Transactions of the Materials Research Society of Japan 24 [1] 105-108 (1999)

Theoretical Calculation of Electronic Properties in the Chain Composed of Ions with and without Correlations between Electrons

Nobuhiro SUE and Yuhei NATSUME

Department of Physics, Faculty of Science, Chiba University, Inage-ku, Chiba 263-8522
Fax: 81-43-290-2874, e-mail:natsume@science.s.chiba-u.ac.jp

The electronic properties of chains for constant chemical potential μ composed of ions (U-sites) with strong correlations are discussed on the basis of numerical calculations. In this model, U-sites are sandwiched by ions without U called N-sites. We use exact diagonalization on these NNUUNN and NNUUUNN chains in grand canonical distribution. Here, the equilibrium number of electrons $\langle N_{el} \rangle$ and the equilibrium electron-addition spectrum expressed as $\beta \cdot \langle (\delta N)^2 \rangle$ are discussed under the condition of constant temperature β and μ. The latter spectrum reflecting the fluctuation of electron-number is related with the conductivity for these systems attached to electrodes with μ. Furthermore, the hopping rates between left and right N-sites trough U-sites are obtained in calculation. The present discussion suggests that the single broad structure appears for the thermodynamic limit in the energy range from lower Hubbard levels and upper Hubbard levels. Such structure has quite characteristic features: they have characters both of strong correlation for many-body systems and simple metallic property for one-body systems.

KEYWORDS: Hubbard sites sandwiched by normal ions, strong correlations, mid-bands, averaged electron number, equilibrium electron-additional spectra, the fluctuation of electron numbers, constant chemical potential, grand-canonical distribution, attachment to electrodes

§1. Introduction

Quite recently, much attention has been paid to the report that the chain composed of several atoms had been skillfully synthesized. Thus, the fundamental problem for the attachment of such mesoscopic systems to electrodes becomes much important.[1] In addition to this essential problem, unparalleled opportunity has been provided to study the relationship between the one-body picture for electrons and many-body effects, by recent extensive investigations on systems of quantum dots. In the last ten years, furthermore, we have had much discussion of the correlation between electrons on a 2-dimensional lattice site, which is made for the purpose of acquiring the insight into the nature of the carriers responsible for superconductivity in transition-metal oxide compounds. This is because the electronic properties of such dots and compounds are dominated by strong electron-electron correlations, as well as the one-body picture for an electrons.

In these situations for the investigation of these materials, a detailed theoretical understanding of models for strongly correlated systems attached to electrodes is needed.

The fundamental model expressing the strong local correlations is given by the Hubbard Hamiltonian. In deed, we have had a lot of work on electronic properties in Hubbard chains where any site has the on-site correlation U under the condition of constant electron numbers. In comparison with these many reports, the study on electronic properties for chains, which are composed by ions with and without U, attached to electrodes of the chemical potential μ, has seemed to be less advanced, up to now. Considering with transport properties which are detected by attaching the electrode with μ to this mesoscopic systems, we need the study of these kinds of materials under the condition of constant μ, nowadays. In other words, we should treat the grand canonical distribution instead of a canonical one.

In this paper, we discuss, therefore, the electronic properties of chains for constant μ composed of ions (called U-sites) with strong correlations expressed by Hubbard U, which are sandwiched by ions (N-sites) without U. We use exact diagonalization on this new model.

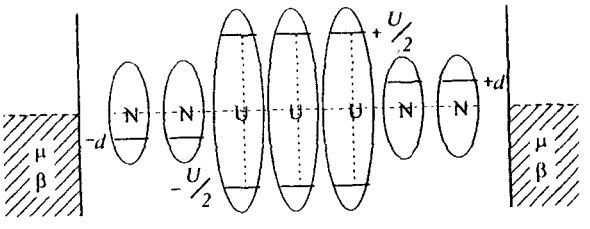

Fig.1. The present model of the one-dimensional chain composed of the series of ions N-N-U-U-U-N-N, where N and U mean the sites of normal ions and characteristic ions with the on-site correlation expressed by Hubbard U, respectively. Here, this chain is treated as the grand canonical distribution with the chemical potential μ and temperature T.

It is the purpose of this paper to argue that the numerical study for this new model leads us the suggestion of the appearance of the anomalous electronic states which has the effect of strong correlation in spite of metallic transport features.

§2. Model

2.1 Chains

As shown in Fig.1, the present model discussed here is the one-dimensional chain composed of the series of ions N-N-U-U-N-N and N-N-U-U-U-N-N.[2-4]

2.2 Hamiltonian

Thus, the present Hamiltonian is expressed as follows by the U sites $i = 3, 4, ...M-2$ and one-body electronic levels ϵ_i of a single ion for N sites $i = 1, 2, M-1, M$:

$$\mathcal{H} = -t \sum_{\ell=1,\sigma}^{M-1} (\hat{c}^{\dagger}_{\ell,\sigma}\hat{c}_{\ell+1,\sigma} + \hat{c}^{\dagger}_{\ell+1,\sigma}\hat{c}_{\ell,\sigma})$$

$$+ \sum_{i=1,\sigma}^{2} \epsilon_i \hat{n}_{i,\sigma} + \sum_{i=M-1,\sigma}^{M} \epsilon_i \hat{n}_{i,\sigma}$$

$$-\frac{U}{2} \sum_{j=3}^{M-2} \{\hat{n}_{j,\uparrow}(1-\hat{n}_{j,\downarrow}) + \hat{n}_{j,\downarrow}(1-\hat{n}_{j,\uparrow})\}$$

$$+\frac{U}{2} \sum_{j=3}^{M-2} \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}.$$

In this Hamiltonian, the transfer energy expressed by t is taken into account for nearest neighbors of ions.

2.3 Averaged electron number and its fluctuation for the grand canonical distribution

Here, we treat the system whose electron number is fluctuated under the condition of constant chemical potenthal μ. In fact, we calculate the equilibrium number of electrons $\langle N \rangle$ and the equilibrium electron-addition spectrum expressed[5] as

$$\beta \cdot \langle (\delta N)^2 \rangle = \beta \cdot [\langle N^2 \rangle - \langle N \rangle^2] = \frac{\partial \langle N \rangle}{\partial \mu},$$

where the temperature T is $1/(k_B\beta)$. Here, the expectation value of operator Θ is defined as

$$\langle \Theta \rangle = \mathrm{Tr}[\Theta \cdot \exp\{-\beta(\mathcal{H} - \mu N)\}]/\mathrm{Tr}[\exp\{-\beta(\mathcal{H} - \mu N)\}].$$

It should be noted that the equilibrium electron-addition spectrum $\beta \cdot \langle (\delta N)^2 \rangle$ corresponds to the fluctuation of $\langle N \rangle$. The adoption of calculation for this spectra to small clusters has been reported by Ugajin.[6,7]

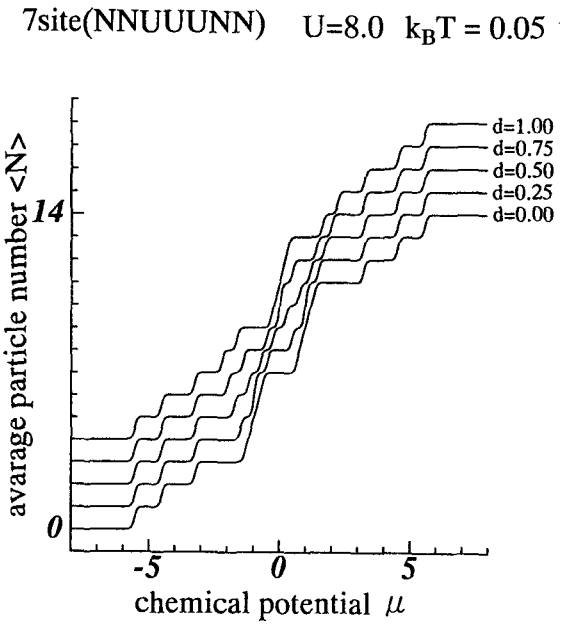

Fig.2. The dependence of equilibrium number of electrons $\langle N \rangle$ on the chemical potential μ for $d = 0, 0.25, 0.5, 0.75, 1.0$. The staircase drawn by the solid line presents $\langle N \rangle$. To be easy to see, $\langle N \rangle + 4d$ is drawn for each value of d. At $\mu = 0$, $\langle N \rangle$ has the value of 7.

2.4 Hopping rate between normal sites

In the next place, we introduce the following hopping rate between normal sites under the condition of μ=constant:

$$h(\mu) = \sum_{\ell=1}^{2} \sum_{k=M-1}^{M} \sum_{\sigma} \langle (\hat{c}^{\dagger}_{\ell,\sigma}\hat{c}_{k,\sigma} + \hat{c}^{\dagger}_{k,\sigma}\hat{c}_{\ell,\sigma}) \rangle. \quad (1)$$

The calculation of this rate in grand canonical distribution is made for the first time in this paper.

§3. Numerical Results and Discussion

We made the numerical calculation for the exact diagonalization for the system of $M = 7$ and $M = 6$ adopting t as the unit of energy. We make the energy difference d to the model. Namely, we fix ϵ_1,ϵ_2 to be $-d$ and ϵ_{M-1},ϵ_M to $+d$, respectively. Considering the dependence of the equilibrium electron-addition spectrum on temperature, we adopt $k_BT = 1/\beta = 0.05$ in this paper.

3.1 Averaged numbers and its fluctuations

The averaged numbers of electrons vs. μ are shown in Fig.2 for various values of d. As for the behavior of $d = 0$, we obtain the quite sim-

ple picture: the bonding and antibonding levels around $\mu \sim 0$ made by the coupling between left and right N sites. This is because these levels are separated from lower $(-U/2)$ and upper $(+U/2)$ Hubbard levels. These structures can be explained by the superposition of localized states for left N sites, U sites and right N sites. If we give the energy difference d to the model, we obtain the more complicated behavior by the coupling between left and right edges via U-sites. In particular, we show both the averaged numbers and its fluctuation in Fig.3, where $d = 0.5$

Here, we find the anomalous structure around $-2 < \mu < +2$. Though it appears at the midpoint between lower $(-U/2)$ and upper $(+U/2)$ Hubbard levels, the step of the staircase for $\langle N \rangle$ is composed of the difference of one electron.

This is the quite different character from that of a simple one-body picture, where the step of $\langle N \rangle$ is 2 electrons by the degeneracy of spins. This remarkable behavior suggest us that we can expect the appearance of the characteristic mid-band in the thermodynamic limit of site number $N_{LR} \to \infty$ both for left and right N sites. This mid-band originating from one-body levels both of left and right N sites yields to the significant influence of strong correlations at U sites.

3.2 Overall structures

Figure.4 presents the 3-dimensinal illustration of the fluctuation $\beta \cdot \langle (\delta N)^2 \rangle$ for M=6 (NNUUNN) at U=8. This figure suggest us that the point d=1 for μ=0 exhibits the transient feature. We expect that the non-local structure connecting left and right N-sites becomes local one (left group and right group) at this point.

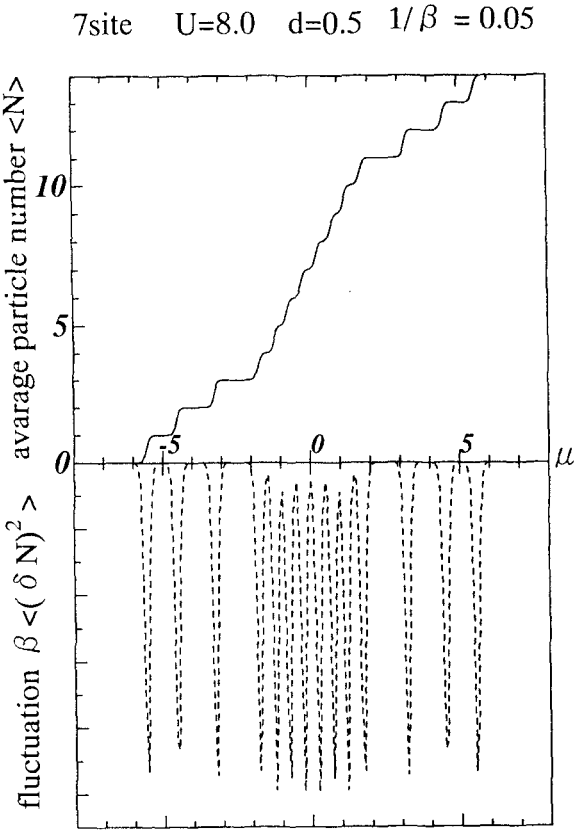

Fig.3. The equilibrium number of electrons $\langle N \rangle$ $\beta \cdot \langle (\delta N)^2 \rangle$ and the equilibrium electron-addition spectrum vs. μ for U=8 and d=0.5. The upper staircase drawn by the solid line presents $\langle N \rangle$, and the lower dashed line denotes $\beta \cdot \langle (\delta N)^2 \rangle$.

Fig.4. The fluctuation $\beta \cdot \langle (\delta N)^2 \rangle$ for M=6 (NNUUNN) at U=8 is shown by 3-dimensional illustration.

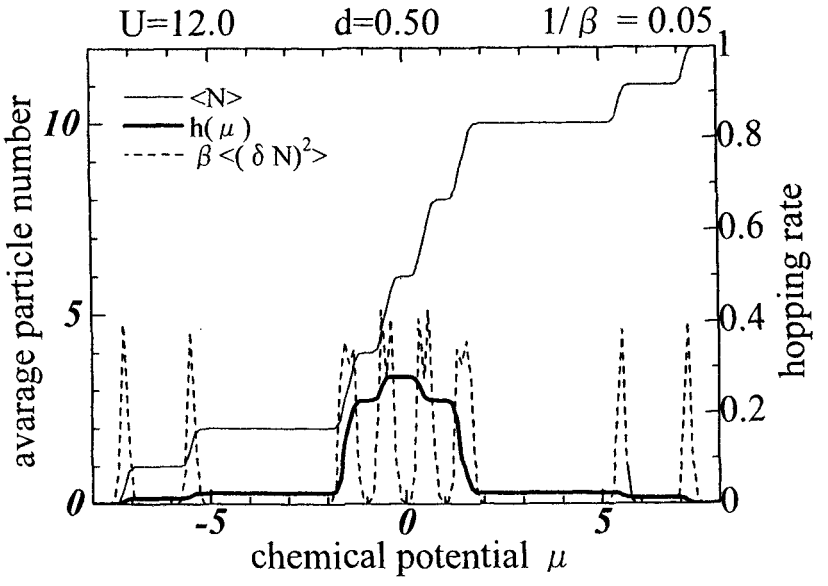

Fig.5. The hopping rate between left and right N-sites $h(\mu)$ vs. μ. Here, we adopt U=12 and d=0.5. We can find the broad structure around $-1.5 < \mu < +1.5$, which is different from that which can be seen in the fluctuation of electron numbers. The detail discussion is made in the text.

3.3 Hopping rates

The hopping rate $h(\mu)$ introduced in 2.3 denotes the coupling between left and right N-sites via U-sites. Figure.5 presents $h(\mu)$ vs. μ for U=12 and d=0.5 in the system of M=6 (NNU-UNN). It should be noted that $h(\mu)$ has different features than the fluctuation of electron numbers, because it dose not need the change of electron numbers: Even for the state at the plateau of electron number, it has the strength by the coupling. We can find the broad structure around $-1.5 < \mu < +1.5$ which has large intensity in comparison with those at lower ($\mu \sim -U/2$) and upper ($\mu \sim +U/2$) Hubbard levels. This fact also supports the appearance of above mentioned mid-band, which connects between left and right N-sites through U-sites.

3.4 Conclusive remark

We would like to point out the following suggestion from discussion made in previous sections: the single broad structure appears from $+U/2$ to $-U/2$, which is expected to become the mid-band for the thermodynamical limit exhibiting quite characteristic features.

Such the mid-band is affected considerably by the strong correlations, though it has the relatively wide metallic band by the significant coupling between left and right N-sites via U-sites.

The authors are indebted to Professor T.Nakayama of Chiba University for stimulating discussion and helpful suggestions.

1) For example, D.K.Ferry and S.M.Goodnick, *Transport in nanostructures* , Cambridge University Press, Cambridge 1997.
2) N. Sue and Y. Natsume, to be submitted to J.Phys.Soc.Jpn.
3) N. Sue and Y. Natsume: Read at the Sectional Meeting of the Phys. Soc. Jpn., Okinawa, September 1998, 28aPS137 (Abstracts Pt.3, p.812).
4) N. Sue and Y. Natsume: Read at the 53rd Annual Meeting of the Phys. Soc. Jpn., Chiba, March 1998, 31aPSA38 (Abstracts Pt.3, p.671). N. Sue and Y. Natsume: Read at the Sectional Meeting of the Phys. Soc. Jpn., Kobe, October 1997, 8aPS94 (Abstracts Pt.3, p.829).
5) C. Kittel: *Elementary Statistical Physics*, (John Wiley & Sons, New York, 1977).
6) Ryuichi Ugajin: J. Phys. Soc. Jpn., **65** (1996) 3952.
7) Ryuichi Ugajin: Physica **E1** (1997) 226.

(Received December 11, 1998; accepted February 28, 1999)