Unambiguous relationship between the Hubbard, t-J and d-p models in One-dimension based on the Luttinger liquid Theory

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Abstract

We examine the one-dimensional (1D) *d-p* model in comparison with typical 1D models such as the 1D Hubbard model and the 1D *t-J* model using the numerical diagonalization method combined with the Luttinger liquid theory. We calculate the spin velocity v_σ, the charge velocity v_ρ and the Luttinger liquid parameter K_ρ for each model. Using these parameters, a relationship between the models is obtained unambiguously. We find that the *d-p* model can be described by the Hubbard model in the wide parameter region, while it can be described by the *t-J* model only in the strong coupling limit.

Key words: Luttinger liquid; *d-p* model; Hubbard model; *t-J* model

Since the discovery of the high-T_c cuprates, strongly correlated electron systems have been extensively studied due to possible relevance to the mechanism of the superconductivity [1,2]. In particular, there has been much theoretical interest in the *d-p* model, the Hubbard model and the *t-J* model. The *d-p* model is widely accepted as a basic model describing the electronic structure of the Cu-O network, while the Hubbard and the *t-J* models are investigated as effective models for low-energy properties [1,2]. Various methods, such as perturbative approach [3] and cluster model calculation [4], have been used to clarify the relationship between these models. Nevertheless, there is no reliable relationship between the parameters of the effective (Hubbard or *t-J*) model and the original *d-p* model available for the whole parameter region.

In this work, we examine the *d-p* model, the Hubbard model and the *t-J* model in one-dimension (1D) by using the numerical diagonalization method combined with the Luttinger liquid theory [5–7]. Although our analysis is limited to 1D systems, it gives a quantitative and unique relationship between these models.

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We consider the *d-p* model simulating a Cu-O chain:

$$H = t_{pd} \sum_{<ij>,\sigma} (p^\dagger_{i\sigma} d_{j\sigma} + h.c.) + \epsilon_d \sum_{j,\sigma} d^\dagger_{j\sigma} d_{j\sigma} + \epsilon_p \sum_{i,\sigma} p^\dagger_{i\sigma} p_{i\sigma} + U_d \sum_j \hat{n}_{dj\uparrow} \hat{n}_{dj\downarrow}, \quad (1)$$

where $d^\dagger_{j\sigma}$ and $p^\dagger_{i\sigma}$ stand for creation operators of a hole with spin σ and $\hat{n}_{dj\sigma} = d^\dagger_{j\sigma} d_{j\sigma}$. Here, the charge-transfer energy Δ is defined as $\Delta = \epsilon_p - \epsilon_d$.

In the Luttinger liquid theory[9,10], low energy properties of 1D models in the Tomonaga-Luttinger regime can be generally described by an effective Hamiltonian:

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

where v_σ, v_ρ, K_σ and K_ρ are the velocities and coupling parameters of spin and charge parts, respectively. The

models considered in this paper are isotropic in spin space and, then, the coupling constant K_σ is renormalized to unity in the low energy limit.

When we scale the energy of every system by v_ρ, the system is identified by using two parameters: v_σ/v_ρ and K_ρ [8]. Then we can indicate every system as a point on the v_σ/v_ρ-K_ρ plane. When two different models are indicated by the same point on the v_σ/v_ρ-K_ρ plane, we recognize that the two models are equivalent in the low energy limit except for the energy unit.

In the weak-coupling regime, so-called g-ology [9] is useful to analyze the 1D models [8]. When we consider only the 'on'-site interaction such as U in the Hubbard model or U_d in the d-p model, the two parameters v_σ/v_ρ and K_ρ are written by only one g-coupling. Eliminating the g-coupling, we obtain $K_\rho = \sqrt{\frac{1+(v_\sigma/v_\rho)^2}{2}}$. It is noted that this result is independent of the band structure of the model. Therefore, the d-p model can be always mapped onto the Hubbard model for any Δ, U_d and any filling n in the weak-coupling limit.

In order to examine the 1D models including strong-coupling regime, we evaluate the two parameters v_σ/v_ρ and K_ρ by numerical diagonalization of finite size systems using the standard Lanczos algorithm. We use 7-unit cells system with 10 holes for the 1D d-p model, and 14-sites system with 8 electrons (6 holes) for the t-J model. Here, the hole density of the t-J model is corresponding to the part of the hole density over the half-filling of the d-p model [2]. In the inset of Fig.1, v_σ/v_ρ vs. K_ρ thus obtained is plotted for the d-p model and the t-J model together with the exact result for the Hubbard model from the Bethe-ansatz method [12]. It is found that the parameter point of the d-p model is close to that of the Hubbard model in the wide parameter region, while it dose not correspond to the t-J model except for the strong coupling region.

Comparing the parameter points of the d-p and the Hubbard models, we can estimate the effective interaction $U_{\rm eff}$ for the d-p model. The value of $U_{\rm eff}$ is defined by the on-site interaction U of the Hubbard model when the Hubbard model is indicated by the same point of the d-p model on the v_σ/v_ρ-K_ρ plane (see the inset). In Fig.1, $U_{\rm eff}$ thus obtained is plotted as a function of U_d for $\Delta = 2$ together with the result from the g-ology. Within the g-ology [7,9,11], $U_{\rm eff}$ is given by $U_{\rm eff} = U_d|\alpha_{k_{\rm F}}|^4 v_{\rm F}^{\rm Hub}/v_{\rm F}^{\rm dp}$, where $|\alpha_{k_{\rm F}}|^2 = \frac{1}{2}(1+\Delta/\sqrt{\Delta^2+4t_{k_{\rm F}}^2})$ with $t_{k_{\rm F}} = 2t_{pd}\cos(\frac{k_{\rm F}}{2})$; $v_{\rm F}^{\rm Hub}$ and $v_{\rm F}^{\rm dp}$ are Fermi velocities of the Hubbard model and the d-p model, respectively. As seen in Fig.1, the result from the numerical method agrees with that from the g-ology in the weak coupling limit. Remarkably, in the strong coupling region, $U_{\rm eff}$ is fairly renormalized and becomes relatively weak.

In summary, we study the relationship between the d-p model, the t-J model and the Hubbard model in one-dimension using the numerical diagonalization method combined with the Luttinger liquid theory. Analysis for the two parameters v_σ/v_ρ and K_ρ shows that the d-p model can be mapped onto the Hubbard model in the wide parameter region, while it can be described by the t-J model only in the strong coupling limit.

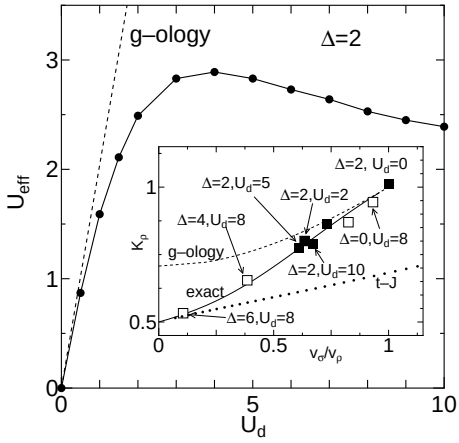

Fig. 1. The effective interaction $U_{\rm eff}$ as a function of U_d from the numerical method (closed circles) and from the g-ology (broken line). Inset shows v_σ/v_ρ vs. K_ρ for the d-p model at U_d=0,1,2,5,10 with $\Delta = 2$ (closed squares) and at Δ=0,1,2,4,6 with $U_d = 8$ (open squares). The result for the t-J model (dotted line) [8] and the exact result for the Hubbard model (solid line) as well as the result from the g-ology (broken line) are also plotted in the inset.

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