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 $v_\sigma$, the charge velocity $v_p$ and the Luttinger liquid parameter $K_p$ 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 \cite{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 \cite{1,2}. Various methods, such as perturbative approach \cite{3} and cluster model calculation \cite{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 \cite{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:

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

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

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

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

$$+ \frac{v_p}{2\pi} \int_0^L dx \left[ K_\rho (\partial_x \theta_\rho)^2 + K_\rho^{-1} (\partial_x \phi_\rho)^2 \right] \quad (2)$$

where $v_\sigma$, $v_p$, $K_\sigma$ and $K_\rho$ 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 $K_\sigma$ is renormalized to unity in the low energy limit.

When we scale the energy of every system by $v_p$, the system is defined by using two parameters: $v_\alpha/v_p$ and $K_\sigma$ [8]. Then we can indicate every system as a point on the $v_\alpha/v_p-K_\sigma$ plane. When two different models are indicated by the same point on the $v_\alpha/v_p-K_\sigma$ 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 $U_\alpha$ in the $d$-$p$ model, the two parameters $v_\alpha/v_p$ and $K_\sigma$ are written by only one $g$-coupling. Eliminating the $g$-coupling, we obtain $K_\sigma = \sqrt{\frac{U}{v_p v_\alpha}}$.

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 $\Delta$, $U_d$ 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 $v_\alpha/v_p$ and $K_\sigma$ by numerical diagonalization of finite size systems using the standard Lanczos algorithm. We use 7-unit cells system with 10 holes for the 1D systems 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, $v_\alpha/v_p$ vs. $K_\sigma$ 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 does 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 $U_{\text{eff}}$ for the $d$-$p$ model. The value of $U_{\text{eff}}$ 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 $v_\alpha/v_p-K_\sigma$ plane (see the inset). In Fig.1, $U_{\text{eff}}$ 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], $U_{\text{eff}}$ is given by $U_{\text{eff}} = \frac{\alpha_{kp}^2}{v_p^T_{\text{Hub}}} v_p^T_{\text{dp}}$, where $\alpha_{kp}^2 = \frac{1}{2}(1 + \Delta/\sqrt{\Delta^2 + 4t_p^2})$ with $t_p = 2t_{pd} \cos (\frac{2\pi}{n})$; $v_p^T_{\text{Hub}}$ and $v_p^T_{\text{dp}}$ 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, $U_{\text{eff}}$ 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 $v_\alpha/v_p$ and $K_\sigma$ 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.

References