Theory of Nonequilibrium Quantum Transport

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Nonlinear conduction in correlated electron systems such as one-dimensional Mott insulators and two-dimensional charge-ordered materials has been of great interest in the past few decades. They offer intriguing subjects of nonequilibrium physics in condensed matter and the possibility for novel functions of electronic devices. Here, we study the relationship between the nonlinear conduction in nano-sized materials and the dielectric breakdown of bulk insulators from a general viewpoint. Then, we study the relationship between the nonlinear conduction and the coexisting charge orders in two-dimensional organic materials.

1. Crossover from Bias-Induced to Field-Induced Breakdown of Insulators[1)]

We focus on quasi-two-dimensional quarter-filled-band charNonequilibrium states induced by an applied bias voltage (V) and the corresponding current–voltage characteristics of one-dimensional models describing band and Mott insulators (Figure 1) are investigated theoretically by using non-equilibrium Green's functions.[2)] We attach the models to metallic electrodes, whose effects are incorporated into the self-energy. Modulation of the electron density and the scalar potential coming from the additional long-range interaction are calculated self-consistently within the Hartree approximation. For both models of band and Mott insulators with length L_C, the bias voltage induces a breakdown of the insulating state, whose threshold shows a crossover as a function of L_C (Figure 2). It is determined basically by the bias $V_{th} \sim \Delta$ for L_C smaller than the correlation length $\xi = W/\Delta$, where W denotes the bandwidth and Δ denotes the energy gap. For systems with L_C much larger than ξ, the threshold is governed by the electric field V_{th}/L_C, which is consistent with a Landau-Zener–type breakdown, where V_{th}/L_C is proportional to Δ^2/W. The spatial dependence of the scalar potential turns out to be crucially important for this crossover: without the scalar potential, the breakdown would occur unnaturally at $V_{th} \sim \Delta$ regardless of the length of the central part L_C.

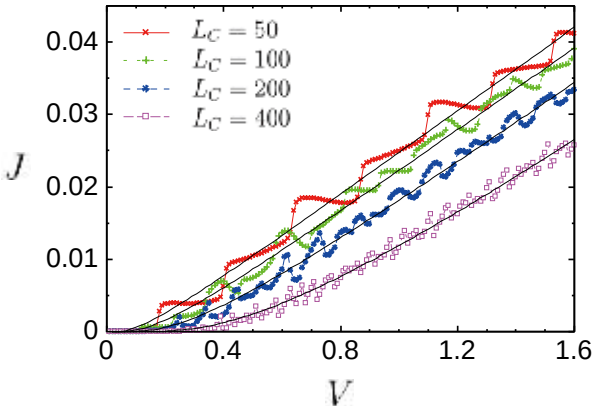

Figure 1. Current (J)–Voltage (V) characteristics of one-dimensional band insulators for several sizes of the central part L_C, with alternation of transfer integrals $\delta t = 0.025$, Coulomb parameter $V_p = 0.1$, and coupling to left and right electrodes $\gamma_L = \gamma_R = 0.1$. The solid lines show the function $J = aV \exp(-V_{th}/V)$, which fits to the results.

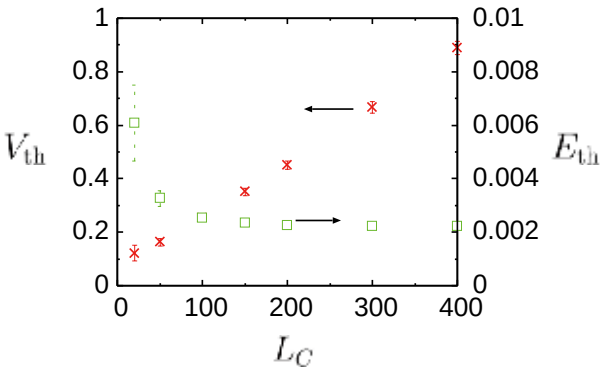

Figure 2. Dependence of the threshold bias voltage V_{th} and the threshold electric field E_{th} on the size of the central part L_C. The other parameters are the same as in Figure 1.

2. Nonlinear Conduction and Melting of Charge Order on a Triangular Lattice[3)]

As described above, a photoinduced insulator-to-metal tranThe observations of the giant nonlinear conduction and spontaneous current oscillation in the organic compounds θ-(BEDT-TTF)$_2$CsM(SCN)$_4$ (M = Co and Zn) have renewed interest since the electric-field-induced behaviors differ in many respects from the sliding of density waves in quasi-one-dimensional materials, where a nesting of the Fermi surface is responsible for their ground states. In quasi-two-dimensional organic conductors θ-(BEDT-TTF)$_2$X, the long-range Coulomb repulsion is mainly responsible for the ground state accompanied with charge orders.

We focus on the mechanism of the peculiar nonlinear conduction in θ-(BEDT-TTF)$_2$X through the melting of stripe-type charge order. An extended Peierls-Hubbard model attached to metallic electrodes (Figure 3) is investigated by a nonequilibrium Green's function technique.[2)] A novel current–voltage characteristics (Figure 4) appears in a coexistent state of stripe-type and non-stripe 3-fold charge orders, where the applied bias melts mainly the stripe-type charge order through the reduction of lattice distortion, whereas the 3-fold charge order survives (Figure 5). These contrastive responses of the two different charge orders are consistent with the experimental observations.

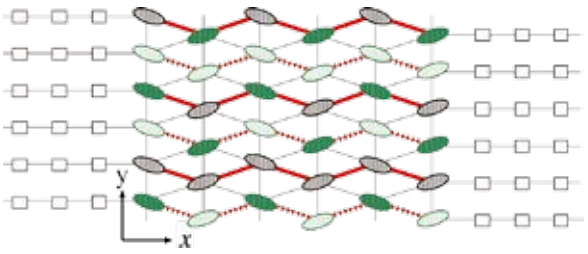

Figure 3. Schematic picture of the model. The left and right electrodes are attached to the central part where the horizontal and 3-fold charge orders coexist.

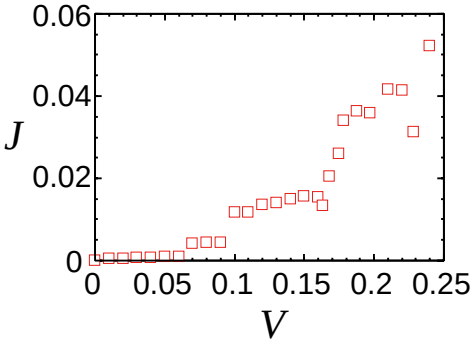

Figure 4. Electric current J, as a function of V.

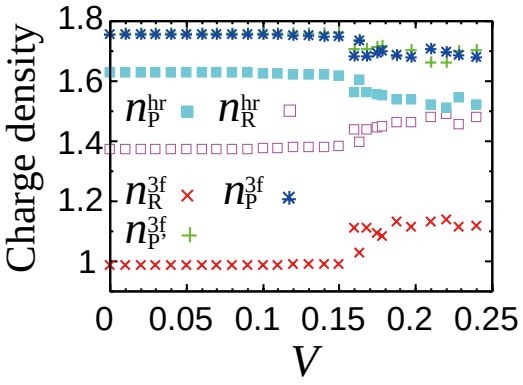

Figure 5. Horizontal (n^{hr}_R and n^{hr}_P) and 3-fold (n^{3f}_R, n^{3f}_P, and $n^{3f}_{P'}$) components of the charge distribution, as a function of V.

When both stripe-type and 3-fold charge orders exist, the density of states at the chemical potential of the central part μ_C, is suppressed compared to the purely 3-fold charge-ordered state (Figure 6). A small current flows because the coexistent state has no energy gap in the thermodynamic limit. Above a threshold bias voltage, the density of states at μ_C is large since the horizontal charge modulation is significantly decreased. This change in the conduction behavior is triggered by the reduction of lattice distortion.

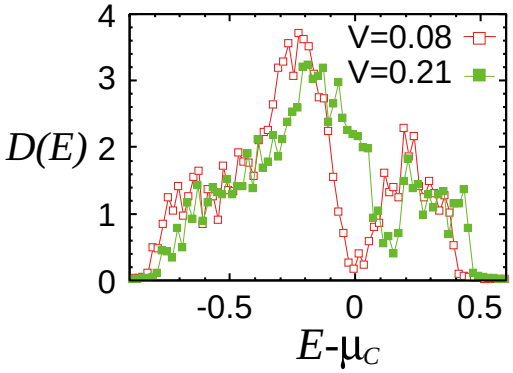

Figure 6. Density of states for V = 0.08 and 0.21.

References

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2) K. Yonemitsu, *J. Phys. Soc. Jpn.* **78**, 054705 (8 pages) (2009).
3) Y. Tanaka and K. Yonemitsu, *Phys. B (Amsterdam, Neth.)* **405**, S211–S213 (2010).

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