

Theory of Nonequilibrium Quantum Dynamics and Transport

Department of Theoretical and Computational Molecular Science
Division of Theoretical Molecular Science II



YONEMITSU, Kenji
YAMASHITA, Yasufumi
TANAKA, Yasuhiro
MIYASHITA, Satoshi
KONDO, Naoko

Associate Professor
Assistant Professor*
IMS Research Assistant Professor
Post-Doctoral Fellow†
Secretary

Nonequilibrium properties of low-dimensional correlated electron systems are investigated from different aspects. Among them, photoinduced transitions are now widely achieved between metals and insulators, between paraelectric and ferroelectric phases, among nonmagnetic, paramagnetic and ferromagnetic phases, and so on.¹⁾ Most of them are realized by changing the temperature also. Here, we focus on a quantum phase transition between neutral quantum- paraelectric and ionic (anti)ferroelectric ground (*i.e.*, zero temperature) states, where photoinduced dynamics are experimentally demonstrated to be different from ordinary ones. In addition, we continue the research for the mechanisms of different rectifying actions. Here, we employ nonequilibrium Green's functions to elucidate differences between strongly-correlated and weakly-correlated insulators.

1. Enhanced Coherent Dynamics near a Quantum Phase Transition²⁾

A quantum phase transition between neutral quantum-paraelectric and ionic antiferroelectric phases is realized in mixed-stack charge-transfer complexes composed of 4,4'-dimethyltetrathiafulvalene (DMTTF) and tetrahalo-*p*-benzoquinones (QBr_{*n*}Cl_{4-*n*}). Recently, photoinduced reflectivity changes are reported. The reflectivity in the energy range where it is sensitive to the ionicity change shows a large-amplitude oscillation near the quantum phase transition point. Then, nonequilibrium dynamics is studied near the quantum phase transition point in the one-dimensional quantum Blume-Emery-Griffiths model. Its pseudospin component S^z represents an electric polarization, and $(S^z)^2$ corresponds to ionicity. This model is one-dimensional and does not distinguish between ferroelectric and antiferroelectric phases. The time-dependent Schrödinger equation is solved for the exact many-body wave function in the quantum-paraelectric phase. After impact force is introduced on a polarization locally in space and time, polarizations [Figure 1(a)] and ionicity [Figure 1(b)] coher-

ently oscillate. The oscillation amplitudes are large near the quantum phase transition point. The dependences of these oscillation amplitudes on the total-energy increment ΔE are shown in Figure 2 for different quantum-tunneling amplitudes h .

The energy supplied by the impact flows linearly into these oscillations, so that the nonequilibrium behavior is uncooperative.

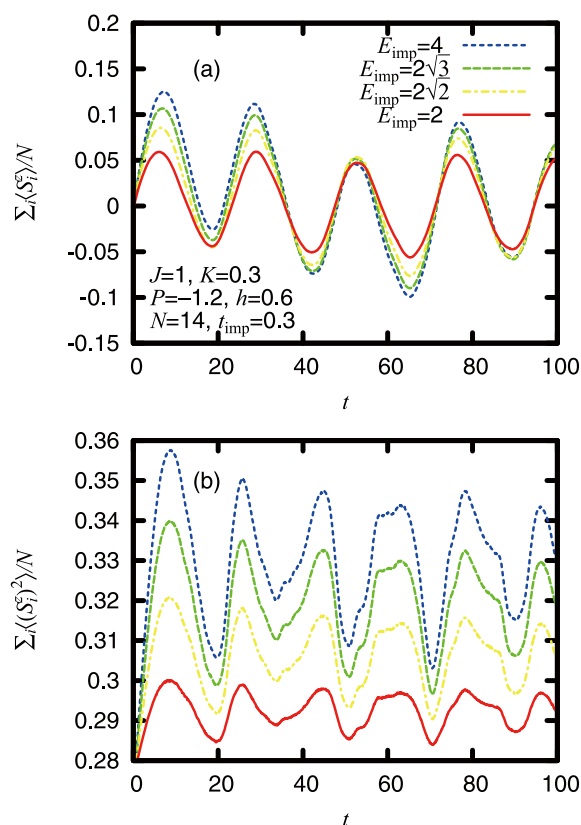


Figure 1. (a) Spatial average of electric polarization S^z and (b) spatial average of ionicity $(S^z)^2$, as a function of time t , after impact force of strength E_{imp} is locally introduced on a polarization.

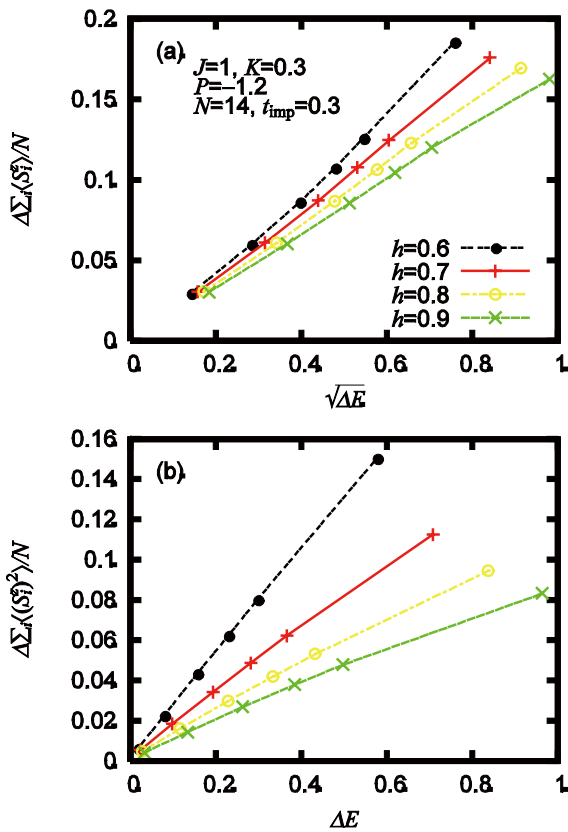


Figure 2. (a) Amplitude of oscillation in spatial average of electric polarization S^z , as a function of square root of energy supplied, and (b) amplitude of oscillation in spatial average of ionicity $(S^z)^2$, as a function of energy supplied ΔE . The quantity h denotes the quantum-tunneling amplitude.

2. Nonequilibrium Green's Functions for Rectification at Metal–Insulator Interfaces³⁾

The suppression of rectification at metal–Mott-insulator interfaces, which was previously shown by numerical solutions to the time-dependent Schrödinger equation and experiments on real devices, is reinvestigated theoretically using nonequilibrium Green's functions. The one-dimensional Hubbard model is used for a Mott insulator. The effects of attached metallic electrodes are incorporated into the self-energy. A scalar potential originating from work-function differences and satisfying the Poisson equation is added to the model. For electron density, we decompose it into three parts. One is obtained by integrating the local density of states over energy to the midpoint of the electrodes' chemical potentials.

Award

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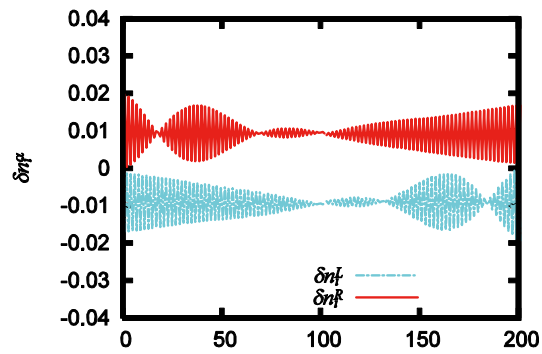


Figure 3. Nonequilibrium part of charge density due to coupling with left electrode, δn_i^L (light blue), and that with right electrode, δn_i^R (red), for Mott insulator with left-going bias.

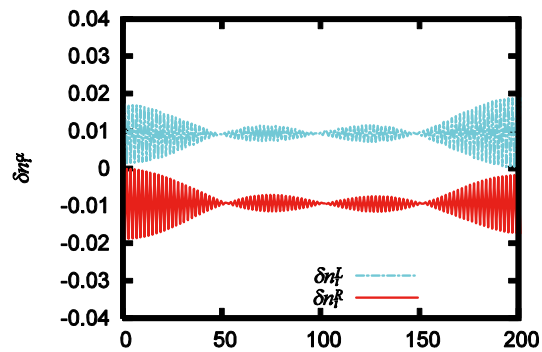


Figure 4. Nonequilibrium part of charge density due to coupling with left electrode, δn_i^L (light blue), and that with right electrode, δn_i^R (red), for Mott insulator with right-going bias.

The others, obtained by integrating lesser Green's functions, are due to couplings with the electrodes and correspond to an inflow and an outflow of electrons (Figures 3 and 4). In Mott insulators, incoming electrons and holes are extended over the whole system, avoiding further accumulation of charges relative to that in the case without bias. Furthermore, the inflow and the outflow of electrons are insensitive to the polarity of the bias. This induces collective charge transport and results in the suppression of rectification.

References

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* Present Address: General Studies, College of Engineering, Nihon University, Koriyama, Fukushima 963-8642

† Present Address: Japan Science and Technology Agency, Chiyoda-ku, Tokyo 102-0075