Quantum Monte Carlo Study of the Hubbard Ladder

Yasuko Munehisa

Faculty of Engineering, Yamanashi University
Kofu, Yamanashi, 400 Japan

Abstract

We present quantum Monte Carlo results for the Hubbard model on a ladder using the re-structuring method which employ eigenstates of two-site system on a rung to construct a complete set.

From technical reasons we concentrate on the case in which the hopping along the leg is much less than the hopping on the rung. We observe the ground state of the half-filled system is made of singlet-like states described in this paper and its first excited state contains one triplet rung. When the system is lightly doped states composed of an electron and a hole appear on some rungs. We find very few hole-pairing on the rung upon doping up to the quarter-filled case.
Section 1 Introduction

Lately strongly correlated systems of electrons on ladders with two or more legs have become quite intriguing from both theoretical and experimental points of view. Various models are numerically investigated by means of exact diagonalization \[1, 2, 3\] and renormalization group approaches \[4, 5, 6\]. Active studies on the quantum spin ladder systems, which correspond to the half-filled fermionic ladders with infinite Coulomb repulsion, are also stimulative \[7\]. Among their results, especially interesting are spin gaps, ground states as well as excited states of the systems and formation of the hole-pair bound state. Presence of spin gaps is reported for several spin systems and for fermion systems such as the \(t-J-t'-J'\) model on a single ladder (two coupled chains) studied in Ref. \[1\], the \(t-J\) model on a single ladder \[2\] and on multi-ladders with even number of coupled chains \[3\], and the two-chain Hubbard Model \[4\]. In Refs. \[1, 2\] emergence of the hole-pairing upon doping, which would indicate the high \(T_c\) superconductivity, is also claimed.

Quantum Monte Carlo techniques based on the Suzuki-Trotter formula, which prove useful for many spin systems \[8, 9\], are difficult to apply to the fermion systems because of the negative sign problem except for those on a single chain \[10\]. Usually studies on the two-dimensional fermion systems have been done after integrating the fermionic degrees of freedom \[11, 12, 13, 14\]. Yet it would be desirable to simulate such electron systems keeping fermionic degrees of freedom and vividly observe how electrons and holes behave on ladders. Recently dynamical properties of the half-filled Hubbard ladder are studied by Scalapino et al. \[6\] using grand canonical quantum Monte Carlo calculations with maximum entropy analytic continuation. In this paper we formulate the Hubbard Model on a single ladder, with or without doping, applying the re-structuring approach \[9\]. Here we employ a complete set composed of sixteen eigenstates of electrons sitting two ends of a rung, including the double occupancy (See the Table). Although our simulations are limited to the case in which the hopping along each chain is much weaker compared to the hopping between sites on a rung, we obtain there Monte Carlo results with satisfactory statistical accuracy on the system’s energy as well as what we call state distribution in this paper, which is defined in section 2, sorted according to values of the third
component of the total spin. At half-filling we observe that in the ground state the
singlet-like state, the ninth eigenstate in the Table, is sitting on all rungs of the
system and the first excited state has a clear gap because of the triplet eigenstate
which appears on one rung of the system. Upon doping the lowest lying state we have
observed contains not a hole-pair eigenstate but some of one-electron eigenstates in
addition to the singlet-like eigenstate. Here we see no spin gap. All our results are
compatible with the corresponding ones in Ref. [4]. For the half-filled ladder our
observations are also in agreement with the \( t-J \) results in Ref. [2].

In the next section we sketch the model and the method used in this paper. In
section 3 the Monte Carlo results are presented. The final section is devoted to the
summary.

**Section 2 the Model**

The model we study is the Hubbard ladder with two legs and \( N \) rungs. Its
Hamiltonian is

\[
\mathcal{H} = -t_c \sum_{i=1}^{N-1} \sum_{\sigma=\uparrow,\downarrow} \left[ (c_{1\sigma}^\dagger(i)c_{1\sigma}(i+1) + c_{2\sigma}^\dagger(i)c_{2\sigma}(i+1)) + \text{H.c.} \right] \\
- t_r \sum_{i=1}^N \sum_{\sigma=\uparrow,\downarrow} \left[ c_{1\sigma}^\dagger(i)c_{2\sigma}(i) + \text{H.c.} \right] + U \sum_{j=1}^2 \sum_{i=1}^N n_{j\uparrow}(i)n_{j\downarrow}(i)
\]

(1)

where \( c_{j\sigma}^\dagger(i) \) is the creation operator for an electron of spin \( \sigma \) on the \( i \)-th rung of the
\( j \)-th leg of the ladder and \( n_{j\sigma}(i) = c_{j\sigma}^\dagger(i)c_{j\sigma}(i) \). From technical reasons we employ
an open boundary condition with a hole at each edge of the legs (See Fig. 1). The
partition function \( Z \) is given by

\[
Z = \text{tr}\{e^{-\beta(\mathcal{H}-\mu \mathcal{N})}\}, \tag{2}
\]

with the inverse temperature \( \beta \), the chemical potential \( \mu \) and

\[
\mathcal{N} = \sum_{j=1}^2 \sum_{i=1}^N \sum_{\sigma=\uparrow,\downarrow} n_{j\sigma}(i) \tag{3}
\]

Let us describe our re-structuring approach briefly. In our representation the
states of the system are given by

\[ | \alpha \rangle = |a_1, a_2, a_3, ..., a_N \rangle, \quad | \beta \rangle = |b_1, b_2, b_3, ..., b_N \rangle, \]
Note that the Hamiltonian $H$ along the chain is noted that $a_m$ and $b_m$ may differ by sign for the same occupants on the two sites of the $m$-th rung because the left site on the rung along the chain $A$ is the right site along the chain $B$ and vice versa.

Then we divide the above Hamiltonian (1) with even $N$ into four parts,

\[ H_{A1} = \frac{1}{4} H_R - t_c \sum_{k=1}^{N/2} \sum_{\sigma=\uparrow,\downarrow} \left[ c_{1\sigma}^\dagger(2k-1)c_{1\sigma}(2k) + \text{H.c.} \right], \]

\[ H_{A2} = \frac{1}{4} H_R - t_c \sum_{k=1}^{N/2-1} \sum_{\sigma=\uparrow,\downarrow} \left[ c_{2\sigma}(2k)c_{2\sigma}(2k+1) + \text{H.c.} \right], \]

\[ H_{B1} = \frac{1}{4} H_R - t_c \sum_{k=1}^{N/2} \sum_{\sigma=\uparrow,\downarrow} \left[ c_{\sigma}^\dagger(2k-1)c_{\sigma}(2k) + \text{H.c.} \right], \]

\[ H_{B2} = \frac{1}{4} H_R - t_c \sum_{k=1}^{N/2-1} \sum_{\sigma=\uparrow,\downarrow} \left[ c_{\sigma}^\dagger(2k)c_{\sigma}(2k+1) + \text{H.c.} \right], \] (4)

where

\[ H_R \equiv -t_r \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} \left[ c_{1\sigma}^\dagger(i)c_{2\sigma}(i) + \text{H.c.} \right] + U \sum_{j=1}^{2} \sum_{i=1}^{N} n_{j\uparrow}(i)n_{j\downarrow}(i). \]

Note that the Hamiltonian $H_{A1} + H_{A2} (H_{B1} + H_{B2})$ describes the Hubbard chain $A(B)$ with the hopping parameters $t_c$ and $t_r/2$ and the Coulomb repulsion $U/2$.

Applying the Suzuki-Trotter formula we obtain

\[ Z_n = \text{tr} \left\{ e^{-\beta(H_{A1}-\mu'N)/n} e^{-\beta(H_{A2}-\mu'N)/n} e^{-\beta(H_{B1}-\mu'N)/n} e^{-\beta(H_{B2}-\mu'N)/n} \right\} \]

\[ = \sum_{\langle \alpha_0 \rangle} \cdots \sum_{\langle \alpha_{2n-1} \rangle} \sum_{\langle \beta_0 \rangle} \cdots \sum_{\langle \beta_{2n-1} \rangle} \langle \alpha_0 | e^{-\beta(H_{A1}-\mu'N)/n} | \alpha_1 \rangle \langle \alpha_1 | e^{-\beta(H_{A2}-\mu'N)/n} | \alpha_2 \rangle \langle \alpha_2 | \beta_0 \rangle \]

\[ \langle \beta_0 | e^{-\beta(H_{B1}-\mu'N)/n} | \beta_1 \rangle \langle \beta_1 | e^{-\beta(H_{B2}-\mu'N)/n} | \beta_2 \rangle \langle \beta_2 | \alpha_3 \rangle \]

\[ : \]

\[ \langle \alpha_{2n-2} | e^{-\beta(H_{A1}-\mu'N)/n} | \alpha_{2n-1} \rangle \langle \alpha_{2n-1} | e^{-\beta(H_{A2}-\mu'N)/n} | \alpha_0 \rangle \langle \alpha_0 | \beta_{2n-2} \rangle \]

\[ \langle \beta_{2n-2} | e^{-\beta(H_{B1}-\mu'N)/n} | \beta_{2n-1} \rangle \langle \beta_{2n-1} | e^{-\beta(H_{B2}-\mu'N)/n} | \beta_0 \rangle \langle \beta_0 | \alpha_0 \rangle, \] (5)

where $n$ is the Trotter number and $\mu' \equiv \mu/4$. 
For later use let us introduce a hermitian operator $O$ defined by

$$
O = \sum_{\{\alpha\}} | \alpha \rangle C_\alpha \langle \alpha |
$$

where $C_\alpha$ denotes a real number. Since

$$
\langle \alpha_0 | O e^{-\beta(HA_1-\mu'N)/n} | \alpha_1 \rangle = \sum_{\{\alpha\}} \langle \alpha_0 | \alpha \rangle C_\alpha \langle \alpha | e^{-\beta(HA_1-\mu'N)/n} | \alpha_1 \rangle
$$

$$
= C_{\alpha_0} \langle \alpha_0 | e^{-\beta(HA_1-\mu'N)/n} | \alpha_1 \rangle,
$$

we obtain

$$
\text{tr}\{O e^{-\beta(H-\mu N)}\}
$$

$$
= \lim_{n \to \infty} \text{tr}\{O [e^{-\beta(HA_1-\mu'N)/n} e^{-\beta(HA_2-\mu'N)/n} e^{-\beta(HB_1-\mu'N)/n} e^{-\beta(HB_2-\mu'N)/n}]^n]\}
$$

$$
= \lim_{n \to \infty} \sum_{\{\alpha_0\}} \sum_{\{\alpha_{2n-1}\}} \sum_{\{\beta_{2n-1}\}} C_{\alpha_0} \times
\langle \alpha_0 | e^{-\beta(HA_1-\mu'N)/n} | \alpha_1 \rangle \langle \alpha_1 | e^{-\beta(HA_2-\mu'N)/n} | \alpha_2 \rangle \langle \alpha_2 | \beta_0 \rangle
\langle \beta_0 | e^{-\beta(HB_1-\mu'N)/n} | \beta_1 \rangle \langle \beta_1 | e^{-\beta(HB_2-\mu'N)/n} | \beta_2 \rangle \langle \beta_2 | \alpha_3 \rangle
\vdots
\langle \alpha_{2n-2} | e^{-\beta(HA_1-\mu'N)/n} | \alpha_{2n-1} \rangle \langle \alpha_{2n-1} | e^{-\beta(HA_2-\mu'N)/n} | \alpha_0 \rangle \langle \alpha_0 | \beta_{2n-2} \rangle
\langle \beta_{2n-2} | e^{-\beta(HB_1-\mu'N)/n} | \beta_{2n-1} \rangle \langle \beta_{2n-1} | e^{-\beta(HB_2-\mu'N)/n} | \beta_0 \rangle \langle \beta_0 | \alpha_0 \rangle.
$$

(7)

With the partition function $Z_n$ in (3) we simulate the system on the $N \times 4n$ checkerboard with the number of rungs $N$ up to 32 and the Trotter number $n = 16$ and 24. We obtain one new configuration by all possible local updates and global updates in both the spacial and the Trotter directions using techniques in Ref. [15]. We do not fix the number of electrons on a ladder so that the system would come to the thermal equilibrium swiftly.

Since one is not free from the negative sign problem with the formulations stated above, our study is limited to the parameter regions where the cancellation is not serious. To check it we measure the $r$ ratio,

$$
r = \frac{Z_+ - Z_-}{Z_+ + Z_-},
$$

(8)

where $Z_+(Z_-)$ is the number of configurations with positive (negative) weight. We refer to the part that survived the cancellation as the whole configurations.
physical quantity \( \langle A \rangle \) is calculated by

\[
\langle A \rangle = \frac{A_+ - A_-}{Z_+ - Z_-},
\]

(9)

with contributions from positively (negatively) signed configurations \( A_+ \) (\( A_- \)).

The physical quantities we measure are the hole doping \( \delta \) and the system’s energy \( \langle E \rangle \). We obtain \( \delta \) by

\[
\delta = 1 - \frac{\langle N_e \rangle}{2N},
\]

(10)

\( N_e \) being the number of electrons on the ladder. As for the system’s energy, we measure the quantity \( G \equiv E - \mu N_e \) using the standard technique in the quantum Monte Carlo method and obtain \( \langle E \rangle \) by

\[
\langle E \rangle = \langle G + \mu N_e \rangle.
\]

(11)

In order to shed some light on the system’s wave function we also measure the frequency distribution for every eigenstate in the Table, which is the ratio of the number of rungs on a ladder occupied by that eigenstate to the total number of rungs \( N \) and will be called state distribution. It should be noted this quantity is physical too, because the operator to represent the number of each eigenstate on a ladder is expressed by \( (\mathbb{E}) \). For the hole-pair eigenstate, for example, \( C_\alpha \) in \( (\mathbb{E}) \) is zero if none of \( a_i \)'s in the state \( |\alpha\rangle \) are equal to \( |00\rangle \), is one if \( |\alpha\rangle \) contains one and only one \( |00\rangle \) state among its \( a_i \)'s, and so on.

The third component of the total spin of the system, \( S_z \), is another measurable quantity in this formalism. We will see \( S_z \) is very helpful to study system’s energy spectra.

**Section 3 Results**

Now let us show our Monte Carlo results. Typically first ten thousand configurations are discarded for the thermalization and next a few ten thousand configurations are used for the measurement. Throughout the rest of the paper we take \( t_r = 1 \) and, unless stated otherwise, \( U = 6 \).

We concentrate on the case \( t_c \ll 1 \), where the negative sign problem is not so serious. In this case the ground state at half-filling is expected to be made of singlet
rungs. We simulate the system with \( t_c = 0.1 \), namely \( t_r/t_c = 10 \). In Fig. 2 we plot the state distribution on the \( N = 16 \) ladder as a function of \( \beta \), with values of \( \mu \) adjusted to ensure \( \delta \) small enough to realize the half-filled system. Values of the \( r \) ratio are between 0.58 and 1 for these \( \beta \) and \( \mu \). We see the mixed state (\( \lambda_1 \)), the ninth state in the Table, dominates as \( \beta \) increases to become almost 100% of the whole at \( \beta = 15 \). We also observe \( S_z = 0 \) for 99.6% of the whole configurations at this value of \( \beta \). These results indicate we can treat the state at \( \beta = 15 \) as the system’s ground state. The ratio of the singlet component in the ground state is \( 2u_1^2 \) (\( u_1 \) being defined in the Table Caption), which is about 0.92 for \( U = 6 \) and goes to 1 as \( U \) goes to infinity. We refer to this state as the singlet-like state.

In order to study the excitation spectrum at half-filling, we examine the value of \( S_z \) at \( \beta = 13 \) and \( \delta \sim 0 \), where we find that 98.85% of the whole configurations has \( S_z = 0 \) and 0.59 (0.56)% has \( S_z = 1 \) (−1). The state distribution with non-zero \( S_z \) shows that 6.235 (6.244)% of the \( S_z = 1 \) (−1) part is occupied by the sixth (the eleventh) eigenstate, namely by the triplet(1) (the triplet(−1)) state, the rest being occupied by the singlet-like state. These results strongly indicate that about 1.73% of the whole configurations at \( \beta = 13 \) (including the triplet(0) state which should be about 0.58/98.85 of the \( S_z = 0 \) part) is in an excited mode in which one of the \( N(= 16) \) singlet-like rungs in the ground state turns to the triplet one.

By measuring system’s energies of \( S_z = 0 \), 1 and −1 configurations separately we estimate the energy of this excited state, \( E_1 \), from energies of \( S_z = \pm 1 \) configurations and the ground state energy, \( E_0 \), from energy of \( S_z = 0 \) configurations and \( E_1 \). The energy gap \( E_1 - E_0 \) thus obtained is 0.608 ± 0.002, which is quite close to the difference of eigenvalues \( -2\mu - (-\lambda_1) \simeq 0.606 \).

Similar results are obtained on the ladders with different \( N \). Figure 3 plots the energy gap as a function of \( 1/N \). The results for \( t_c = 0.1 \) up to \( N = 32 \) indicate that the energy gap of this excitation mode, namely the spin gap, remains finite in the thermodynamic limit. Results for \( t_c = 0.2 \) up to \( N = 16 \) and for \( t_c = 0.3 \) and \( N = 8 \) plotted together also support the presence of the gap. Measurement of the gap for larger ladders or larger \( t_c \) was unsuccessful because of the decreasing value of \( r \).
Let us see what happens to the system upon doping, which is done by reducing the value of the chemical potential. More cancellation due to the negative sign problem is observed at intermediate values of $\delta$, yet it is not difficult to obtain statistically meaningful results except for the region near $\delta \sim 0.25$. Fig. 4 shows state distribution at $\beta = 13$ for various values of $\delta$. Here we observe, from half-filling ($\delta = 0$) to nearly quarter-filling ($\delta = 0.5$), the singlet-like state diminishes as $\delta$ grows and the ratio of the one-electron states increases instead. As is plotted together, only the second and the fourth eigenstate, which are even in the site-exchange, appear as the one-electron states. Note that for $\delta < 0.5$ we see very few hole-pairs on rungs. For $\delta > 0.5$ the distribution changes drastically because the number of holes exceeds the number of electrons, but we pursue this region no longer.

Since we do not fix the number of electrons in the updating processes, configurations with different numbers of electrons can emerge in the simulation even when the chemical potential is adjusted to result in integer values of $\langle N_e \rangle$. In simulations at half-filling this causes no problem because we observe that for large values of $\beta$ very few configurations have $N_e$ different from $2N$. For the doped system, however, we find the contamination is serious at any available $\beta$. In search for the ground state of the system with $2(N - N_0)$ electrons ($N_0 = 1, 2, \cdots$), we therefore have to discard configurations with $N_e \neq 2(N - N_0)$ in the measurements of the state distribution and the energy spectra at the cost of statistical accuracy. The results thus obtained at $\beta = 9$ for the $N = 16$ ladder with $N_0 = 1$ (i.e. for $\delta = 0.0625$) show us that the ratio of the second, the fourth and the ninth eigenstates in the Table (namely the even one-electron state with up spin, with down spin and the singlet-like state) is about $1/16 : 1/16 : 7/8$ for $S_z = 0$ whereas it is $1/8 : 0 : 7/8 (0 : 1/8 : 7/8)$ for $S_z = 1 (-1)$ and contributions from other states are negligible. Consistently with these results, we do not see any energy gap here; the energies are $\langle E \rangle = -10.69 \pm 0.01, -10.67 \pm 0.02$ and $-10.63 \pm 0.02$ for $S_z = 0, 1$ and $-1$, respectively. It should be noted that these values of $\langle E \rangle$ are smaller than $-10.48$, the value with $t_c = 0$ directly calculated from the eigenvalues of the rungs. We also simulate the $N = 32$ ladder with $N_0 = 2$ at $\beta = 9$ and obtain statistically meaningful results on $S_z = 0, -1$ configurations which suggest that the system has
two (one) even one-electron rungs with up spin, two (three) even one-electron rungs with down spin and 28 singlet-like rungs for $S_z = 0$ ($-1$). The energy on this ladder is $\langle E \rangle = -21.30 \pm 0.05$ ($-21.29 \pm 0.07$) for $S_z = 0$ ($-1$), which indicates that the finite-size effect is small.

Section 4 Summary

In this paper we carry out Monte Carlo simulations of the Hubbard model on a ladder by the re-structuring method we proposed in Ref. [9]. Having constructed the complete set in the Suzuki-Trotter formula from the eigenstates for two electrons on a rung, our method works satisfactorily when the hopping along the chain is much weaker compared to the hopping within rungs. At half-filling we obtain numerical results which indicate that the ground state is of singlet-like eigenstate only, the first excited state contains one triplet rung besides singlet-like ones and the spin gap persists in the thermodynamic limit. When the system is doped we observe that on some rungs the eigenstates which contain one electron and one hole appear instead of the singlet-like ones seen in the half-filled case.

We did not observe any hole-pair formation in the parameter region we could study. Whether the doped system realizes hole-pairing or not on ladders with larger hopping parameters along the chain is an open question so far. Although it seems difficult to obtain data for such ladders straightforwardly, detailed study on the system's wave function which is possible in this formulation would be useful to understand properties of the system.

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Table Caption

Eigenstates, eigenvalues for the partial Hamiltonian of two-site system on one rung,

$$h - \mu n_e \equiv -t_r \sum_{\sigma=\uparrow,\downarrow} (c_1^\dagger c_2\sigma + H.c.) + U \sum_{j=1}^{2} n_{j\uparrow} n_{j\downarrow} - \mu \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{2} n_{j\sigma},$$

with $t_r$ and $U$ in the Hamiltonian (1) and the chemical potential $\mu$ in (2), and their names used in this study.

$|S_l, S_r\rangle$ in the Table represents the state on a rung whose left (right) site is occupied by $S_l(S_r)$, where $S_l(S_r)$ is either 0 (hole), $\uparrow$ (an up-spin electron), $\downarrow$ (a down-spin electron) or $\uparrow\downarrow$ (an electron pair).

Parameters $u_1$ and $u_2$ and eigenvalues $\lambda_1$ and $\lambda_2$ in the ninth and the tenth eigenstates are defined as

$$u_1 \equiv \frac{1}{2} \left[ \frac{1 + \frac{U}{\sqrt{U^2 + 16t_r^2}}}{2} \right],$$

$$u_2 \equiv \frac{1}{2} \left[ \frac{1 - \frac{U}{\sqrt{U^2 + 16t_r^2}}}{2} \right],$$

$$\lambda_1 \equiv \frac{1}{2} (4\mu - U + \sqrt{U^2 + 16t_r^2}),$$

$$\lambda_2 \equiv \frac{1}{2} (4\mu - U - \sqrt{U^2 + 16t_r^2}).$$

Figure Captions

Figure 1

A schema to show the ladder we study. The open circle on each edge of the ladder denotes a hole. The thin solid (dashed) line is to indicate the chain $A$ ($B$) described in section 2.
Figure 2
The state distribution $R$ for the $t_r = 1$, $t_c = 0.1$, $U = 6$ and $N = 16$ Hubbard ladder as a function of $\beta$ with $|\delta| < 7 \times 10^{-3}$. The Trotter number $n$ is 16. The open circles, right triangles, left triangles and down triangles denote the ratios for the first, eighth, tenth and sixteenth eigenstate in the Table, respectively. The filled diamonds denote the ninth eigenstate which is referred as singlet-like state in the paper. The open squares (asterisks) denote the sum of the contributions from the second to the fifth (from the twelfth to the fifteenth) eigenstates, which is the contribution of all one-electron (three-electron) states. The open diamonds denote the contribution of all triplet states, namely the sixth, the seventh and the eleventh eigenstates. Statistical errors are within symbols.

Figure 3
The spin gap $\Delta \equiv E_1 - E_0$ at half-filling with $t_r = 1$ and $U = 6$ as a function of $1/N$, $N$ being the number of rungs of the ladder. The system’s energy defined by (11) is measured for the ground state which is made of $N$ singlet-like rungs ($E_0$) and for the excited state where $(N - 1)$ rungs are singlet-like and one rung is occupied by the triplet(1) (or triplet(-1)) eigenstate ($E_1$). The open circles denote results for $t_c = 0.1$, $\beta = 13$ and $n = 16$, the open square for $t_c = 0.1$, $\beta = 13$ and $n = 24$, the open triangles for $t_c = 0.2$, $\beta = 9$ and $n = 16$, the open diamond for $t_c = 0.3$, $\beta = 7$ and $n = 16$. Statistical errors are within symbols except for the $t_c = 0.3$ datum.

Figure 4
The state distribution $R$ for the $t_c = 0.1$, $U = 6$ and $N = 16$ Hubbard ladder as a function of $\delta$ with $\beta = 13$. The Trotter number $n$ is 16. The open circles, filled diamonds, open squares and open diamonds denote contributions of the hole-pair state, the singlet-like state, all one-electron states and all the triplet states, respectively. Contribution from the even one-electron states, namely from the second and the fourth eigenstates, is also plotted by the crosses. The open triangles are the contribution of the rest. Statistical errors are within symbols.
| No. | eigenstate | eigenvalue | Name                              |
|-----|------------|------------|-----------------------------------|
| 1   | | 00⟩       | 0         | hole-pair                         |
| 2   | \( \frac{1}{\sqrt{2}}(|↑ 0⟩ + | 0 ↑⟩) \) | \(-(μ + t_r)\) | one electron (up,even)            |
| 3   | \( \frac{1}{\sqrt{2}}(|↑ 0⟩ - | 0 ↑⟩) \) | \(-(μ - t_r)\) | one electron (up,odd)             |
| 4   | \( \frac{1}{\sqrt{2}}(|↓ 0⟩ + | 0 ↓⟩) \) | \(-(μ + t_r)\) | one electron (down,even)          |
| 5   | \( \frac{1}{\sqrt{2}}(|↓ 0⟩ - | 0 ↓⟩) \) | \(-(μ - t_r)\) | one electron (down,odd)           |
| 6   | | ↑↑⟩       | \(-2\mu\) | triplet (1)                       |
| 7   | \( \frac{1}{\sqrt{2}}(|↑↓⟩ + |↓↑⟩) \) | \(-2\mu\) | triplet (0)                       |
| 8   | \( \frac{1}{\sqrt{2}}(|↕ 0⟩ - | 0 ⬇⟩) \) | \(-(2\mu - U)\) | an electron-pair and a hole       |
| 9   | \( u_1(|↑ ↓⟩ - | ↓ ↑⟩) + u_2(|↓ 0⟩ + | 0 ↓⟩) \) | \(-\lambda_1\) | mixed state (\(\lambda_1\))      |
| 10  | \( u_2(|↑ ↓⟩ - | ↓ ↑⟩) - u_1(|↓ 0⟩ + | 0 ↓⟩) \) | \(-\lambda_2\) | mixed state (\(\lambda_2\))      |
| 11  | | ↓↓⟩       | \(-2\mu\) | triplet (−1)                      |
| 12  | \( \frac{1}{\sqrt{2}}(|↑↑⟩ + |↑↓⟩) \) | \(-(3\mu - U - t_r)\) | three electrons (up,even)         |
| 13  | \( \frac{1}{\sqrt{2}}(|↑↓⟩ - |↑↑⟩) \) | \(-(3\mu - U + t_r)\) | three electrons (up,odd)          |
| 14  | \( \frac{1}{\sqrt{2}}(|↓↑⟩ + |↓↓⟩) \) | \(-(3\mu - U - t_r)\) | three electrons (down,even)       |
| 15  | \( \frac{1}{\sqrt{2}}(|↓↓⟩ - |↓↑⟩) \) | \(-(3\mu - U + t_r)\) | three electrons (down,odd)        |
| 16  | | ⬇⬇⟩       | \(-(4\mu - 2U)\) | electron-pairs                     |
Fig. 1
Fig. 2
