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Nonlinear electrical-transport phenomena in regular and disordered Hubbard chains

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A quantum-mechanical transport theory is developed to nonlinear electrical-transport phenomena in Hubbard chains. The intrasite Coulomb repulsion is assumed to be sufficiently strong, and the electron-transfer term is treated as a perturbation. The interaction between electrons and intrasite vibrations is taken into account by two types of coupling terms. The effects of the electron-phonon interaction and structural disorder are discussed. dc current peaks and negative resistance are found and explained by considering four possible carrier-transfer processes between sites. In disordered systems, new current peaks characterized by the disorder are also found.

I. INTRODUCTION

During the last decade, the Hubbard model has been used extensively to investigate the electrical and magnetic properties of the systems with narrow energy bands. Corresponding substances are, for example, transition metals, their oxides, and quasi-one-dimensional organic charge-transfer salts. The Hubbard Hamiltonian represents probably the simplest way to take into account the electron-correlation effect. This effect yields significant influences on the thermodynamic behavior of the system.

Extensions of the Hubbard model were considered by including additional interactions, for example, the interatomic Coulomb repulsion and exchange interaction between nearest-neighbor sites.[1,2] However, apart from the long-range properties in the electron-electron interaction, one of the most significant physical extensions of the Hamiltonian is taking into account the electron-phonon or electron-excitation interaction. In fact, tetracyanoquinodimethane (TCNQ) salts like (*N*-methylphenazinium) *N*MP-TCNQ are strongly polarizable materials. The coupling of electrons to phonons or to localized modes involving polarization plays essential roles on the Peierls instability,[3] intramolecular vibrations,[4] and small polaron formation.[5]

The interaction between electrons and intrasite vibrations has been considered by two types of coupling terms. One is the linear interaction term between the electron in one molecular site and the lattice displacement coordinate on that site. Bari[6] discussed the electrical conductivity and thermoelectric power including this type of coupling terms. The other type of coupling terms was introduced by Pincus.[4] This denotes a change of intrasite Coulomb repulsion induced by the molecular-stretching vibrational mode.

In a previous paper,[7] the author discussed the effects of those two types of coupling terms on the electrical conductivity in a Hubbard chain with structural disorder. In the theoretical investigation based upon the Hubbard model, structural disorder is also an important factor to be discussed. In real materials disorder is usually present. An important problem on disorder is what effects the disorder yields to the physical properties of the system. In *N*MP-TCNQ, for example, structural disorder is caused by the random orientation of methyl groups in *N*MP$^+$ ions.[8] Consequently, electrons will be moving along the TCNQ$^-$ chain under the influence of a random potential. In several TCNQ salts, the magnetic susceptibility behaves at low temperature as $T^{-\gamma}$, $\gamma < 1$.[9] Theodrou[10] explained such unusual behavior by the structural disorder based upon a disordered Hubbard model. On the other hand, the effects of disorder on the Peierls instability have been investigated by many authors.[11]

The electrical-transport phenomena in a regular Hubbard chain have been also studied by many authors.[5,12] However, the discussion was based upon the linear-response theory, and therefore, restricted to the weak electric field case. Nonlinear phenomena have currently received much attention in various systems. To the author's knowledge, nonlinear electrical-transport properties have not been studied in the Hubbard model. The purpose of the present paper is to investigate nonlinear electrical-transport phenomena in Hubbard chains. The interaction between electrons and intrasite vibrations is taken into account by two types of coupling terms as mentioned above. The effects of structural disorder on nonlinear dc current are also discussed. The electron-transfer term is assumed to be much smaller than that of the intrasite Coulomb repulsion. Further we assume that the Peierls instability[3] is quenched by the strong Coulomb repulsion.[4,13]

II. FORMULATION ON NONLINEAR ELECTRICAL TRANSPORT

A quantum theory of nonlinear electrical-transport phenomena is developed in this section. The starting point is the equation of motion for the density of matrix:

$$i\hbar\frac{\partial\rho_T}{\partial t}=i\hbar\frac{\partial\rho'}{\partial t}=[H_T,\rho_T]=[H_T,\rho']+[V,\rho] \quad , \tag{1}$$

where

$$H_T=H+V, \quad \rho_T=\rho+\rho' \quad . \tag{2}$$

H_T and ρ_T are the Hamiltonian and density matrix of the system, respectively, H and ρ are those in the absence of the external field, V denotes the interaction with the external field, and ρ' stands for a change of the density matrix caused by the interaction V.

From Eq. (1) we obtain

$$\rho'=-\frac{i}{\hbar}\int_0^t dt'\exp[-iH_T(t-t')/\hbar][V,\rho] \times\exp[iH_T(t-t')/\hbar] \quad . \tag{3}$$

The electric current is given by

$$J(t)=\mathrm{Tr}(\rho_T\hat{J})=\mathrm{Tr}(\rho'\hat{J}) \quad , \tag{4}$$

where $\hat{J}$ is the current operator.

We now consider a Hubbard chain described by the following Hamiltonian:

$$H=H_0+H' \quad , \tag{5}$$

where

$$\begin{aligned}H_0=&\sum_{i\sigma}\epsilon_i n_{i\sigma}+\sum_i U_i n_{i\uparrow}n_{i\downarrow}\\&+\sum_{i\lambda}Q_{i\lambda}[V_{i\lambda}(n_{i\uparrow}+n_{i\downarrow})+W_{i\lambda}n_{i\uparrow}n_{i\downarrow}]\\&+\sum_{i\lambda}\tfrac{1}{2}\hbar\Omega_{i\lambda}(P_{i\lambda}^2+Q_{i\lambda}^2) \quad ,\end{aligned} \tag{6}$$

$$H'=-\sum_{ij\sigma}t_{ij}a_{i\sigma}^{\dagger}a_{j\sigma} \quad , \tag{7}$$

$$\begin{aligned}Q_{i\lambda}&=\frac{1}{\sqrt{2}}(b_{i\lambda}^{\dagger}+b_{i\lambda}),\\P_{i\lambda}&=\frac{i}{\sqrt{2}}(b_{i\lambda}^{\dagger}-b_{i\lambda}) \quad .\end{aligned} \tag{8}$$

Here $a_{i\sigma}^{\dagger}\,(a_{i\sigma})$ is the creation (annihilation) operator for an electron with spin σ at the ith site of the chain, and $n_{i\sigma}=a_{i\sigma}^{\dagger}a_{i\sigma}$. The parameters ϵ_i and U_i are the single-site energy and Coulomb repulsion at the ith site, respectively, and t_{ij} is the electron-transfer integral between nearest-neighbor sites. Further, $b_{i\lambda}^{\dagger}$ $(b_{i\lambda})$ is the creation (annihilation) operator of phonons for the vibrational mode λ at the ith site with frequency $\Omega_{i\lambda}$. The phonon system is taken to be an array of dispersionless Einstein oscillators. Vibrations at different sites are supposed to be uncoupled. The parameters $V_{i\lambda}$ and $W_{i\lambda}$ are the electron-phonon coupling constants at the ith site: $V_{i\lambda}$ denotes the interaction between electron density and lattice displacement coordinate, and $W_{i\lambda}$ denotes a change of the Coulomb repulsion introduced by Pincus.

We regard H' as a perturbation and perform the following unitary transformation to H_0 in Eq. (6):

$$\overline{H}=e^{-S}H_0e^{S}=\sum_i\overline{H}_i \quad , \tag{9}$$

where

$$S=\sum_{i\lambda}\frac{i}{\hbar\Omega_{i\lambda}}[V_{i\lambda}(n_{i\uparrow}+n_{i\downarrow})+W_{i\lambda}n_{i\uparrow}n_{i\downarrow}]P_{i\lambda} \quad , \tag{10}$$

$$e^{-S}b_{i\lambda}^{\dagger}e^{S}=b_{i\lambda}^{\dagger}-\frac{1}{\sqrt{2\hbar}\,\Omega_{i\lambda}}[V_{i\lambda}(n_{i\uparrow}+n_{i\downarrow})+W_{i\lambda}n_{i\uparrow}n_{i\downarrow}] \quad , \tag{11}$$

$$\overline{H}_i=\overline{\epsilon}_i(n_{i\uparrow}+n_{i\downarrow})+\overline{U}_i n_{i\uparrow}n_{i\downarrow}+\sum_\lambda\hbar\Omega_{i\lambda}(b_{i\lambda}^{\dagger}b_{i\lambda}+\tfrac{1}{2}) \quad . \tag{12}$$

Here $\overline{\epsilon}_i$ and $\overline{U}_i$ are given by

$$\begin{aligned}\overline{\epsilon}_i&=\epsilon_i-\sum_\lambda\frac{V_{i\lambda}^2}{2\hbar\Omega_{i\lambda}} \quad ,\\\overline{U}_i&=U_i-\sum_\lambda\frac{1}{2\hbar\Omega_{i\lambda}}(2V_{i\lambda}^2+4V_{i\lambda}W_{i\lambda}+W_{i\lambda}^2) \quad .\end{aligned} \tag{13}$$

The single-site energy ϵ_i and Coulomb repulsion U_i are renormalized by the electron-phonon interaction, and reduced to $\overline{\epsilon}_i$ and $\overline{U}_i$, respectively.

Using the invariance of the trace with respect to the transformation, the unperturbed partition function is given by

$$\begin{aligned}Z&=\mathrm{Tr}\exp[-\beta(H_0-\mu\hat{N})]\\&=\prod_i Z_i\left\{\prod_\lambda\tfrac{1}{2}\operatorname{csch}\tfrac{1}{2}\beta\hbar\Omega_{i\lambda}\right\} \quad ,\end{aligned} \tag{14}$$

where $\hat{N}=\sum_i(n_{i\uparrow}+n_{i\downarrow})$, $\beta=(kT)^{-1}$, k is the Boltzmann constant, μ the unperturbed chemical potential, and

$$Z_i=1+2\exp[-\beta(\overline{\epsilon}_i-\mu)] +\exp[-\beta(2\overline{\epsilon}_i+\overline{U}_i-2\mu)] \quad . \tag{15}$$

The relation between the total number of electrons N_e and the unperturbed chemical potential μ is expressed as

$$\begin{aligned}N_e&=kT\frac{\partial}{\partial\mu}\ln Z\\&=\sum_i\frac{2}{Z_i}\{\exp[-\beta(\overline{\epsilon}_i-\mu)]\\&\qquad+\exp[-\beta(2\overline{\epsilon}_i+\overline{U}_i-2\mu)]\} \quad .\end{aligned} \tag{16}$$

The interaction between electrons and the external field F is written

$$V=-\sum_{i\sigma} eFR_i a_{i\sigma}^{\dagger} a_{i\sigma} \ , \tag{17}$$

where R_i is the component of the lattice-site position vector parallel to the external field, and $e<0$. The current operator is given by

$$\hat{J}=\frac{ie}{\hbar}\left[H,\sum_{i\sigma} R_i n_{i\sigma}\right]=\frac{ie}{\hbar}\sum_{ij\sigma} t_{ij}(R_i-R_j)a_{i\sigma}^{\dagger}a_{j\sigma} \ . \tag{18}$$

The density matrix ρ is expanded with respect to t_{ij} as follows:

$$\rho=\rho_0+\rho_1+\cdots \ . \tag{19}$$

Here ρ_0 and ρ_1 are the zeroth and first-order terms, respectively, and written

$$\rho_0=\frac{1}{Z}\exp[-\beta(H_0-\mu\hat{N})] \ , \tag{20}$$

$$\rho_1=\frac{-1}{Z}\exp[-\beta(H_0-\mu\hat{N})] \times\int_0^{\beta} dt_1 \exp[t_1(H_0-\mu\hat{N})]H' \times\exp[-t_1(H_0-\mu\hat{N})] \ . \tag{21}$$

We calculate the dc current $J(t)$ up to the second order of t_{ij}. The validity of this approximate calculation is limited to the regime $U_{i,j} >> |t_{ij}|$, $kT>|t_{ij}|$. In such a regime, H_T and ρ in Eq. (3) can be put as (H_0+V) and $(\rho_0+\rho_1)$, respectively. The commutation relation $[V,\rho]$ in Eq. (3) is reduced to $[V,\rho_1]$, because we have $[V,\rho_0]=0$. Consequently, within the second order of t_{ij}, the dc current $J(t)$ of Eq. (4) is written

$$J(t)=\frac{F}{Z}\mathrm{Tr}\Big(\exp[-\beta(H_0-\mu\hat{N})]\int_0^{t} d\tau \exp[-i(H_0+V)\tau/\hbar]\int_0^{\beta} dt_1 \exp[t_1(H_0-\mu\hat{N})] \times \hat{J}\exp[-t_1(H_0-\mu\hat{N})]\exp[i(H_0+V)\tau/\hbar]\hat{J}\Big) \ . \tag{22}$$

Here we have used

$$\frac{i}{\hbar}[V,H']=\frac{i}{\hbar}eF\sum_{ij\sigma} t_{ij}(R_i-R_j)a_{i\sigma}^{\dagger}a_{j\sigma}=F\hat{J} \ . \tag{23}$$

The steady-state current J is evaluated by taking the limit $t\rightarrow\infty$ in Eq. (22). The details of the calculation are given in Appendix. As a result, J is expressed as

$$J=2\frac{\sqrt{\pi}}{\hbar}e\sum_{ij} t_{ij}^2 a_{ij}[\exp(\beta eFa_{ij})-1]\frac{K_{ij}(eFa_{ij})}{(Z_iZ_j)} \ , \tag{24}$$

where $a_{ij}=R_i-R_j$ and

$$\begin{aligned} K_{ij}(x)=&\left(\sum_{\lambda} G_{i\lambda}+G_{j\lambda}\right)^{-1/2}\exp\left[-\left(x+\epsilon_j-\epsilon_i+\sum_{\lambda}\Gamma_{i\lambda}\right)^2\Big/\left(\sum_{\lambda} G_{i\lambda}+G_{j\lambda}\right)-\beta(\bar{\epsilon}_i-\mu)\right]\\ &+\left(\sum_{\lambda} G_{i\lambda}+G'_{j\lambda}\right)^{-1/2}\exp\left[-\left(x+\epsilon_j+U_j-\epsilon_i-\sum_{\lambda}(\Gamma'_{j\lambda}-\Gamma_{i\lambda})\right)^2\Big/\left(\sum_{\lambda} G_{i\lambda}+G'_{j\lambda}\right)-\beta(\bar{\epsilon}_j+\bar{\epsilon}_i-2\mu)\right]\\ &+\left(\sum_{\lambda} G'_{i\lambda}+G_{j\lambda}\right)^{-1/2}\exp\left[-\left(x+\epsilon_j-\epsilon_i-U_i+\sum_{\lambda}\Gamma'_{i\lambda}(2+X_{i\lambda})\right)^2\Big/\left(\sum_{\lambda} G'_{i\lambda}+G_{j\lambda}\right)-\beta(2\bar{\epsilon}_i+\bar{U}_i-2\mu)\right]\\ &+\left(\sum_{\lambda} G'_{i\lambda}+G'_{j\lambda}\right)^{-1/2}\exp\left[-\left(x+\epsilon_j+U_j-\epsilon_i-U_i-\sum[\Gamma'_{j\lambda}-(2+X_{i\lambda})\Gamma'_{i\lambda}]\right)^2\Big/\left(\sum_{\lambda} G'_{i\lambda}+G'_{j\lambda}\right)\right.\\ &\left.-\beta(\bar{\epsilon}_j+2\bar{\epsilon}_i+\bar{U}_i-3\mu)\right] \ . \end{aligned} \tag{25}$$

Here the following parameters are introduced:

$$G_{i\lambda}=V_{i\lambda}^2\coth(\tfrac{1}{2}\beta\hbar\Omega_{i\lambda}),\quad \Gamma_{i\lambda}=\frac{V_{i\lambda}^2}{\hbar\Omega_{i\lambda}},\quad X_{i\lambda}=\frac{W_{i\lambda}}{V_{i\lambda}} \ ,\quad \Gamma'_{i\lambda}=(1+X_{i\lambda})\Gamma_{i\lambda},\quad G'_{i\lambda}=(1+X_{i\lambda})^2G_{i\lambda} \ . \tag{26}$$

In the regular system with a half-filled band, the chemical potential μ is equal to $(\bar{\epsilon}_i + \frac{1}{2}\bar{U}_i)$ from Eq. (16), and the current J is written

$$J = \frac{\sqrt{\pi}\, eaN_S t^2}{2\hbar(1+e^{\beta\bar{U}/2})^2}[A(eaF) - A(-eaF)] \ , \tag{27}$$

where a and N_S are the lattice constant and the number of sites, respectively. The function $A(x)$ is defined as

$$\begin{aligned} A(x) = (e^{\beta x}-1)\Bigg\{ & \left(\sum_\lambda 2G_\lambda\right)^{-1/2} \exp\left[-\left(x+\sum_\lambda \Gamma_\lambda\right)^2 \Big/ \left(\sum_\lambda 2G_\lambda\right) + \tfrac{1}{2}\beta\bar{U}\right] \\ & + \left(\sum_\lambda G_\lambda + G'_\lambda\right)^{-1/2} \exp\left[-\left(x+U-\sum_\lambda \Gamma_\lambda X_\lambda\right)^2 \Big/ \left(\sum_\lambda G_\lambda + G'_\lambda\right) + \beta\bar{U}\right] \\ & + \left(\sum_\lambda G_\lambda + G'_\lambda\right)^{-1/2} \exp\left[-\left(x-U+\sum_\lambda (2+X_\lambda)\Gamma'_\lambda\right)^2 \Big/ \left(\sum_\lambda G_\lambda + G'_\lambda\right)\right] \\ & + \left(\sum_\lambda 2G'_\lambda\right)^{-1/2} \exp\left[-\left(x+\sum_\lambda (1+X_\lambda)\Gamma'_\lambda\right)^2 \Big/ \left(\sum_\lambda 2G'_\lambda\right) + \tfrac{1}{2}\beta\bar{U}\right]\Bigg\} \ . \end{aligned} \tag{28}$$

The indices (i,j) for the parameters are abbreviated in Eqs. (27) and (28). If only the first-order terms in F are taken in Eqs. (24) and (27), we obtain the known result of the linear-response theory.[7]

III. DISCUSSION

Nonlinear dc electrical-transport properties in Hubbard chains are discussed in what follows. There are four processes of charge transfer between nearest-neighbor sites: (1) transfer from a singly occupied site to an empty site; (2) transfer from a singly occupied site to a site already occupied by an opposite-spin electron; (3) transfer from a doubly occupied site to an empty site; (4) transfer from a doubly occupied site to a site already occupied by an opposite-spin electron. In Eq. (25) the Gaussian peak centered at $-eFa_{ij} = E^p$ $(p = 1 \sim 4)$ is related to the process (p) in the carrier transfer from the ith site to the jth site, where E_p is expressed as

$$\begin{aligned} E_1 &= \epsilon_j - \epsilon_i + \sum_\lambda \Gamma_{i\lambda} \ , \\ E_2 &= \epsilon_j + U_j - \epsilon_i - \sum_\lambda (\Gamma'_{j\lambda} - \Gamma_{i\lambda}) \ , \\ E_3 &= \epsilon_j - \epsilon_i - U_i + \sum_\lambda \Gamma'_{i\lambda}(2+X_{i\lambda}) \ , \\ E_4 &= \epsilon_j + U_j - \epsilon_i - U_i - \sum_\lambda [\Gamma'_{j\lambda} - (2+X_{i\lambda})\Gamma'_{i\lambda}] \ . \end{aligned} \tag{29}$$

From the expression of G_{ij} in Eq. (26), we see the Gaussian peaks become more broad as temperature and the strength of the electron-phonon interaction increase.

From the above consideration, it is expected that current peaks and negative resistance will be found. When $-eF|a_{ij}| >> |E_p|$ $(p = 1 \sim 4)$, the carrier-transfer rate of any process is very small, and $J = 0$ in the limit $F \rightarrow \infty$. But such consideration is reasonable only for the systems with narrow energy bands. Further, the validity is restricted to the cases in which the interband transition of carriers and breakdown of the system do not occur. If the energy gap between adjacent bands is narrow, the interband transition of carriers will occur in a high-field region.

In Fig. 1, lines A and B denote the variation of dc current with the external field in the regular A and B systems. Temperature is fixed at $T = 0.1\,U_A$ in the figure. The indices A and B are attached to the parameters for the A and B systems, respectively. For simplicity, only one vibrational mode is considered, i.e., $\lambda = 1$. The values of the parameters are determined to satisfy the following relations: $U_A - U_B = 2(\epsilon_B - \epsilon_A)$, $\bar{U}_A - \bar{U}_B = 2(\bar{\epsilon}_B - \bar{\epsilon}_A)$, and $N_e = N_S$, i.e., half-filled band case is considered. Irrespective of temperature, the chemical potential μ is $\bar{\epsilon}_A + \frac{1}{2}\bar{U}_A$ in both the A and B systems. The energies E_p of Eq. (29) are evaluated as

$$E_1 \sim \pm 10^{-3} U_{A,B}, \quad E_2 \sim \pm U_{A,B} \ ,$$
$$E_3 \sim \pm U_{A,B}, \quad E_4 \sim \pm 10^{-3} U_{A,B} \ .$$

In Fig. 1, a peak of current appears near $-eaF = 2 \times 10^{-2} U_A$. This value of $-eaF$ does not coincide with that of $|E_1|$ or $|E_4|$. When the applied field is weak, i.e., $-eaF \sim 10^{-3} U_{A,B}$ and $-eaF << kT = 0.1\,U_A$, the current J of Eq. (27) increases almost linearly with increasing F. In the function $A(\pm eaF)$, the term $[\exp(\pm\beta eaF) - 1]$ is more dominant for the current than the Gaussian terms. As the applied field becomes strong, the Gaussian terms become more dominant than the term $[\exp(\pm\beta eaF) - 1]$. Consequently, a peak of current appears in a higher field region $(-eaF \sim 10^{-2} U_A)$ than the Gaussian peaks related to the processes (1) and (4). Negative resistance is found in a region $-eaF \gtrsim 2 \times 10^{-2} U_A$. However,

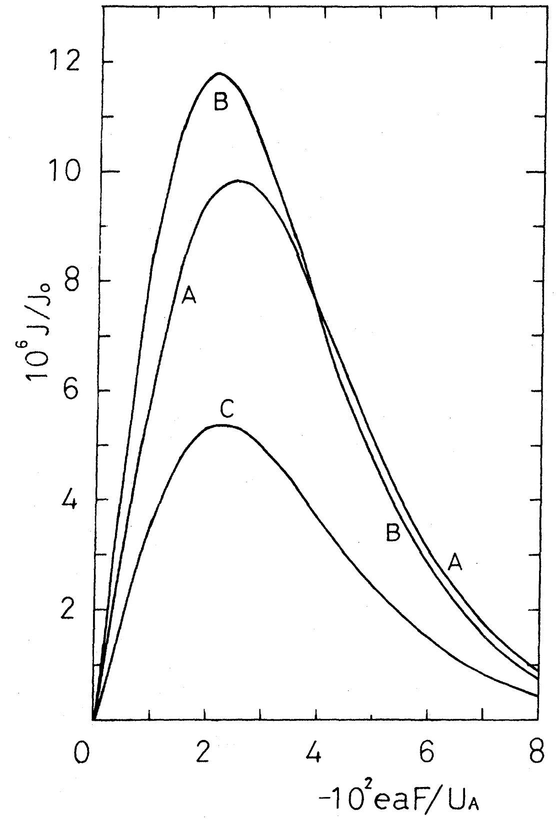

FIG. 1. Nonlinear dc current J vs external field F. Lines A and B show J in the regular A and B systems, respectively. Line C shows J in a substitutionally disordered system composed of A and B species. The values of the parameters used in the calculation are as follows: $kT/U_A=0.1$, $\epsilon_A/U_A=0.1$, $\epsilon_B/U_A=-0.1$, $U_B/U_A=1.4$, $t_{AA}/U_A=0.01$, $t_{BB}/U_A=0.03$, $t_{AB}/U_A=0.02$, $V_A/U_A=0.02$, $V_B/U_A=0.015$, $W_A/U_A=0.01$, $W_B/U_A=0.011$, $\hbar\Omega_A/U_A=0.3$, $\hbar\Omega_B/U_A=0.2$, $C_A=C_B=0.5$. The quantity J_0 is given by $-eaN_S U_A \hbar^{-1}$.

current does not decrease monotonically. The other peak of current appears near $-eaF=U_{A,B}$, although it is not shown in Fig. 1. The carrier transfer processes (2) and (3) are dominant around that peak.

We next discuss the effects of structural disorder. If the parameters are random variables, many Gauss-

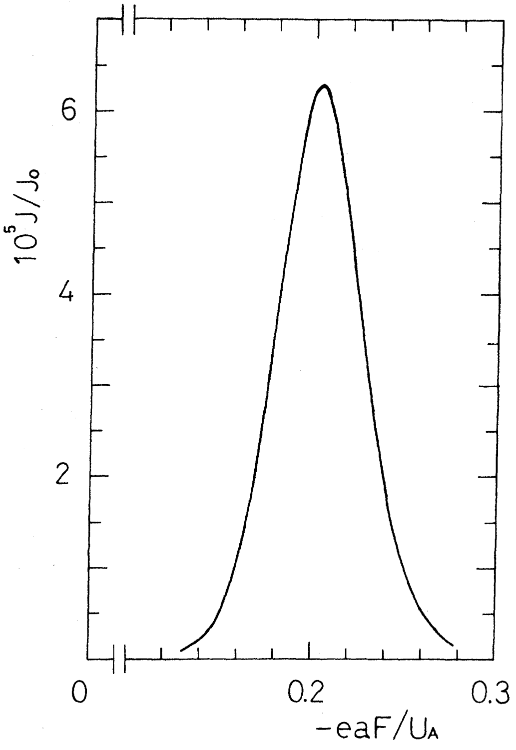

FIG. 2. Nonlinear dc current vs external field F in a substitutionally disordered system. The values of the parameters are those used in Fig. 1.

ian peaks will appear in Eq. (25). Therefore, current peaks are changed variously by structural disorder. They reflect the properties of the disorder. There are many parameters influenced by the disorder. For simplicity, we consider a substitutionally disordered system composed of A and B species. The distribution of A and B species is assumed to be completely random. When the summation with respect to sites is taken in Eq. (24), we neglect the configurational correlation of species. Consequently, within the second order of t_{ij}, the current J is approximately given by

$$J=2\frac{\sqrt{\pi}}{\hbar}eaN_S\left[(e^{\beta eaF}-1)\left(C_A^2\frac{t_{AA}^2}{Z_A^2}K_{AA}(eaF)+C_AC_B\frac{t_{AB}^2}{Z_AZ_B}[K_{AB}(eaF)+K_{BA}(eaF)]+C_B^2\frac{t_{BB}^2}{Z_B^2}K_{BB}(eaF)\right)-\cdots\right], \tag{30}$$

where the ellipsis represents the term with a → $-a$ and $C_A(C_B)$ is the concentration of $A\,(B)$ species, and therefore, $C_A+C_B=1$.

In Fig. 1, the electric current in a substitutionally disordered system is shown by line C. The half-filled band case is considered and the chemical potential of the disordered system is $\bar{\epsilon}_A+\frac{1}{2}\bar{U}_A$ because we consider the case of $C_A = C_B = 0.5$. In the figure, the shape of line C is similar to those of lines A and B. But the current is considerably diminished by the substitutional disorder. As shown in Fig. 2, a Gaussian peak of current reflecting the substitutional disorder appears in a high-field region ($-eaF \sim 0.2U_A$). In Eq. (29), the energies $|E_1|$ and $|E_4|$ for the carrier transfer between A and B sites are nearly equal to $0.2U_A$. Therefore, the transfer processes (1) and (4) between A and B sites can easily occur around $-eaF = 0.2U_A$.

We have discussed some of the features associated with nonlinear electrical-transport phenomena in Hubbard chains. However, in the present treatment, the interband transition caused by the applied field is not taken into account. The substitutional disorder is mainly discussed in the present paper, but the disorder expected in TCNQ salts is not substitutional one. Nonlinear transport properties in Hubbard systems should be investigated more extensively.

ACKNOWLEDGMENT

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APPENDIX

In this Appendix, the current J is calculated using Eq. (22). Since $[H_0, V] = [H_0, \hat{N}] = [\hat{N}, V] = 0$, we change the order of the operators in the trace. Accordingly, J is written as

$$J = \frac{F}{2Z}\int_0^\infty d\tau \int_0^\beta dt_1 \,\mathrm{Tr}\{\exp[-\beta(H_0-\mu\hat{N})]\exp[t_1(H_0-\mu\hat{N})][\hat{J}(\tau)+\hat{J}(-\tau)]\exp[-t_1(H_0-\mu\hat{N})]\hat{J}\} \ , \qquad (\mathrm{A1})$$

where

$$\hat{J}(\tau) = \exp[-i(H_0+V)\tau/\hbar]\hat{J}\exp[i(H_0+V)\tau/\hbar] \ . \qquad (\mathrm{A2})$$

To evaluate Eq. (A1), we use

$$e^{-\hat{A}n_{i\sigma}}a_{i\sigma}^\dagger e^{\hat{A}n_{i\sigma}} = e^{-\hat{A}}a_{i\sigma}^\dagger, \quad e^{-\hat{A}n_{i\sigma}}a_{i\sigma}e^{\hat{A}n_{i\sigma}} = e^{\hat{A}}a_{i\sigma} \ , \qquad (\mathrm{A3})$$

where $\hat{A}$ is an arbitrary operator which satisfies

$$[\hat{A}, a_{i\sigma}^\dagger] = [\hat{A}, a_{i\sigma}] = 0 \ .$$

Further, in the trace of Eq. (A1), we use the operator S of Eq. (10) and perform the same unitary transformation as that of Eq. (9). As a result, we obtain

$$J = \frac{e^2F}{2\hbar^2}\sum_{ij\sigma} t_{ij}^2 \frac{(R_i-R_j)^2}{Z_iZ_j}\int_0^\beta dt_1 \exp[Fe(R_i-R_j)t_1] \times \int_0^\infty d\tau\,\mathrm{Tr}\left\{\left[D_i\left(t_1-\frac{i}{\hbar}\tau\right)D_j\left(-t_1+\frac{i}{\hbar}\tau\right)+D_i\left(t_1+\frac{i}{\hbar}\tau\right)D_j\left(-t_1-\frac{i}{\hbar}\tau\right)\right]n_{i\sigma}(1-n_{j\sigma})\right\} \ , \qquad (\mathrm{A4})$$

where

$$D_i(t) = \exp\{-\beta[(\bar{\epsilon}_i-\mu)(n_{i\uparrow}+n_{i\downarrow})+\bar{U}_i n_{i\uparrow}n_{i\downarrow}]\} \times \exp\left[t\left(\epsilon_i - eFR_i + U_i n_{i-\sigma} - \sum_\lambda \frac{1}{\hbar\Omega_{i\lambda}}[V_{i\lambda}(n_{i\uparrow}+n_{i\downarrow})+W_{i\lambda}n_{i\uparrow}n_{i\downarrow}](V_{i\lambda}+W_{i\lambda}n_{i-\sigma}) + \sum_\lambda (V_{i\lambda}+W_{i\lambda}\,n_{i-\sigma})Q_{i\lambda}\right)\right] \times \exp\left(-\beta\sum_\lambda \hbar\Omega_{i\lambda}(b_{i\lambda}^\dagger b_{i\lambda}+\tfrac{1}{2})\right)\Big/ \mathrm{Tr}\exp\left(-\beta\sum_\lambda\hbar\Omega_{i\lambda}(b_{i\lambda}^\dagger b_{i\lambda}+\tfrac{1}{2})\right) \ . \qquad (\mathrm{A5})$$

On the thermal average with respect to phonon operators, the following identity is present[14]:

$$\frac{\mathrm{Tr}\exp[-\beta\hbar\Omega_{i\lambda}(b_{i\lambda}^\dagger b_{i\lambda}+\frac{1}{2})]e^{\eta Q_i}}{\mathrm{Tr}\exp[-\beta\hbar\Omega_{i\lambda}(b_{i\lambda}^\dagger b_{i\lambda}+\frac{1}{2})]} = \exp[\tfrac{1}{4}\eta^2\coth(\tfrac{1}{2}\beta\hbar\Omega_{i\lambda})] \ , \qquad (\mathrm{A6})$$

where η is an arbitrary parameter. Using Eq. (A6) and the integral formula

$$\int_0^\infty d\tau\,\{\exp[-\eta(\tau+i\xi)^2]+\exp[-\eta(\tau-i\xi)^2]\} = \sqrt{\pi/\eta} \ ,$$

the current J of Eq. (A4) is reduced to Eq. (24).

[1] R. Kishore and S. K. Joshi, J. Phys. C 4, 2475 (1971).

[2] G. Röpke, B. Albani, and W. Schiller, Phys. Status Solidi B 69, 45 (1975).

[3] R. E. Peierls, *Quantum Theory of Solids* (Oxford, London, 1955), Chap. V.

[4] P. Pincus, Solid State Commun. 11, 51 (1972).

[5] P. Chaikin, A. F. Garito, and A. J. Heeger, J. Chem. Phys. 58, 2336 (1973).

[6] R. A. Bari, Phys. Rev. B 9, 4329 (1974).

[7] K. Hattori, J. Phys. Soc. Jpn. 49, 638 (1980).

[8] C. J. Fritchie, Jr., Acta Crystallogr. 20, 892 (1966).

[9] L. N. Bulaevskii, A. V. Zvarykina, Yu. S. Karimov, R. B. Lyubovskii, and I. F. Shchegolev, Zh. Eksp. Teor. Fiz. 62, 725 (1972) [Sov. Phys.–JETP 35, 384 (1972)].

[10] G. Theodorou, Phys. Rev. B 16, 2264, 2273 (1977).

[11] P. N. Sen and C. M. Varma, Solid State Commun. 15, 1905 (1974); L. J. Sham and B. R. Patton, Phys. Rev. B 13, 3151 (1976); C. Tannous and A. Caillé, Solid State Commun. 33, 951 (1980).

[12] R. A. Bari and T. A. Kaplan, Phys. Rev. B 6, 4623 (1972); D. Ihle and B. Lorenz, Phys. Status Solidi B 69, K117 (1975); D. Cabib, Phys. Rev. B 12, 2189 (1975).

[13] R. A. Bari, Phys. Rev. B 3, 2662 (1971).

[14] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Chap. XII.