) = (10, 0) and N =16 and constructed the MBWF by unitary transformation of these states. Quantitative agreement of the charge model and the method of MBWFs is confirmed for N = 40; see Fig. 2(a). We successfully obtained the converged optical conductivity spectra with respect to the system size as seen in Fig. 2(b).

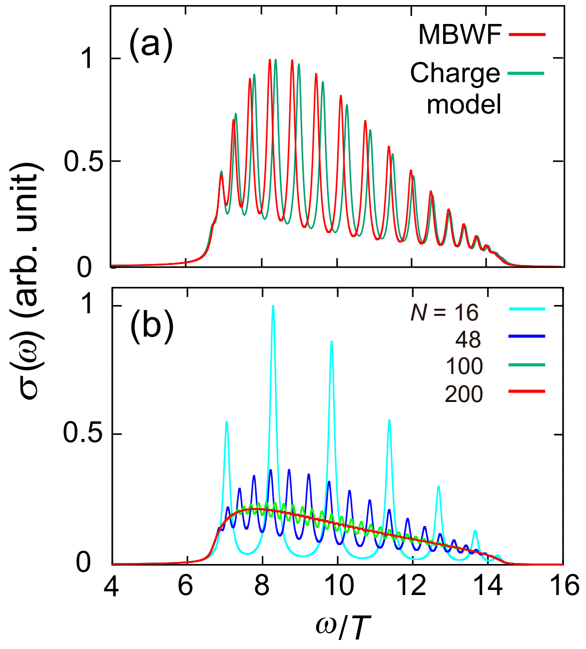

Figure 2: (a) Comparison of the conductivity spectra σ(ω) calculated by using the many-body Wannier functions (MBWFs) and the charge model. (b) Size dependence of σ(ω) calculated by using the MBWFs. Reprinted figures with permission from [2] Copyright (2019) by the American Physical Society.

In summary, we have developed the charge model as an effective model of the extended Hubbard model and found that both the spin-charge separation and the charge fluctuations play essential roles in the realistic U/T region. We also constructed many-body Wannier functions based on the charge model and succeeded in obtaining the optical conductivity spectrum for a large enough system to compare with experimentally observed spectra. We expect that our new model and method will help clarify the photoexcitation processes in strongly correlated systems.

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