Effective Interactions of the One-Dimensional d-p Model Based on the Luttinger Liquid Theory

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We examine effective interactions of the 1D d-p model mapped to a typical one-dimensional(1D) model such as the Hubbard model or the t-J model by the numerical diagonalization method combined with the Luttinger liquid theory. Analysis of the effective coupling constants of the mapped model gives the relationship between these models without ambiguity. We find that the renormalized interaction is relatively weak, though the repulsion of the d-p model at Cu-sites is very strong. We also find that the d-p model corresponds to not the t-J model but the Hubbard model for wide range of the parameters. It suggests that the Hubbard model is more favorable than the t-J model as a effective model of the d-p model in the low energy limit.

KEYWORDS: d-p model, electronic structure, Hubbard model, Luttinger liquid, t-J model

§1. Introduction

The one-dimensional(1D) d-p model, simulating a Cu-O linear chain with the strong Coulomb repulsion U_d at Cu-sites and the charge-transfer energy Δ between Cu-sites and O-sites, may be a good target for investigating quasi one-dimensional cuprates and a possible mechanism of the high-T_c superconductivity.[1–3] To achieve a solid understanding of this kind of problem, numerical diagonalization studies of finite size systems combined with the Luttinger liquid theory are highly desirable.[4–7] We consider the following model Hamiltonian for the Cu-O chain in the hole picture:

$$H = t_{pd} \sum_{<ij>,\sigma} (p^\dagger_{i\sigma} d_{j\sigma} + h.c.) + \epsilon_d \sum_{j,\sigma} d^\dagger_{j\sigma} d_{j\sigma} + \epsilon_p \sum_{i,\sigma} p^\dagger_{i\sigma} p_{i\sigma} + U_d \sum_j \hat{n}_{dj\uparrow} \hat{n}_{dj\downarrow}, \tag{1.1}$$

where $d^\dagger_{j\sigma}$ and $p^\dagger_{i\sigma}$ stand for creation operators of a hole with spin σ in the Cu(d) orbital at site j and of a hole with spin σ in the O(p) orbital at site i, respectively, and $\hat{n}_{dj\sigma} = d^\dagger_{j\sigma} d_{j\sigma}$. Here, t_{pd} stands for the transfer energy between the nearest-neighbor d and p sites and will be set at unity (t_{pd}=1) hereafter in this study. The atomic energy levels of d and p orbitals are given by ϵ_d and ϵ_p, respectively. The charge-transfer energy Δ is defined as $\Delta = \epsilon_p - \epsilon_d$.

In this work, we obtain effective interactions of the 1D d-p model mapped to a typical 1D model based on the Luttinger liquid theory.[8–10] In the Luttinger liquid theory, an effective Hamiltonian of 1D models in the Tomonaga-Luttinger regime is generally given by

$$H = H_\sigma + H_\rho = \frac{v_\sigma}{2\pi} \int_0^L \mathrm{d}x \left[K_\sigma (\partial_x \theta_\sigma)^2 + K_\sigma^{-1} (\partial_x \phi_\sigma)^2 \right] + \frac{v_c}{2\pi} \int_0^L \mathrm{d}x \left[K_\rho (\partial_x \theta_\rho)^2 + K_\rho^{-1} (\partial_x \phi_\rho)^2 \right] \tag{1.2}$$

where v_s, v_c, K_σ and K_ρ are the velocities and coupling parameters of spin and charge parts, respectively. In the model which is isotropic in spin space, the coupling constant K_σ is renormalized to unity in the low energy limit. When we scale the energy of systems by v_c, two parameters v_s/v_c and K_ρ are required for identification of the system. These two parameters are given by numerical diagonalization of finite size systems using the Lanczos method. Comparing with these parameters, we determine the effective interactions of the model.

§2. Numerical diagonalization

We numerically diagonalize the Hamiltonian (1.1) up to 16 sites (8 unit cells) using the standard Lanczos algorithm. To carry out a systematic calculation, we use the periodic boundary condition for $N_h = 4m + 2$ and the antiperiodic boundary condition for $N_h = 4m$, where N_h is the total hole number and m is an integer. The filling n is defined by $n = N_h/N_u$, where N_u is the total number of unit cells (each unit cell contains a d and a p orbital). We also diagonalize the Hamiltonians of the the 1D Hubbard model,

$$H = -t \sum_{i,\sigma} (c^\dagger_{i\sigma} c_{i+1\sigma} + h.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \tag{2.1}$$

and 1D t-J model,

$$H = -t \sum_{i,\sigma} (\tilde{c}^\dagger_{i\sigma} \tilde{c}_{i+1\sigma} + h.c.) + J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} \hat{n}_i \hat{n}_{i+1}), \tag{2.2}$$

where $\tilde{c}^\dagger_{i\sigma} = c^\dagger_{i\sigma}(1 - \hat{n}_{i-\sigma})$ and $\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$.

The uniform charge susceptibility χ_c is obtained from the numerical differential of the ground state energy of the systems by the usual method[4–6] The critical exponent K_ρ is related to the charge susceptibility χ_c and the Drude weight D

$$K_\rho = \frac{1}{2} (\pi \chi_c D)^{1/2}, \tag{2.3}$$

with $D = \frac{\pi}{N_u} \frac{\partial^2 E_0(\phi)}{\partial \phi^2}$, where $E_0(\phi)$ is the total energy of the ground state as a function of a magnetic flux $N_u \phi$.[10]

We can also determine the K_ρ using the charge velocity v_c,

$$K_\rho = \frac{D}{2v_c}, \tag{2.4}$$

with $v_c = \frac{N_u}{2\pi}(E_1 - E_0)$,where $E_1 - E_0$ is the lowest charge excitation energy.[4,10] Using these two independent equations for K_ρ, we can check the consistency of the Luttinger liquid relations. In the previous work,[6] we have confirmed that the numerical results of K_ρ obtained through eqs.(2.3) and (2.4) are consistent with each other. However, the finite size effect of eq.(2.3) is usually smaller than that of eq.(2.4) in our experience. Therefore, we mainly use eq.(2.3).

§3. Effective exchange interaction

At first, we consider the 1D *d-p* model at half-filling. Because charge-gap opens, degrees of freedom of spin-part only remains in the low energy limit and spin velocity v_s becomes the only relevant parameter. In this case, the value of v_s directly leads the effective interaction. We compare the spin velocity v_{s-dp} of the *d-p* model to the spin velocity v_{s-H} of the Heisenberg model. The effective exchange interaction $\tilde{J}$ is defined by v_{s-dp}/v_{s-H}, where v_{s-H} is given by $\pi/2$.[11] We use the system of 4, 6 and 8 unit cells and calculate $\tilde{J}$ by the extrapolation.

In Fig.1, we show $\tilde{J}$ with the result of the 2nd order perturbation[12] and the result of the *d-p* ladder model estimated by Jeckelmann et al.[13] Values of $\tilde{J}$ for both models are very similar to each other for $\Delta \gtrsim 4$. It also indicates that our analysis is consistent with the perturbation for large Δ and the perturbation is not applicable to the case of $\Delta \lesssim 4$. The difference of $\tilde{J}$ between the *d-p* chain and the *d-p* Ladder may come of the difference of geometry of both models. Inset shows the size dependence of $\tilde{J}$ the *d-p* model and suggests that the finite size effect is small.

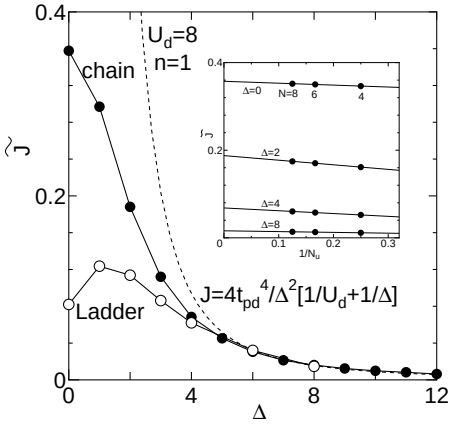

Fig. 1. Effective interaction $\tilde{J}$ as a function of Δ for 1D *d-p* model and the *d-p* ladder model estimated by Jeckelmann et al. at $U_d = 8$. The broken line represents the results of the 2nd order perturbation. The solid lines are guides for the eye. Inset shows the size dependence of $\tilde{J}$ for 1D *d-p* model.

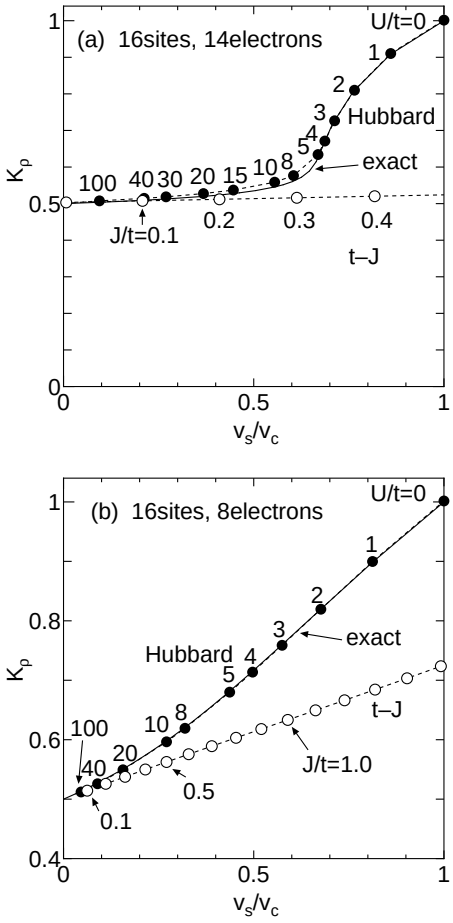

Fig. 2. The parameters v_s/v_c and K_ρ of the Hubbard model and the *t-J* model for various U and J on the v_s/v_c-K_ρ plane. Hole densities n are 1/8 (a) and 1/2 (b). The solid lines represent the result of the infinite system of the Hubbard model by the Bethe anzatz method. The broken lines are guides for the eye. Open circles represent the result of the *t-J* model at J/t=0.1,0.2,0.3,0.4 (a) and at J/t=0.1,0.2,0.3,....,1.5 (b) ,respectively. Solid circles represent the result of the Hubbard model.

§4. Parameters v_s/v_c and K_ρ

Next, we consider the doping case. A pair of parameters v_σ/v_ρ and K_ρ stands a state of the Luttinger liquid described in the effective Hamiltonian (1.2). We show the coupling parameters as a point on the v_s/v_c-K_ρ plane. If points of any two systems have been close to each other on the plane, we recognize that two models are equivalent to each other in the low energy limit. In Figs.2, we show the parameters v_s/v_c and K_ρ of the Hubbard model and the *t-J* model on the v_s/v_c-K_ρ plane.. We use 16-sites systems with 14electrons (2holes) (a) and 8electrons(8holes) (b) for the both models. We have confirmed that the values v_s and v_c of the *t-J* model are consistent with the result of Ogata et al.[4] We also show the exact result of the infinite system of the Hubbard model by the Bethe anzatz method.[14] Figures show that the exact result agrees with the result of the finite size systems and the finite size effect may be small.

As well known, the Hubbard model in the limit of the on-site repulsion $U \to \infty$ corresponds to the *t-J* model in the limit of the $J \to 0$.[15] The effective exchange interaction of the Hubbard model is written by $\tilde{J} \simeq 4t^2/U$. In

the light doping case, it is consistent with our result. For example, the state of the the Hubbard model at $U = 40$ is close to the state of the t-J model for $J = 0.1$ at $n = 1/8$. At $n = 1/2$, however, the deviation of $\tilde{J}$ from the above relation seems to be larger. It means that the mapping to the t-J model from the Hubbard model is not so valid for the over doping case.

In Figs.3, we show the parameters v_s/v_c and K_ρ of the 1D d-p model, the Hubbard model and the t-J model. We use 7-unit cells system with 8-holes (a) and 10-holes (b) for the 1D d-p mode and 14-sites system with 12-electrons (2holes) (a) and 8-electrons(6-holes) (b) for the Hubbard model and the t-J model. It is noted that the hole density of the Hubbard model and the t-J model is corresponding to the part of the hole density over the half-filling of the d-p model ($n = 1$). In the 8-holes case for the 1D d-p model, we cannot calculate K_ρ by eq.(2.3), since the number of holes over the half-filling is too small and the numerical differential which gives χ_c is not defined. So, we use eq.(2.4), though it leads larger finite size effect than eq.(2.3).[16] For the others, we calculate K_ρ by eq.(2.3).

We change the value of Δ at fixed U_d and change the value of U_d at fixed Δ for the 1D d-p model. Our result indicates that the parameter point of the d-p model is close to that of the Hubbard model for large Δ at fixed U_d. When Δ is fixed to 2, the d-p model is well mapped to the Hubbard model with relatively weak U. For example, the point of $U_d = 8$ and $\Delta = 2$ is corresponding with the point of $U \simeq 4$ for $n = 8/7$ and the point of $U \simeq 3$ for $n = 10/7$. This result suggests that the effective repulsion of U_d is fairly renormalized and weak. Figures also show that the d-p model corresponds to not the t-J model but the Hubbard model for wide range of the parameters. It may suggest that the Hubbard model is more favorable than the t-J model as an effective Hamiltonian of the d-p model in the low energy limit.

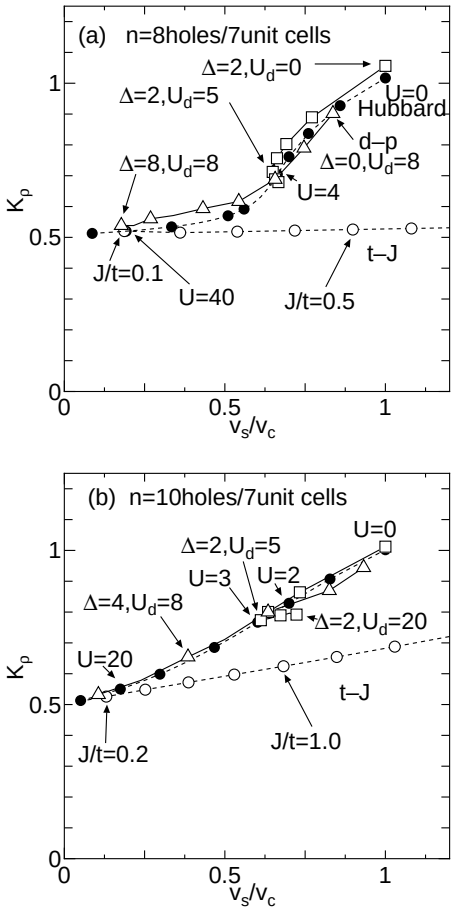

Fig. 3. The parameters v_s/v_c and K_ρ of the d-p model, the Hubbard model and the t-J model for various U_d, Δ, U and J on the v_s/v_c-K_ρ plane. Hole density n is 8/7 (a) and 10/7 (b). Open circles represent the result of the t-J model at J/t=0.1,0.2,0.3,..,0.6 (a) and at J/t=0.2,0.4,0.6,....,1.4 (b) ,respectively. Solid circles represent the result of the Hubbard model at U =0,1,2,3,4,8,10,20,40,100 (a) and at U =0,1,2,3,5,10,20,100 (b) ,respectively. Open squares stand the result of the d-p model at U_d=0,1,2,3,5,8,11 (a) and at U_d=0,1,2,5,10,20 (b) for $\Delta = 2$,respectively. Open triangles stand the result of the d-p model at Δ=0,1,2,3,4,6,8 (a) and at Δ=0,1,2,4,10 (b) for $U_d = 8$,respectively.

§5. Summary

We have considered the effective interactions of the 1D d-p model mapped to the Hubbard model and/or the t-J model by the numerical diagonalization method combined with the Luttinger liquid theory. The analysis gives the relationship between these 1D models without ambiguity. We find that the repulsive interaction of the d-p model is renormalized and relatively weak. Furthermore, the electronic state of the 1D d-p model seems to correspond to not the t-J model but the Hubbard model for wide range of the parameters. It suggests that the physics of the 1D d-p model is well described by the Hubbard model in the low energy limit.

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