Multi-fermion excited states in a two-dimensional spinless fermion model

K. Iwano[1] and H. Matsufuru[2]

[1] *Institute of Materials Structure Science, High Energy Research Organization (KEK), Tsukuba, Ibaragi 305-0801, Japan*

[2] *Computing Research Center, High Energy Research Organization (KEK), Tsukuba, Ibaragi 305-0801, Japan*

In the solid-state physics, new phenomena named "photoinduced phase transitions (PIPTs)" are now attracting much attention. While usual phase transitions are caused by the change of the static external parameters such as temperature, pressure, and so on, the PIPTs are triggered by light. We emphasize that the PIPTs are closely related to the collective nature of optically excited states. A rough picture of this remark is that only a single photon "moves" more than one electrons, being against an ordinary common sense that one photons excites only one electron. We expect that such a multi-excited cluster of electrons will play the role of a seed leading to a global phase change. Apart from the phase transition, the collective natures of the electrons are somewhat similar to those among nucleons. We believe that numerical developments in the treatment of the excited states will give benefit to both the fields.

Returning to the study of the PIPTs, the above-mentioned picture has already been confirmed for a certain types of one-dimensional systems [1]. Meanwhile, it is not known yet whether the picture is valid in two-dimensional systems, although an experiment strongly suggests the existence of multi-electron excitations tied with one photon [2]. Motivated by such suggestion, we have started the study of two-dimensional systems, as the first target being a spinless fermion model, the hamiltonian of which is written as

$$H = -t_0 \Sigma_{(l,l')}(C_l^\dagger C_{l'} + H.c.) + V \Sigma_{(l,l')} n_l n_{l'} , \qquad (1)$$

where the creation and annihilation operators are those of the fermion, and t_0 and V are the electron transfer energy and the intersite repulsion energy, respectively. Both terms are limited to nearest-neighbor site pairs. Since the periodic-boundary condition is imposed on both the ends, the system can be regarded as a two-dimensional torus. For this lattice, we place the fermions of which the number is half that of the lattice sites. We thus have a ground state in which the fermions occupy the sites with a checker-board-like pattern.

In FY2012, we have challenged a full diagonalization of the system of 6×6, following that based on a restricted dimension for the Hilbert space in the preceding year (FY2011). The restriction of the dimension was defined by setting an upper bound for the number of occupied nearest-neighboring sites (i.e., bonds). In the preceding year, the size of the dimension was 1,468,366,616 for the maximum of fifteen bonds. We now enlarge it to a full dimension, that is, 9,075,135,300, which is halved by applying the particle-hole symmetry rigorously. We then find that the enlargement is accomplished without any numerical difficulty for the Lanczos and continued-fraction methods for the determination of the ground state and the optical spectrum, respectively. The memory usage is roughly 4TB, consuming almost all the available memory in the 4-node job. In the calculation of a conjugate-gradient (CG) method that determines the excited-state vector, however, the memory slightly exceeds the upper limit and makes it still difficult to execute the CG calculation in the full dimension. In Fig. 1, we compare a spectrum obtained for $V=2t_0$ by the Lanczos and continued fraction methods with that obtained by a dynamical density-matrix renormalization group (DDMRG). The latter method is also applied to nuclear physics [3]. The coincidence between the two spectra of $\sigma(\omega)$ is satisfactory, while the number of excited fermions, $N_{ex}(\omega)$, shows some difference, and this seems to indicate an imperfection of the present latter calculation, namely, a shortage in the allowed number of states per "block."
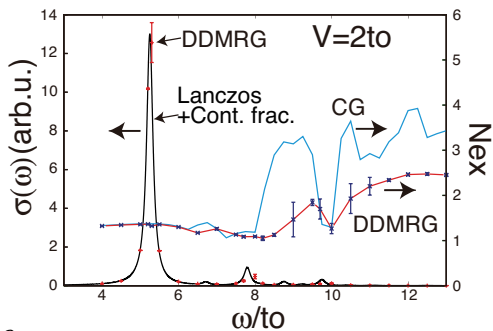

Figure 1: Optical conductivity spectrum, $\sigma(\omega)$, and the number of fermion excitations, $N_{ex}(\omega)$, for $V=2t_0$. Two results from the direct diagonalization and the DDMRG are shown for comparison. For $\sigma(\omega)$, the solid line is for the result calculated by the direct method and the dots with an errorbar are for that by the DDMRG. Note that $N_{ex}(\omega)$ by the direct method is calculated under the restriction of the dimension, because the CG method still does not work in the full dimension.

References

[1] K. Iwano, Phys. Rev. Lett. **97**, 226404 (2006), and *ibid.* **102**, 106405 (2009).

[2] S. Iwai *et al.*, Phys. Rev. Lett. **98**, 097402 (2007).

[3] J. Dukelsky, S. Pittel, S. S. Dimitrova and M. V. Stoitsov, Phys. Rev. C **65**, 054319 (2002) [nucl-th/0202048].