Eliminating interactions between non-neighboring qubits in the preparation of cluster states in quantum molecules

Guo-Ping Guo,* Xiao-Jie Hao, Tao Tu,† Zhi-Cheng Zhu, and Guang-Can Guo

Key Laboratory of Quantum Information, University of Science and Technology of China,
Chinese Academy of Sciences, Hefei 230026, People’s Republic of China

(Dated: April 1, 2022)

We propose a scheme to eliminate the effect of non-nearest-neighbor qubits in preparing cluster state with double-dot molecules. As the interaction Hamiltonians between qubits are Ising-model and mutually commute, we can get positive and negative effective interactions between qubits to cancel the effect of non-nearest-neighbor qubits by properly changing the electron charge states of each quantum dot molecule. The total time spent on the present multi-step cluster state preparation scheme is only doubled for one-dimensional qubit chain and tripled for two-dimensional qubit array comparing with the time spent on previous protocol leaving out the non-nearest-neighbor interactions.

PACS numbers: 03.67.Mn, 03.67.Lx, 73.23.Hk

Keywords: non-neighboring qubits, cluster state, double-dot quantum molecule

Semiconductor quantum dot (QD) is believed to be one of the most promising systems for quantum information processing [1, 2]. Recently, quantum molecule, formed by coupled double quantum dots, has attracted many interests. A lot of experimental [3, 4, 5, 6] and theoretical [7, 8, 9] work has been done on the two-electron states of the double-dot molecule. It is argued that by encoding in singlet and triplet states of quantum molecule, qubits can be protected from low-frequency noise and the dominant source of decoherence from hyperfine interactions can be suppressed [3, 10, 11, 12, 13, 14]. Universal quantum gates and a fault-tolerant architecture for quantum computation have been proposed for these qubits encoding in the two-electron states of quantum molecule [8, 15]. In the reference [16], we proposed a one-step scheme to prepare large cluster states with QD molecules, which can act as a general source for one-way quantum computation [17]. As in most of the solid-state quantum computation protocols, only interactions between neighboring qubits are considered in this scheme. However, all these protocols directly explore the long range Coulomb interaction of the electrons between different molecules [8, 15, 16]. There are unwanted small interactions between non-nearest-neighbor molecules. Generally, this kind of unwanted interactions between non-nearest-neighbor qubits will act as an additional decoherence source and affect the proposed quantum processing fidelity, for example, the fidelity of prepared states or quantum gates. It is well known that there is a decoupling and refocusing technique in standard nuclear-magnetic-resonance field [18, 19]. Many works explores this idea to simulate quantum dynamics [20], construct universal quantum computation with some Hamiltonian forms [21]. Here we focused on a particular physical system of double-dot quantum molecules, and propose an efficient scheme to eliminate the effect of the interactions between non-nearest-neighbor qubits in the preparation of cluster state with QD molecules. By properly changing the electron charge states in each QD molecule, the effective interactions between qubits can be switched as positive, zero and negative. As the interaction Hamiltonians between qubits are all Ising-model and mutually commute, the effect of non-nearest-neighbor qubits interactions can be efficiently canceled through a multi-step preparation process. In addition, the total time for the present multi-step cluster state preparation scheme is only several times comparing with the time of previous protocol neglecting the non-nearest-neighbor interactions.

For each double-dot quantum molecule, the notation \((n_u, n_l)\) can be used to indicate the number of electrons in the upper and lower QDs. Define a bias parameter \(\Delta\) to represent the potential offset between the three possible charge states of each molecule \((0, 2), (1, 1)\) and \((2, 0)\). We can adiabatically sweep \(\Delta\) of each molecule by tuning gate-bias voltages of each molecule or applying an external electrical field. The charge states \((0, 2), (1, 1)\) and \((2, 0)\) respectively correspond to the case of \(\Delta = E_c, 0\) and \(-E_c\) as shown in Fig.1 [3, 7].

For the charge state \((1, 1)\), there are four spin states: \(|S\rangle = (|↑↓⟩ - |↓↑⟩)/\sqrt{2}, |T\rangle = (|↑↑⟩ + |↓↓⟩)/\sqrt{2}, |T_+\rangle = |↑↑⟩, and |T_-⟩ = |↓↓⟩\). The two triplet states \(|T_\pm\rangle\) can be largely separated from the singlet state \(|S\rangle\) and triplet state \(|T\rangle\) by Zeeman splitting, which enables us to exclude them in the following [8]. The qubit can be encoded in the near-degenerate \((1, 1)\) charge states \(|T\rangle = |0\rangle\) and \(|S\rangle = |1\rangle\), which are separated due to weak tunneling between the two dots of each molecule. As a result of Pauli blockade, only the singlet state \(|S\rangle\) can be tuned into charge state \((0, 2)\) or \((2, 0)\) by sweeping \(\Delta\). The triplet state \(|T\rangle\) will be kept in the charge state \((1, 1)\) in the processing of sweeping.

---

*Electronic address: gpguo@ustc.edu.cn
†Electronic address: tutao@ustc.edu.cn
As the Coulomb interaction between the two electrons inside each molecule can be excluded, we only consider the interaction between electrons of different molecules [15, 22]. For any two quantum molecules, different charge states can result in different Coulomb interactions as shown in Fig.2. When the bias voltage of two molecules are both set on $\Delta = 0$, these two molecules can be both in the charge state $(1, 1)$ (see Fig.2(a)). In this case, the Coulomb interaction energy between them can be directly written as:

$$E_0(a, b) = \frac{1}{4\pi\epsilon} \left( \frac{2\epsilon^2}{b} + \frac{2\epsilon^2}{\sqrt{a^2 + b^2}} \right). \quad (1)$$

Here and in the following text, $\epsilon$ is dielectric constant of GaAs, $a$ is the distance between the two QDs in one molecule and $b$ is the distance between the two molecules. When one of two molecules remains in the charge state $(1, 1)$ by keeping its $\Delta = 0$ and the other molecule is changed to other charge state $(0, 2)$ or $(2, 0)$ by sweeping its $\Delta$ to $E_c$ or $-E_c$, the interaction between them can remain in the form $E_0(a, b)$ as shown in Fig.2(b). When the two molecules are both in the charge state $(0, 2)$ or $(2, 0)$ by tuning their bias parameter $\Delta$, the interaction energy between them can then be written as $E_1(a, b) = \frac{1}{4\pi\epsilon} \frac{4\epsilon^2}{\sqrt{a^2 + b^2}}$ as shown in Fig.2(c). As only the singlet state $|S\rangle$ can be tuned into charge state $(0, 2)$ or $(2, 0)$ and the triplet state $|T\rangle$ will be kept in the charge state $(1, 1)$ by sweeping $\Delta$, this interaction Hamiltonian between two neighboring qubits can be written in the basis $|TT\rangle$, $|TS\rangle$, $|ST\rangle$ and $|SS\rangle$ as [16]:

$$H_+(a, b) = \text{diag} \{ E_0(a, b), E_0(a, b), E_0(a, b), E_1(a, b) \}. \quad (2)$$

Taking the interaction energy $E_0(a, b)$ as zero point of the effective interaction energy between two qubits, we can write the interaction Hamiltonian as:

$$H_+(a, b) = H_0(a, b) + H'_+(a, b), \quad (3)$$

where we define:

$$H_0(a, b) = E_0(a, b) \times \text{diag} \{ 1, 1, 1, 1 \}; \quad (4)$$

$$H'_+(a, b) = \text{diag} \{ 0, 0, 0, E_1(a, b) \}, \quad (5)$$

where $E_+(a, b) = E_1(a, b) - E_0(a, b) = \frac{1}{4\pi\epsilon} \left( \frac{2\epsilon^2}{b} - \frac{2\epsilon^2}{\sqrt{a^2 + b^2}} \right)$ is positive. When one of two molecules is in the charge state $(0, 2)$ and the other one is in the charge state $(2, 0)$ as shown in Fig.2(d), the interaction energy between them can be written as $E_2(a, b) = \frac{1}{4\pi\epsilon} \frac{4\epsilon^2}{\sqrt{a^2 + b^2}}$. Similarly, we can also get effective interaction in the basis $|TT\rangle$, $|TS\rangle$, $|ST\rangle$ and $|SS\rangle$ as:

$$H_-(a, b) = \text{diag} \{ E_0(a, b), E_0(a, b), E_0(a, b), E_2(a, b) \} = H_0(a, b) + H'_-(a, b), \quad (6)$$

where

$$H'_-(a, b) = \text{diag} \{ 0, 0, 0, E_-(a, b) \}, \quad (7)$$

and $E_-(a, b) = E_2(a, b) - E_0(a, b) = -E_+(a, b)$ is negative.

The effective interaction between two non-neighboring qubits can also be written in the above forms, except that the parameter $b$ is replaced by the distance between the two non-neighboring molecules. Therefore, we can set the effective interaction between any two quantum molecules as positive, zero and negative by properly changing the charge state of each molecule. The property enables us to cancel the effect of non-nearest-neighbor qubits interactions with a multi-step preparation process for cluster state of QD molecules.

Firstly, all qubits are initialized in the states $(|S\rangle + |T\rangle)/\sqrt{2}$. In this case, all molecules are in the $(1, 1)$ charge state and the effective interaction between any two qubits is closed. Sweeping $\Delta$ of all molecules by tuning gate-bias voltages of each molecule or applying a globe external electrical field, the qubits in the $|S\rangle$ state can be changed into $(0, 2)$ charge state. With this operation, Ising-model interactions as Eq.2 are switched on between all quantum molecules. As in our previous scheme [16], if there are only interactions between nearest-neighbor quantum molecules, we can
prepare cluster state simply with this operation. However, there are small interactions between non-nearest-neighbor QD molecules. For example, there is interaction between qubit \( i \) and qubit \( i+k \) in the following form:

\[
H_+(a, kb) = E_0(a, |k|b) \times \text{diag}\{1, 1, 1, 1\} + \text{diag}\{0, 0, 0, E_+(a, |k|b)\} = H_0(a, kb) + H_+^k(a, kb).
\]

(8)

Here \( kb \) represents the distance between molecule \( i \) and \( i+k \); \( k = \pm 1, \pm 2, \ldots \); when \( k < 0 (k > 0) \), \( i+k \) correspond to the qubits of left(right) side neighbor. We describe the effect of non-nearest-neighbor qubits by the ratio of all the non-nearest-neighbor interactions to the nearest-neighbor interaction (based on the following discussion, the effect of \( H_0(a, kb) \) can be ignored):

\[
R(a, b) = \sum_{k=2}^{+\infty} E_+(a, kb)/E_+(a, b).
\]

(9)

For a typical value of \( a \) and \( b = 10a \), the ratio \( R(a, 10a) \approx 20\% \). Therefore, we need to include interactions between non-nearest-neighbor qubits to generate a cluster state with higher fidelity.

Including the non-nearest-neighbor interactions, the total interaction Hamiltonian can be written as:

\[
H = \sum_{i=-\infty}^{+\infty} \left( H_{i,i+1}^+ (a, b) + \sum_{k=2}^{+\infty} H_{i,i+k}^+ (a, kb) \right).
\]

(10)

The superscripts in Eq.10 indicate the two qubits which the interactions acting on. It is noted that the interaction Hamiltonians between any two molecules are Ising-model and mutually commute, so the order of application of the time evolution operations does not matter. We can then describe the system time evolution as follows:

\[
U(t) = \exp \left( \frac{it}{\hbar} \sum_{i=-\infty}^{+\infty} \left( H_{i,i+1}^+ (a, b) + \sum_{k=2}^{+\infty} H_{i,i+k}^+ (a, kb) \right) \right)
\]

\[
= \prod_{i=-\infty, k=1}^{+\infty} U_{i,i+k}^+ (t)
\]

\[
= \prod_{i=-\infty, k=2}^{+\infty} U_{i,i+k}^+ \otimes \prod_{i=-\infty}^{+\infty} U_{i,i+1}^+.
\]

(11)

Here

\[
U_{i,i+k}^+ (t) = \exp \left( \frac{it H_{i,i+k}^+ (a, kb)}{\hbar} \right)
\]

\[
= e^{i\phi(k,t)} \text{diag}\left\{1, 1, 1, \exp \left( \frac{iE_+(a, |k|b)t}{\hbar} \right) \right\},
\]

(12)

where

\[
e^{i\phi(k,t)} = \exp \left( \frac{iE_0(a, |k|b)t}{\hbar} \right),
\]

(13)

is a constant phase, which only affect the trivial global phase of final state. That means we can ignore the \( H_0(a, kb) \) part in \( H_{i,i+k}^+ (a, kb) \). For briefness, we use \( H_{i,i+k}^+ (a, kb) = H_{i,i+k}^+ (a, kb) \).

If there are only interactions between nearest-neighbor quantum molecules, the evolution operator includes simply the term \( \prod_{i=-\infty}^{+\infty} U_{i,i+1}^+ \), with which the system can evolve into cluster state for a proper time \( t = t_0 \) \([16]\). In order to eliminate the effect of non-nearest-neighbor qubit interaction, we need to cancel the operation \( \prod_{i=-\infty, k=2}^{+\infty} U_{i,i+k}^+ \) (The constant phases caused by each \( H_{i,i+k}^+ (a, kb) \) can be added together as a global phase, which has no effect to the final state fidelity). As shown above, we can get negative Ising-model interaction \( H_{i,i+k}^- (a, kb) = -H_{i,i+k}^+ (a, kb) \) by changing the molecule charge state. If the system successively evolves under \( H_{i,i+k}^+ (a, kb) \) and \( H_{i,i+k}^- (a, kb) \) for a same time interval, the system will return to its origin states. Thus we can split the cluster state preparation into several steps to eliminate the effect of non-nearest-neighbor qubits: after the first step operation \( U(t) \), we can properly switch on negative
interaction $H_-(a, kb)$ to cancel the effect of the operator $\prod_{i=-\infty}^{+\infty}U_{i,i+k}$. The number of the steps depends on how many non-nearest-neighbor qubit interactions we want to cancel.

For example, to eliminate the effects of the next-nearest-neighbor qubits, we can use a three-step process as given in Fig.3 and Table.I to generate cluster state. Firstly, after initialization, we tune bias parameter $\Delta$ of each molecule to move qubits $i + 4n$, $i + 4n + 1$ (the number $n = 0, 1, 2, \ldots$) into the charge state $(0, 2)$ and qubits $i + 4n + 2$, $i + 4n + 3$ into the charge state $(2, 0)$ for a time interval of $t_1 = t_0/2$ (Fig.3(a)). Here, $t_0$ is the time we need to generate cluster state without considering the interactions between non-nearest-neighbor qubits. Then we move the qubits $i + 4n$, $i + 4n + 3$ into the charge state $(0, 2)$ and qubits $i + 4n + 1$, $i + 4n + 2$ into $(2, 0)$ for a time interval of $t_2 = t_0/2$ (Fig.3(b)). Finally, we can move all molecules into the charge state $(0, 2)$ for a time interval of $t_3 = t_0$ (Fig.3(c)). Through these three steps causing a time of $2t_0$, we can prepare a cluster state where the effect of all the $(4n + 2)$-nearest-neighbor qubits ($n = 0, 1, 2, \ldots$), including next-nearest-neighbor qubits ($n = 0, -1$), are eliminated. Here $(4n + 2)$-nearest-neighbor means the qubit separated $4n + 2$ sites from qubits $i$. By indicating the effective interaction energies of each step in Table.I, we can understand this preparation process more clearly. Although the interactions between qubit $i$ and qubit $i + 4n$ are doubled, the ratio of the residual non-nearest-neighbor interaction to the nearest-neighbor interaction is reduced to the value $R'$ through this three-step process:

$$R' = \frac{\sum_{n=1}^{+\infty}(E_+(a, (4n \pm 1)b) + 2E_+(a, 4nb))}{E_+(a, b)} \approx 9\%, \ (b = 10a).$$

(14)

To eliminate more non-nearest-neighbor interactions, we can use a more-step process as shown in Table.II. To cancel the effect of $(mn + 2)$-nearest-neighbor to $(mn + m - 2)$-nearest-neighbor qubits ($m$ is an integer larger than 3, and $n = 0, 1, 2, \ldots$), firstly, we move the qubits $i + mn$, $i + mn + 1$ into $(0, 2)$ state and the others into $(2, 0)$ state for a time interval of $t_1 = t_0/4$ ($t_0$ is the same as before). Secondly, we move the qubits $i + mn - 1$, $i + mn$ into $(0, 2)$ state and the others into $(2, 0)$ state for a time interval of $t_2 = t_0/4$. Thirdly, we move the qubits $i + mn - 2$, $i + mn - 1$ into $(0, 2)$ state and the others into $(2, 0)$ state for a time interval of $t_3 = t_0/4$. Similarly shift the charge state sequence one qubit to the left for a time interval of $t_0/4$ as above $m$ times. After that, we move all the molecules into the charge state $(0, 2)$ for a time interval of $t_{m+1} = (8 - m)t_0/4$. All the effective interactions between qubit $i$ and qubit $i + k$ in this process are shown in Table.II. It is demonstrated that after the above $m + 1$ steps, only the interactions between qubit $i$ and $i + nm$, $i + nm$ are left (the interactions between qubit $i$ and $i + nm$ are doubled). Thus we can prepare a cluster state through this process, where the effect of $(mn + 2)$-nearest-neighbor to $(mn + m - 2)$-nearest-neighbor qubits is eliminated. To satisfy $t_{m+1} = (8 - m)t_0/4 \geq 0$ (the time interval of the last step should be positive), $m$ must be no larger than 8. The ratio of the residual non-nearest-neighbor interactions to the nearest-neighbor interaction is reduced to the value $R''$:

$$R'' = \frac{\sum_{n=1}^{+\infty}(E_+(a, (mn \pm 1)b) + 2E_+(a, mnb))}{E_+(a, b)} \approx 1\%, \ (b = 10a, m = 8).$$

(15)

The total time we need to prepare cluster state in this multi-step process is only doubled. It is noted that this above process only can be applicable for the case $4 \leq m \leq 8$. When $m = 3$, it corresponds to the case of eliminating the effect of next-nearest-neighbor qubits. There are still some non-nearest-neighbor interactions left in this cluster state generation process. However, as we can turn on or off the interaction $H_+(a, kb)$ or $H_-(a, kb)$ between any two qubits, the remaining non-nearest-interactions can also be eliminate by a more-step process, where the negative interactions $H_-(a, kb)$ are properly switched on and off to cancel the effect of non-nearest-neighbor interactions $H_+(a, kb)$. It is noted that the present idea can only be applicable when the interaction Hamiltonians between qubits mutually commute.

In the above section, only one-dimensional qubit chain is considered. We can expand the above idea to a two-dimensional qubit array, where the two dots in each molecule can be fabricated in different layers of a bilayer system as shown in Fig.4 [23, 24, 25, 26]. Each molecule can be transferred among $(0, 2)$, $(1, 1)$ and $(2, 0)$ charge states by tuning the voltage of top gates and back gates. For example, we can eliminate the effect of the next-nearest-neighbor (diagonal) qubits interactions in a three-step cluster state preparation process. Firstly, we move qubits $(i + 2m, j + 2n)$ to $(0, 2)$ state, qubits $(i + 2m + 1, j + 2n + 1)$ to $(2, 0)$ state and the other qubits to $(1, 1)$ state for a time interval of $t_0$ (Here $m, n = 0, 1, 2, \ldots$). Secondly, we move qubits $(i + 2m, j + 2n + 1)$ to $(0, 2)$ state, qubits $(i + 2m + 1, j + 2n)$ to $(2, 0)$ state and the others to $(1, 1)$ state for a time interval of $t_0$. Finally, we add a negative voltage on the top gates to move all the initialized qubits to $(0, 2)$ charge state for a time interval of $t_0$. With these three steps causing a total time of $3t_0$, we can prepare a two-dimensional cluster state while the next-nearest-neighbor (diagonal) qubits interactions are eliminated. Similarly, with a more-step process, other non-nearest-neighbor interactions can also be eliminated by properly switching on the positive or negative interactions between each two qubits.
In real experiment, there are unavoidable randomness in the the distances between quantum dots (the value of a and b). This randomness will greatly affect the fidelity of final state, especially when the interactions between non-neighboring qubits are included. As in the present protocol, the interactions of non-neighboring qubits are canceled by switched to negative and positive value. The randomness in the distances between non-neighboring qubits is also eliminated.

For a wide class of so-called “toy models” in quantum computation, most researches focus on the idea rather than its quantitative development in real systems. Nevertheless, the importance and efficiency of those simplified models are still very high, since they usually provide physical ground for more involved theories. Moreover, the lack of pronounced results in up-to-date experimental efforts in realization of even prototypical quantum registers, composed of tens of qubits, forces us to consider and to analyze all proposed frameworks of quantum computations. Our results may stimulate further theoretical investigations of perspectives of one-way quantum computations for which the existence of reliable mechanism of cluster state preparation is crucial. And it be interesting and useful for researchers dealing with this area of investigations.

In conclusion, we propose a multi-step cluster state generation protocol for double-dot molecules to eliminate the effect of the interactions between non-nearest-neighbor qubits. As the interaction Hamiltonians between qubits are Ising-model and mutually commute, the order of application of the time evolution operations does not matter. We can get positive and negative effective interactions between qubits to cancel the effect of non-nearest-neighbor qubits by properly tuning the electron charge states of each QD molecule. The total time for the present multi-step cluster state preparation scheme is only doubled for one-dimensional qubit chain and tripled for two-dimensional qubit array compared with the time of previous protocol neglecting the non-nearest-neighbor interactions.

This work was funded by National Fundamental Research Program, the innovation funds from Chinese Academy of Sciences and National Natural Science Foundation of China (Grant No.60121503 and No.10604052).

[1] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, New York, 2000).
[2] Loss, D. and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998).
[3] J. R. Petta, A. C. Johnson, J. M. Taylor, E. A. Laird, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Science 309, 2180 (2005).
[4] F. H. L. Koppens, C. Buizert, K. J. Tielrooij, I. T. Vink, K. C. Nowack, T. Meunier, L. P. Kouwenhoven, L. M. K. Vandersypen, Nature 442, 766 (2006).
[5] J. M. Taylor, J. R. Petta, A. C. Johnson, A. Yacoby, and M. D. Lukin, cond-mat/0602470 (2006).
[6] A. C. Johnson, J. R. Petta, M. P. Hanson, and A. C. Gossard, cond-mat/0604024 (2006).
[7] J. M. Taylor, T. M. van Heumen, and L. M. K. Vandersypen, Science 306, 1246 (2004).
[8] E. A. Laird, C. Barthel, E. I. Rashba, C. M. Marcus, M. P. Hanson, A. C. Gossard, cond-mat/0702055 (2007).
[9] J. R. Petta, A. C. Johnson, J. M. Taylor, A. Yacoby, and M. D. Lukin, Nature Physics 1, 177 (2005).
[10] R. Hanson and G. Burkard, Nature 435, 925 (2005).
[11] R. de Sousa, S. Das Sarma, Phys. Rev. B 76, 153301 (2007).
[12] D. Stepanenko and G. Burkard, Phys. Rev. B 75, 205324 (2007).
[13] S. R. Eric Yang, J. Schliemann, and A. H. McaDonald, Phys. Rev. A 65, 040301 (2002).
[14] C. Santori, D. Fattal, J. Vuckovic, G. S Solomon and Y. Yamamoto, Nature 436, 925 (2005).
[15] Hui Zhang, Guo-Ping Guo, Tao Tu and Guang-Can Guo, Phys. Rev. A 76, 012335 (2007).
### TABLE I: Interaction energies between qubit $j$ and qubit $j+k$ in the process of eliminating the next-nearest-neighbor interactions in preparation of cluster state (qubit $j$ is any qubit in the molecule chain). The rows begin with (a), (b) and (c) are corresponding to the Fig.3(a), Fig.3(b) and Fig.3(c) in Fig.3, respectively. And the numbers in last four lines indicate the effective intense of the interaction between qubit $j$ and qubit $j+k$ (Units: $E_+ (a, kb)$).

| $k$ | 1   | 2   | 3   | 4   | 5   | 6   | 7   |
|-----|-----|-----|-----|-----|-----|-----|-----|
| (a) | $-1/2$ | $-1/2$ | $-1/2$ | $+1/2$ | $+1/2$ | $-1/2$ | $-1/2$ |
| (b) | $-1/2$ | $-1/2$ | $+1/2$ | $+1/2$ | $-1/2$ | $-1/2$ | $+1/2$ |
| (c) | $+1$  | $+1$  | $+1$  | $+1$  | $+1$  | $+1$  | $+1$  |
| Total | $+1$ | $0$  | $+1$  | $+2$  | $+1$  | $0$  | $+1$  |

### TABLE II: Interaction energies between qubit $j$ and qubit $j+k$ in the process of eliminating the non-nearest-neighbor interactions in preparation of cluster state (qubit $j$ is any qubit in the molecule chain). The signs and numbers indicate the effective intense of the interaction between qubit $j$ and qubit $j+k$ (Units: $E_+ (a, kb)/4$).

| $k$ | 1   | 2   | 3   | m-2 | m-1 | m   | m+1 | m+2 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| (1) | $+$ | $-$ | $-$ | $\cdots | $-$ | $+$ | $+$ | $-$ |
| (2) | $-$ | $-$ | $-$ | $\cdots | $+$ | $+$ | $-$ | $-$ |
| (3) | $+$ | $+$ | $+$ | $\cdots | $+$ | $-$ | $-$ | $-$ |
| (4) | $+$ | $+$ | $+$ | $\cdots | $+$ | $+$ | $+$ | $+$ |
| (m-2) | $+$ | $+$ | $-$ | $\cdots | $+$ | $+$ | $+$ | $+$ |
| (m-1) | $+$ | $-$ | $-$ | $\cdots | $+$ | $+$ | $+$ | $+$ |
| (m) | $-$ | $-$ | $+$ | $\cdots | $+$ | $+$ | $+$ | $-$ |
| (1)~(m) | m-4 | m-8 | m-8 | $\cdots | m-8 | m-4 | m-4 | m-8 |
| (m+1) | 8-m | 8-m | 8-m | $\cdots | 8-m | 8-m | 8-m | 8-m |
| Total | 4   | 0   | 0   | $\cdots | 0   | 4   | 8   | 4   | 0
FIG. 1: Energy level structure of the quantum molecule system as a function of potential offset $\Delta$ between the three possible charge states.

FIG. 2: Relation between electron charge states and the interaction between two QD molecules. $a$ is the distance between two QDs in one QD molecules and $b$ is the distance between two QD molecules. Hollow circles stand for Quantum Dots, and solid circles stand for electrons. Every QD molecule (qubit) has two electrons. And the interaction of two qubit depends on the electrons distribution in the QD molecules. (a)(b) Effective interaction is zero. (c) Effective interaction is $H_+$. (d) Effective interaction is $H_-$. See text for details.
FIG. 3: Scheme of eliminating the interactions between the qubits and their next-nearest-neighbor qubits. The time shown in the right bottom of each subfigure means the time interval of this kind of interaction.

FIG. 4: Drawing of two-dimensional QD molecule array. Each QD molecule is fabricated across the two layers of the system. The squares in the gate layer stand for the control gates, and the circles in the two-dimensional electron gas (2DEG) layers stand for quantum dots. When the gates are tuned properly, the corresponding qubit electron charge states can be modified.