Phase diagrams of electronic state  
on One Dimensional d-p Model  

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Abstract  

We investigate the one-dimensional (1D) d-p model, simulating a Cu-O linear chain with strong Coulomb repulsion, by using the numerical diagonalization method. Using the Luttinger liquid theory, we obtained phase diagrams of the ground state on $U_d - U_{pd}$ plane, where $U_d$ and $U_{pd}$ represent on-site interaction at d-sites and the nearest-neighbor interaction between p- and d-sites respectively. In the weak coupling region, they agree with the g-ology; a superconducting phase (SC(I)) is restricted to attractive interaction $U_{pd} < 0$. On the other hand, in the strong coupling region, we found a novel superconducting phase (SC(II)) for repulsive interaction $U_{pd} > |U_d|$ and a insulating state with a charge gap for $U_d > U_{d}^c$ and $U_{pd} > U_{pd}^c$ with critical values $U_{d}^c$ and $U_{pd}^c$ at half-filling. Away from half-filling, another superconducting phase (SC(III)) appears for $U_d >> U_{pd} > 0$; which has been found for $U_d \rightarrow \infty$ in the previous paper [Physica C205 (1993) 170]. An analysis of the spin gap suggests that the SC(I) and SC(II) include the Luther-Emery region (with spin-gap) in part, while the SC(III) belongs to Tomonaga-Luttinger region (without spin-gap) in whole.
I. INTRODUCTION

Since the discovery of copper oxides superconductors, strongly correlated electron systems have been extensively studied. In particular, there is much theoretical interest in the electronic state of the d-p model because of the possible relevance of high-temperature superconductivity[1-12]. In the previous work, the present authors have studied the one-dimensional d-p model, simulating a Cu-O linear chain with infinite intra-site interaction \(U_d\)at the Cu-(d-)sites and the nearest neighbor interaction \(U_{pd}\) between the O-(p-)sites and d-sites, is solved exactly by using the numerical diagonalization method [13]. By assuming the Luttinger liquid relations, the superconducting correlation is found to be dominant compared with the CDW and SDW correlations in the proximity of the phase boundary towards the phase separation. Recently, A.Sudbø et al. showed that the d-p chain with large \(U_{pd}\) exhibits flux quantization with charge 2\(e\) and slow algebraic decay of the singlet superconducting correlation function on oxygen sites [14]. These works demonstrate that the numerical diagonalization studies of finite sizes systems combined the Luttinger liquid theory have supplied us with unambiguous and important information about the complicated electronic systems such as the d-p model [13–17].

In this paper, we study the one-dimensional d-p model by the numerical diagonalization method. To clarify the role of the inter- and intra-site interaction for the electronic structure of d-p model, we turn our attention to \(U_d\) and \(U_{pd}\). In the weak coupling regime, we will take advantage of the weak coupling theory (so-called g-ology) to analyze numerical results. For \(U_{pd} \to \infty\), we find some exact results which agree with numerical results. This paper is organized as follows. In the next section, we define the model Hamiltonian. The Luttinger liquid relation is also discussed. In Sec.3, we present our numerical results of phase diagram on the \(U_d - U_{pd}\) plane by using the Luttinger Liquid relation. We also analyze a spin gap. The conclusion of this work is presented in Sec. 4.

II. MODEL AND LUTTINGER LIQUID RELATION

We consider the following model Hamiltonian for the Cu-O chain:

\[
H = -t \sum_{<ij>,\sigma} (p_{i\sigma}^\dagger d_{j\sigma} + h.c.) + \epsilon_d \sum_{j,\sigma} d_{j\sigma}^\dagger d_{j\sigma} + \epsilon_p \sum_{i,\sigma} p_{i\sigma}^\dagger p_{i\sigma} \\
+ U_d \sum_{j} n_{d_j\uparrow} n_{d_j\downarrow} + U_{pd} \sum_{<ij>,\sigma\sigma'} n_{p_{i\sigma}} n_{d_{j\sigma'}} ,
\]

(1)

where \(d_{j\sigma}^\dagger\) and \(p_{i\sigma}^\dagger\) stand for creation operators of a electron with spin \(\sigma\) in the d-orbital at site \(j\) and of a electron with spin \(\sigma\) in the p-orbital at site \(i\), respectively. \(n_{d\sigma} = d_{j\sigma}^\dagger d_{j\sigma}\) and \(n_{p\sigma} = p_{i\sigma}^\dagger p_{i\sigma}\). \(t\) stands for the transfer energy between the nearest neighbor d- and p-sites, which will be set to be unity \((t=1)\) hereafter in the present study. The atomic energy levels of p- and d-orbitals are given by \(\epsilon_p\) and \(\epsilon_d\), respectively. The charge-transfer energy \(\Delta\) is defined as \(\Delta = \epsilon_p - \epsilon_d\).

The fillingness \(n\) is defined by \(n = N_e/N_u\), where \(N_u\) is the total number of unit cells (each unit cell contains a d- and a p- orbital), \(N_e\) is the total electron number and the Fermi
wave number $k_F$ is given as $k_F = \frac{\pi}{2} n$. In the non-interacting limit with $U_d = U_{pd} = 0$, the hybridized bands are given as

$$E^\pm(k) = \frac{\epsilon_p + \epsilon_d \pm \sqrt{\Delta^2 + 4t^2}}{2}, \quad (2)$$

where $t_k = 2t\cos(k/2)$ and $k = 2\pi l/N_u \quad (l = 0, \pm 1, \pm 2, \ldots)$. Here, $E^+(k)$ and $E^-(k)$ stand p- and d- like bands respectively.

To achieve systematic calculation, we use the periodic boundary condition for $N_e = 4m + 2$ and antiperiodic boundary condition for $N_e = 4m$ with an integer $m$. This choice of the boundary condition removes accidental degeneracies so that the ground state is always a singlet with zero momentum. We numerically diagonalize the Hamiltonian with up to 12 sites (6 unit cells) using the standard Lanczos algorithm. We have calculated the ground state energies per unit cell for different sizes of systems. The relative difference is of order of $10^{-3} \sim 10^{-4}$ for typical values of parameters involved in the model. It indicates that size dependence in the ground state energies is negligible.

The chemical potential $\mu(N_e, N_u)$ is defined by

$$\mu(N_e, N_u) = \frac{E_0(N_e + 1, N_u) - E_0(N_e - 1, N_u)}{2}, \quad (3)$$

where $E_0(N_e, N_u)$ is the ground state energy of a system with $N_u$ unit cells and $N_e$ electrons. When the charge gap vanishes in the thermodynamic limit, the uniform charge susceptibility $\chi_c$ is obtained from

$$\chi_c(N_e, N_u) = \frac{2/N_u}{\mu(N_e + 1, N_u) - \mu(N_e - 1, N_u)}. \quad (4)$$

We will discuss the correlation functions in connection with the Luttinger liquid theory \cite{18-20}. Some relations obtained in the Luttinger liquid theory have been established as universal relations in various one-dimensional models. Some of one-dimensional models can be solved rigorously by the combined use of the Bethe ansatz method with the numerical methods and/or the conformal field theory \cite{21-23}. In these theories, the critical exponents describing the power-law decay of various types of correlation functions have been determined. The bosonization theory on the Tomonaga-Luttinger model \cite{24,25} and the Luther-Emery model \cite{26} and the week coupling renormalization group theory (known as g-ology) also provides us with some rigorous information about the critical exponents \cite{27,28}. In the Luttinger liquid theory, the critical exponents of correlation functions are determined by a single parameter $K_\rho$ for isotropic models in spin space, or more explicitly, some correlation functions in momentum space have singularities as follows:

1) Tomonaga-Luttinger (T-L) regime (without spin-gap)

$$C_{CDW}(k) \quad \text{and} \quad C_{SDW}(k) \sim |k - 2k_F|^{K_\rho} \quad \text{for} \quad k \sim 2k_F, \quad (5.a)$$

$$C_{SS}(k) \sim \begin{cases} |k|^{\frac{1}{K_\rho}} & \text{for} \quad k \sim 0, \\ |k - 2k_F|^{\frac{1}{K_\rho} + K_\rho^{-1}} & \text{for} \quad k \sim 2k_F. \end{cases} \quad (5.b)$$
\[ C_{TS}(k) \sim |k|^{\frac{1}{K_\rho}} \quad \text{for} \quad k \sim 0 \quad , \quad (5.b) \]

2) Luther-Emery (L-E) regime (with spin-gap)

\[ C_{CDW}(k) \sim |k - 2k_F|^{K_\rho - 1} \quad \text{for} \quad k \sim 2k_F \quad , \quad (6.a) \]

\[ C_{SS}(k) \sim |k|^{\frac{1}{K_\rho} - 1} \quad \text{for} \quad k \sim 0 \quad , \quad (6.b) \]

\[ C_{SDW}(k) \quad \text{and} \quad C_{TS}(k) \quad \text{no singularity} \quad , \quad (6.c) \]

where \( C_{CDW}, C_{SDW}, C_{SS} \) and \( C_{TS} \) stand for Charge Density Wave (CDW), Spin Density Wave (SDW), Singlet Superconducting and Triplet Superconducting correlation functions respectively. In the Luther-Emery regime, the spin excitation spectrum has a gap, while in the Tomonaga-Luttinger regime, the spin is gapless. In the T-L regime, spin excitation, the SS and TS correlation have the same critical exponent apart from a logarithmic correction. On the other hand, in the L-E regime, the real space correlation functions of SDW and TS decrease exponentially with distance \( r \). The parameter \( K_\rho \) is related to the charge susceptibility \( \chi_c \) and the charge velocity \( v_c \) by the relations \[ K_\rho = \frac{\pi}{2} v_c \chi_c \quad , \quad (7) \]

\[ v_c = \frac{N_u}{2\pi}(E_1 - E_0) \quad , \quad (8) \]

where \( E_1 - E_0 \) is the lowest charge excitation energy. These relations tell us that the enhancement of \( \chi_c \) leads to increase of absolute value of the critical exponent in the superconducting correlations and decrease of those in the CDW and the SDW correlations.

For the one-dimensional d-p model in the weak coupling regime, T. Matsunami and M. Kimura \[23\] have calculated critical exponents in some correlation functions by the renormalization group analysis. They showed that the d-p model is mapped onto \( g \)-model with spin independent couplings:

\[ g_1 = U_d |\alpha_{k_F}^+|^4 + 4U_{pd} \cos(k_F)|\alpha_{k_F}^-|^2|\alpha_{k_F}^+|^2 \quad (9.a) \]

\[ g_2 = U_d |\alpha_{k_F}^+|^4 + 4U_{pd} |\alpha_{k_F}^-|^2|\alpha_{k_F}^+|^2 \quad (9.b) \]

where \(|\alpha_{k_F}^\pm|^2 = \frac{1}{2}(1 \pm \Delta/\sqrt{\Delta^2 + 4t_k^2})\). The T-L regime corresponds to the case with \( g_1 > 0 \), while the L-E regime corresponds to the case with \( g_1 < 0 \). In the most divergent approximation, the critical exponent \( K_\rho \) is given by \( K_\rho = 1 + (g_1 - 2g_2)/(2\pi v_F) \). The superconducting phase appears in the region of \( g_1 - 2g_2 > 0 \). The transformed phase diagram on the \( U_d-U_{pd} \) plane is shown in Fig.1.

### III. NUMERICAL RESULTS

In the non-interacting case, the critical exponent \( K_\rho \) is unity at any \( \Delta \) and any filling for infinite systems. Numerical results of \( K_\rho \) indicate that \( K_\rho \) is equal to 0.92 for the system of
6-unit cells with 8-electrons and 0.90 for 4-unit cells with 4-electrons at $\Delta = 2$. It suggests that the size dependence of $K_\rho$ are not so large even the 4-units system.

For finite coupling case, the numerical values of $K_\rho$ are 0.86 (0.91), 0.80 (0.81), and 0.77 (0.72) for $U_d = 0.5$, 1.0, and 1.5 respectively in the system of 6-unite cells with 8-electrons at $\Delta = 2$ and $U_{pd} = 0$, where the values in parentheses are obtained by the g-ology. The consistency of both results is good in the weak coupling regime. We expect that our numerical results are sufficiently reliable for the strong coupling regime.

### A. Phase diagram at half-filling

First we investigate the electronic state at half-filling ($n=1$). In Fig.2, we show the contour map for $K_\rho$ on the $U_d - U_{pd}$ plane at $\Delta = 2$ for the system of 6-unit cells with 6-electrons, where the contour lines are drawn by using the spline interpolation. The numerical result agrees with the result of g-ology in the weak coupling regime. It indicates that the superconducting phase (SC(I)) appears in the lower half-plane ($U_{pd} < 0$). The attractive interaction $U_{pd}$ accounts for this superconducting phase. Moreover, in the strong repulsive regime, a novel superconducting phase (SC(II)) appears for the large repulsive interaction $U_{pd}$ in the proximity of the phase separation (PS(II)). These results seem to be similar to that of the one band model (U-V model) obtained in the previous work \[16,17\].

We also evaluate the charge excitation gap $\Delta_C$ by the discontinuity in the chemical potential at half-filling ($n = 1$) and show the region of the insulating state with finite $\Delta_C$ in Fig.2. For large $U_d$ and $U_{pd}$, we find that the charge gap exists on a large area.

In the case of $U_d = \infty$, we have shown that the charge gap $\Delta_C$ is roughly proportional to $\Delta$ for large $\Delta$ \[13\]. By using the least square method, we estimate $\Delta_C$ in more detail as a function of $\Delta$ for $U_d = \infty$ and $U_{pd} = 0$ in Fig.3. It indicates that $\Delta_C$ is roughly proportional to $\Delta - 2t^2/\Delta$ for large values of $\Delta$ \[30\]. The effect of $U_{pd}$ is to increase $\Delta_C$ by roughly $2U_{pd}$, which corresponds to the mean field contribution of $U_{pd}$ to $\Delta_C$. Accounting this effect, we estimate the critical value $U_{pd}^c$ of the metal-insulator transition at $\Delta = 2$. In this case, we get $\Delta_C \sim 1.3$ for $U_{pd} = 0$ and $U_{pd}^c = -\Delta_C/2 \sim -0.7$. This result consists with the numerical result in Fig.2.

On the other hand, in the limit $U_{pd} \to \infty$, the problem becomes very simple and we can get some exact results. The exact wave function of the insulating state is given by

$$|\text{ins} > = |......, 1, 0, 1, 0, 1, 0, 1, 0, 0, 1, 0, ...... >,$$

where each underlined number denotes the number of electrons at a Cu-site and another does the number of electrons at a O-site. The energy of this insulating state is $E_{\text{ins}} = 0$. We also consider a metallic state defined by the first charge-excited state from the insulating state, whose element is presented by

$$|\text{metal} > = |......, 0, 1, 0, 2, 0, b, 0, 1, 0, ...... >,$$

where "2" denotes a doubly occupied site (we call this electron pair dimer) and "h" denotes a hole which can move freely in the d-like band. The energy of the metallic state
is $E_{metal} = U_d + E^-(k = 0)$, where $E^-(k)$ is defined by \( E^-(k = 0) = -1.236 \) in the case of $\Delta = 2$. When $E_{metal} > E_{ins}$, the insulating state is the ground state. Then, the metal-insulator transition occurs at $U_d^c = -E^-(k = 0)$ in the limit $U_{pd} \to \infty$. Our numerical result agrees with the exact result mentioned above.

When $U_d$ is smaller than $U_d^c$, many charge excitation occur; which make dimers and holes. To gain the kinetic energy of holes, dimers are required to aggregate each other. Therefore, the phase separation (PS(II)) occurs such as

$$|\text{PS(II)}> = |\ldots, 2, 0, 2, 0, 2, 0, 2, 0, 1, 0, 0, 1, 0, 0, 0, 0, \ldots >$$

as seen in Fig.2. When $U_d$ becomes large negative value, all of the electron make dimers and the phase separation disappears.

### B. Phase diagram away from half-filling

Next we investigate the electronic state away from half-filling. In Fig.4, we show the phase diagram on the $U_d - U_{pd}$ plane for $n = 4/3$ (8-electrons per 6-unit cells).

In the attractive coupling regime with $U_d < 0$ or $U_{pd} < 0$, the phase diagram is similar to that of half-filling. In the repulsive coupling regime with $U_d > 0$ and $U_{pd} > 0$, the phase separation region (PS(III)) appears instead of the insulator phase seen in half-filling. Furthermore, the new superconducting phase (SC(III)) is also found in the proximate region towards the phase separation. The mechanism of the phase separation PS(II) can be understood as well as that of the half-filling case. However, for PS(III), the mechanism of the phase separation changes completely, since double occupancy of electrons on each Cu-site is prohibited and doped electrons (they make dimers) must sit at O-sites at the cost of the atomic energy difference $\Delta$. In the limit of $U_d$ and $U_{pd} \to \infty$, a schematic wave function of PS(III) is given as

$$|\text{PS(III)}> = |\ldots, 0, 2, 0, 2, 0, 2, 0, 0, 1, 0, 1, 0, 0, 1, 0, \ldots >$$

Again, dimers are aggregated each other to gain the kinetic energy. Of course, for $U_d < 2\Delta$, dimers can sit also on Cu-sites and the above type of the phase separation vanishes. It agree with our numerical result in Fig.4.

### C. Analysis of Spin gap

Finally, we consider the energy gap in the spin excitation spectrum. For weak coupling regime, the boundary line between T-L regime and L-E regime obtained by the gology on the $U_d - U_{pd}$ plane is $g_1 = 0$, i.e., $U_d = -4U_{pd}\cos(k_F)|\alpha_{k_F}^-|^2/|\alpha_{k_F}^+|^2$ (See Fig.1). For a fixed value of $U_{pd}$, the spin gap vanishes at a critical value $U_d^c$. In the weak coupling regime, $U_d^c$ increases with $U_{pd}$ for $n < 1(k_F < \pi/2)$. On the other hand, in the strong coupling limit $U_{pd} \to \infty$, the spin gap vanishes at the critical value $U_d^s = 2E^-(k = 0) = -2.472$ exactly [32]. To presume the boundary line for intermediate coupling regime, we will estimate the
spin gap numerically. The spin excitation energy for a finite size system is obtained from the energy difference between the lowest triplet state and the singlet ground state. We assume that the size dependence of the spin gap as

$$\Delta_S(N_u)^2 = \Delta_S(\infty)^2 + C/N_u^2,$$  \hspace{1cm} (10)

where $\Delta_S(N_u)$ is the spin gap of $N_u$-site system and $C$ is a constant. Sano and Takano [31] have shown that this finite size scaling is successful in the estimation of the spin gap for $t - J - J'$ model. Hereafter, we denote the $\Delta_S(\infty)$ as $\Delta_S$ for simplicity.

We calculated the $\Delta_S$ as a function of $U_d$ under fixed values of $U_{pd}$ using the eq.(8) with the $N_u = 3$ and 6 systems for $n = 4/3$. Fig.5 shows that a large spin gap opens in the region $U_d < \sim -2$. It decreases with increasing $U_d$ and seems to close to zero at $U_d \sim 0$ for $U_{pd} = 0$. We get $U_d^* > -0.5$ for $U_{pd} = 1, 2$ and 3 and $U_d^* \sim -1$ for $U_{pd} = 5$. Because of the finite size effect, it is difficult to determine the $U_d^*$ accurately. The result of the limiting case $U_{pd} \to \infty$ ($U_d^* = -2.472...$), the g-ology and the numerical data for $U_{pd} \leq 5$ suggest that the superconducting phases SC(I) and SC(II) belong to L-E regime in part, while the another superconducting phase SC(III) belong to L-E regime in whole [33].

IV. SUMMARY AND DISCUSSION

In summary, we have numerically diagonalized the one-dimensional $d-p$ model with finite sizes. Paying special attention to the role of $U_{pd}$ in the strong coupling regime, we have calculated the critical exponent of correlation functions, charge gap and spin gap in the systems. On the $U_d - U_{pd}$ plane, the obtained phase diagram consists with the result of g-ology in the weak coupling regime. On the other hand, in the strong coupling regime, more complicated phases are obtained. Using the Luttinger liquid relations, we found the three superconducting phases (SC(I),SC(II) and SC(III)) in the proximity of the phase separation region (PS(I),PS(II) and PS(III) ) respectively. The relation (8) tells us that the enhancement of $\chi_c$ leads to increase of absolute value of the critical exponent in the superconducting correlations and decrease of those in the CDW and the SDW correlations. Thus, unstable phase is accompanied by the superconducting phase.

We speculate that the three types of mechanism of phase separation produce the three types of superconducting phases. The origin of unstable phase PS(I) and the superconducting phase SC(I) are explained by the attractive interaction $U_d$ and/or $U_{pd}$. The large repulsion $U_{pd}$ produces the unstable phase PS(II) and the superconducting phase SC(II) at half-filling (similar phase has been obtained in the 1D $U - V$ model) [16,17]. Away from half-filling, the third unstable phase PS(III) and the superconducting phase SC(III) appear in the region $U_d >> 0$ and $U_{pd} > 0$. Our result suggests that $U_{pd}$ enhances the charge fluctuation which promotes the superconducting correlation. It is noted that the parameter region of SC(III) is corresponding to the charge transfer insulator region at half-filling. We believe that this result have the relevance to the high-temperature superconductivity which is realized by doping to the charge transfer insulator.

The spin gap analysis suggests that the SC(I) and SC(II) phases partially include the Luther-Emery region (with spin-gap). At the same time, the whole SC(III) phase belongs
to Tomonaga-Luttinger liquid (without spin-gap). Generally, in realistic parameter region \( U_d \gg U_{pd} > 0 \), the system belongs to the T-L regime. It is also checked as follows. we investigate the finite size correction to the ground state energy \( E_0 \). The conformal filed theory predicted the size dependence of \( E_0 \) as

\[
E_0/N_u = \epsilon - \frac{\pi c(v_c + v_s)}{6 N_u^2} + o(N_u^{-4}),
\]

where \( v_s \) is the spin velocity and \( c \) is the central charge. If the system is a Luttinger liquid, we should have \( c=1 \). This was shown explicitly for 1D Hubbard model as well as for the 1D-supersymmetric \( t-J \) model. For 1D \( d-p \) model, we calculate the central charge numerically by fitting the ground state energy to the formula of the above equation by taking \( n = 4/3 \) with the system size \( N_u = 3, 6 \). The charge and spin velocity, \( v_c \) and \( v_s \) are estimated for the largest 6-unit cluster. It turned out that \( c \) is almost constant \((0.9 < c < 1.1)\) in the region \( U_{pd} = 0.0 \sim 11.5 \) for \( \Delta = 4 \) and \( U_d = \infty \). It suggests that the 1D \( d-p \) model behaves as the Tomonaga-Luttinger liquid for \( U_d \gg 0 \).

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[30] The charge gap $\Delta_C$ is calculated by the second-order perturbation with respect to $t$ for large $\Delta$. We choose the initial state $|\ldots,0,1,0,1,0,1,0,\ldots>$ and intermediate state of the charge transfer type as $|\ldots,0,1,0,1,1,0,\ldots>.$
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[32] In the limit $U_{pd} \rightarrow \infty$, a ground state for large negative $U_d$ is given as

$$|G.S> = |\ldots,0,2,0,2,0,2,0,0,0,0,0,0,2,0,\ldots>.$$ 

In this case, the kinetic energy of electrons is zero and the ground state energy $E_g$ is $(N_u/2)U_d$ where we set $\epsilon_d = 0$. If the charge excited occur, a dimer brakes up and two electrons can move freely. Thus, the energy $E_{ex}$ of this excitation state is $(N_u/2-1)U_d - 2E_-(k=0)$. When $U_d = -2E_-(k=0)$, the excitation energy is zero and the spin gap vanishes.
[33] For $n = 1$, the $g$-ology shows the boundary line ($g_1 = 0$) is given by $U_d = 0$. Numerical data of $\Delta_S$ seem to suggest that the line borders the left of the boundary of the superconducting phase SC(II) in Fig.2.
Figure Captions

**Fig.1** The phase diagram on the \( U_d - U_{pd} \) plane obtained by the g-ology, where \( g_1 \) is given by eq.(10.a) and \( g_1 - 2g_2 = -(U_d|\alpha_{kF}^+|^4 + 4U_{pd}|\alpha_{kF}^-|^2|\alpha_{kF}^+|^2(2 - \cos(k_F))) \). Note that, in the repulsive regime \( U_d > 0 \) and \( U_{pd} > 0 \), \( (g_1 - 2g_2) \) is always negative and then the superconducting phase does not appear within the g-ogy.

**Fig.2** Contour map for the \( K_\rho \) on the \( U_d - U_{pd} \) plane at \( \Delta = 2 \). We used the 6-unit 6-electron system (\( n=1 \)) and calculated the values of \( K_\rho \) at points of \( U_d = -5, -4, ..., 10 \) for \( U_{pd} = -2, -1, ..., 10 \). The contour lines are plotted by using the spline interpolation.

**Fig.3** The charge gap \( \Delta_C \) as a function of \( \Delta \) for \( n = 1 \). A dotted line represents \( \Delta - 2t^2/\Delta \), which is obtained the second order perturbation method (See Ref. [30]).

**Fig.4** Contour map for the \( K_\rho \) on the \( U_d - U_{pd} \) plane for \( n=4/3 \) at \( \Delta = 2 \). We used the 6-unit 8-electron system.

**Fig.5** The spin gap \( \Delta_S \) as a function of \( U_d \) for \( U_{pd}=0,1,2,3 \) and 50 at \( n = 4/3 \).