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DOUBLE QUANTUM DOT OF GRAHENE NANORIBBON QUBIT FOR QUANTUM INFORMATION

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ABSTRACT

Weak hyperfine interaction as well as spin-orbit interaction enforced that graphene quantum dot qubit material rather than other semiconductor qubits material. So; we suggest here a Hamiltonian model of a graphene nanoribbon double quantum dot qubit based on the functionalization of graphene nanoribbon by hydrogen atoms to produce a theoretical studied on a quantum computer. We are using the Dirac equation and the Heisenberg exchange approach to solve our model. Then we determine the exchange interaction J_{ex}. We investigate the effects of potential barrier height Ω_b and barrier thickness **d** on exchange coupling J_{ex}. Our results show a great variation of J_{ex} depends on these parameters, and how this parameter affected on J_{ex} at special value. Also, we can use the variation of J_{ex} with both potential barrier height Ω_b and barrier thickness **d** to represent how the information can transfer, which is important to gate operation necessary for quantum information.

Keywords: qubit; electron spin; graphene; exchange interaction

1. Introduction

After doing a lot of scientific research on graphene, research on its properties and applications remains uninterrupted. However, its greatest importance lies in the application of electronic devices. The exceptional electronic properties of graphene have ensured a rapid growth of interest as the base material for electronic circuitry [1]. Graphene-based quantum dot considers the best candidate for this device and can be implemented for quantum computers [2, 3, 4]. This computer works depending on superposition and entanglement phenomena [5, 6], where the spin of electrons acts as a quantum bit (qubit) [7-10]. The scalability of that electronic system is considered in the protection of information stored in qubit [11], since decoherence time should be 104 times longer than the gate time to transfer information. Several types of research worked on how to preserve coherence time longer as we need to gate to do its operation. Graphene can perfectly solve this problem. Owing to the band structure of graphene, the low- energy electrons in it behave like massless chiral fermions. That governed by the Dirac-Weyl equation. In this situation, the confinement of electrons becomes quite a challenging task, due to the so-called Klein tunneling [12, 13]. Previously Trauzettel, Bulaev, Loss, and Burkard [14] introduce a model for overcoming this difficult and confined electron as a spin qubit in a graphene nanoribbon with armchair boundary condition [15, 16, 17]. Here we introduce a model of double quantum dot-based on the functionalization of graphene nanoribbon by hydrogen atoms, where the electron can be confined on a quantum dot between two barrier regions. The electrons spin are coupled via exchange coupling and the coupling controlled by barrier voltage represented by low energy effective Hamiltonians:

$$\mathcal{H}(t)=J_{12}(t)\, S^1.S^2. \tag{2}$$

where J_{12}(t) is the exchange coupling constant between the two spins S^1 and S^2.

This coupling with a combination of single spin rotation is sufficient to form a required universal quantum gate [18].

2. Theoretical model

A single quantum dot of functionalized graphene nanoribbon is formed when a single layer of graphene deposited on sio_2 substrate which is exposed to hydrogen atoms. The dots region is fully passivated to hydrogen atoms, while the barrier region is a non-hydrogen passive region [19]. A gapless region is formed in passive hydrogen corresponding to quantum dot, while a gaped region formed with non-hydrogenated passive corresponding to barrier region as shown in Fig. 1.

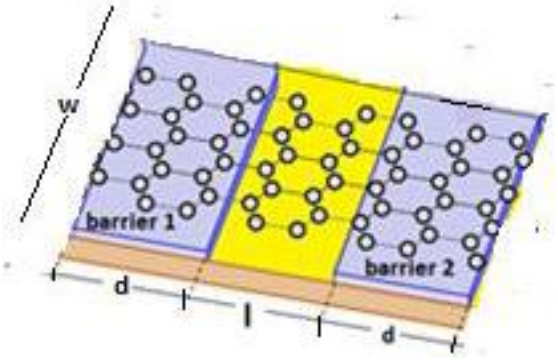

Fig. 1. Single quantum dot of functionalized GNB deposited on quartz substrate (yellow) confined between two barrier regions (blue)

The electronic wave function of graphene system describes by:

$$\Phi = \begin{pmatrix} \Phi^{A}_{k} \\ \Phi^{B}_{k} \\ -\Phi^{A}_{k'} \\ -\Phi^{B}_{k'} \end{pmatrix} \tag{1}$$

where k, k' related to the two valleys in the Brillion zone of graphene, and A, B refer to the two components of the pseudospin. The low energy massless electron describes by Dirac equation:

In the dot region (where $0 \le y \le L$)

$$-i\hbar v \begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix} \Phi + eV\Phi = E\,\Phi$$

and in the barrier region [19] (where y < 0 or y > L)

$$-i\hbar v \begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix} \Phi + \Delta \begin{pmatrix} 0 & \partial_z \\ \partial_z & 0 \end{pmatrix} \Phi - \eta\, V_\sigma \Phi = E\,\Phi \tag{3}$$

where $\hbar$ is Planck's constant, v is the Fermi velocity of graphene, ∂_x, ∂_y and ∂_z are Pauli matrices, η=±1 related to spin up and spin down, 2Δ is the gap induced by the substrate, 2 V_σ is the splitting energy of spin

V is the electrical confining potential along the y-axis, (e*V) is the electrical confining energy in units of $\hbar v q_0$, where q_0 is the quantization of ground state wave vector in x-direction that given by:

$$q_0 = \frac{\pi}{3\,W}$$

where W is the ribbon width

In the case of double quantum dot-separated by a barrier thickness d with potential barrier height Ω_b. The ribbon whose length L and width W (Fig. 2). the dots length is l along the y-axis and catching one electron with an electric potential V (y) along the y-direction [14].

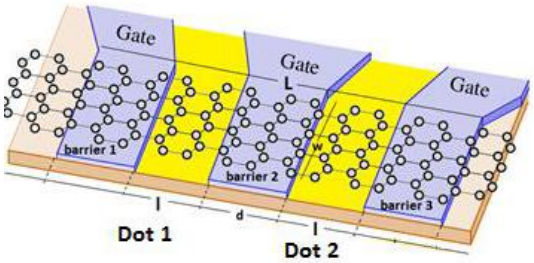

Fig. 2. Structured of double quantum dot of GNB deposited on quartz substrate (yellow) separated by barrier thickness d (blue)

The electric potential can be tuned to appropriate value via gate voltage, so electrons are tunneling between dots and spin qubits are coupled. The exchange interaction occurs between them giving an anti-symmetric total wave function.

The model can describe by Hamiltonian:

$$\mathcal{H} = \sum_{i=1,2} \mathcal{H}_i + C \quad (4)$$

$\mathcal{H}_i$ is the single-particle Hamiltonian for a Dirac particle that can be defined by the Dirac equation obtains in eq. (2) [20].

C is the Coulomb interaction in two-dimension given by:

$$C = \frac{e^2}{4\pi\epsilon\sqrt{(r_1 - r_2)^2}}$$

The solution of eq. (4) gives an electron wave as:

$$|\Phi(x,y)\rangle = \frac{1}{\sqrt{wL}} \begin{pmatrix} a_\beta e^{iq_n x} \\ a_\beta e^{-iq_n x} \end{pmatrix} \mathrm{Cos}[kLy] \quad (5)$$

β = A, B. The basis vectors for the two-component pseudo spinor are:

$$a_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$a_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The total wave function of coupled electrons can be written as the product of the spatial wave function and the corresponding two-particle spinor for the singlet (triplet) state.

$$|\Phi_{+/-}\rangle = \frac{1}{\sqrt{2(1 \pm s^2)}} (|LR\rangle \pm |RL\rangle) \quad (6)$$

L/*R* denotes a four-component single-particle wave function located at the left (right) quantum dot, and S =⟨ L |R⟩, which is the overlap between them.

To evaluate the exchange coupling J_{ex}=E_T - E_S from the Schrodinger equation:

$$E_{S/T} = \langle \Phi_{+/-} | \mathcal{H} | \Phi_{+/-} \rangle / \langle \Phi_{+/-} | S | \Phi_{+/-} \rangle \quad (7)$$

From Eq. (4), (6) and (7) we can solve J_{ex} analytical and result:

$$J_{ex} = \langle \Phi_- | \mathcal{H} | \Phi_- \rangle - \langle \Phi_+ | \mathcal{H} | \Phi_+ \rangle$$

$$J_{ex} = [\langle R|R\rangle\langle L|\mathcal{H}_i|L\rangle + \langle L|L\rangle\langle R|\mathcal{H}_i|R\rangle \mp \langle L|\mathcal{H}_i|R\rangle\langle R|L\rangle \mp \langle L|R\rangle\langle R|\mathcal{H}_i|L\rangle + \langle RL|c|RL\rangle \mp \langle LR|c|RL\rangle] \quad (8)$$

3. Results

3.1. The potential barrier height Ω_b

We represent the ribbon of width W= 0.5 q_0^{-1} and its length L = 18 q_0^{-1}, where q_0=1/20 $(nm)^{-1}$.

Owing to the potential barrier height Ω_b represents a resistance for the electron to stay on the same dot. So, at the beginning when the barrier height is small, the exchange interaction between two electrons is strong, indicating that the two electrons located on the same dot, two dots behave as a single dot and electrons must be in a singlet state. This behavior can produce for small barrier distance only, in our model for d= 2 q_0^{-1} and *l*=5 q_0^{-1}(Fig. 3a). As soon as the barrier height Ω_b increases, the allowance for double electrons to be on the same dot is never occurring and the exchange interaction axiomatically in triplet state indicating by negative J_{ex}. The transition occurs from singlet to triplet at about 0.9 $\hbar v q_0$. For large barrier thickness d, the small and large barrier height Ω_b keeps the exchange interaction in always triplet state as in Fig. 3b where d=5 q_0^{-1} and *l*=5 q_0^{-1}. Fig. (4) Shows that the value of J_{ex} for short and long **d** is nearly close to each other as the barrier height reaches the value of the bandgap of GNB ≈ 2 $\hbar v q_0$. This phenomenon is a special character for GNB whereas the barrier is high; the Klien tunneling occurs. The same result obtained if we change the length of dots *l*=3 q_0^{-1} at barrier thickness d=1.5 q_0^{-1} and d=3 q_0^{-1}(Figs. 5 and 6).

3.2. The barrier distance d

The behavior for barrier distance d (Fig. 7) is nearly the same as in the case of the potential barrier Ω_b, where the exchange interaction J_{ex} is reversely proportional to **d**. For so small **d** at nearly 2 q_0^{-1} and at Potential barrier equal zero, the exchange interaction is positive and decay

exponential as d increase until reach to zero at ≈ 4.9 q_0^{-1} then change its sign to negative at a value of d greater than d=5 q_0^{-1}. This behavior can be explained as in the previous section, where for small d the two dots behave as a single one and the electron must be in a singlet state. For large d the exchange interaction becomes negative represent triplet state. If the value of barrier height increases at Ω_b=1.3 $\hbar v q_0$ *and* 1.95 $\hbar v q_0$, this value is close to the bandgap value, and the exchange interaction is always in triplet state but the value of J_{ex} for Ω_b=1.95 $\hbar v q_0$ is greater than that for Ω_b=1.3 $\hbar v q_0$ due to Kline tunneling effect.

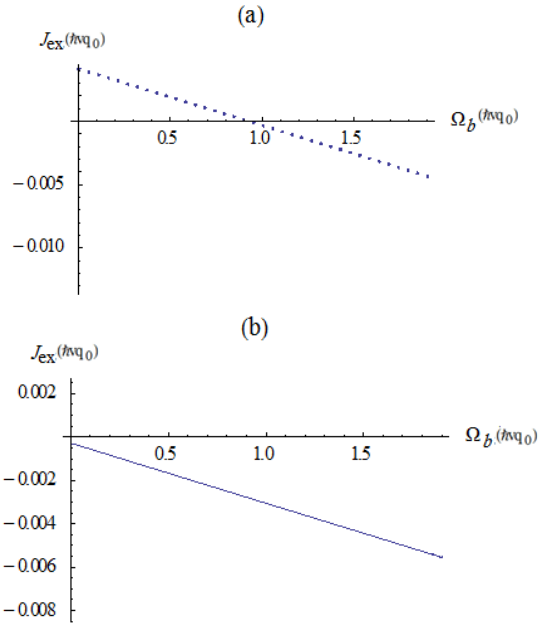

Fig. 3. The exchange coupling J_{ex} $(\hbar v q_0)$ as a function of barrier height Ω_b $(\hbar v q_0)$. For l= 5 q q_0^{-1} and q_0=1/20 $(nm)^{-1}$ (a) at d=2 q_0^{-1} (b) at d=5 q_0^{-1}

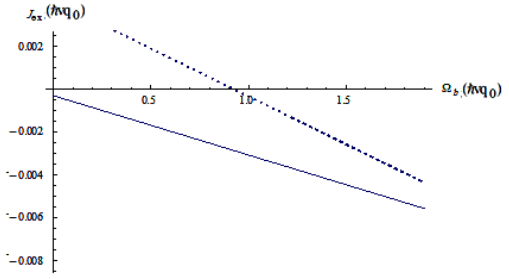

Fig. 4. The exchange coupling J_{ex} $(\hbar v q_0)$ as a function of barrier height Ω_b $(\hbar v q_0)$ at l= 5 q_0^{-1}, q_0=1/20 $(nm)^{-1}$ and d=2 q_0^{-1} (dot line), d=5 q_0^{-1} (solid line).

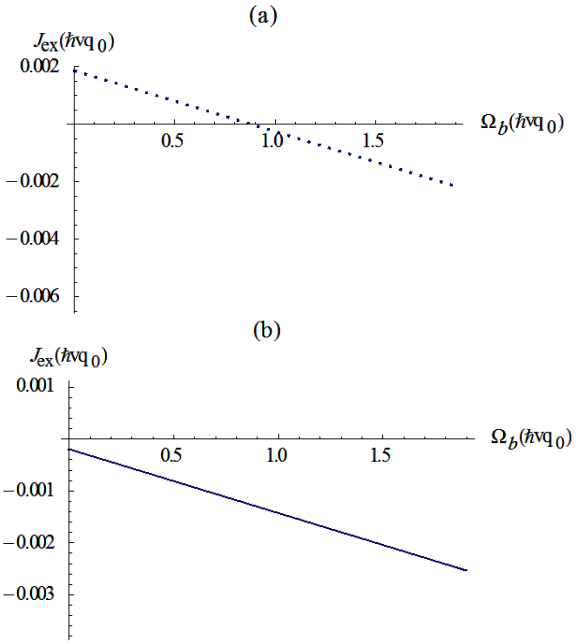

Fig. 5. The exchange coupling J_{ex} $(\hbar v q_0)$ as a function of barrier height Ω_b $(\hbar v q_0)$. For l= 3 q_0^{-1} and q_0=1/20 (nm)-1 (a) at d=1.5 q_0^{-1} (b) at d=3 q_0^{-1}

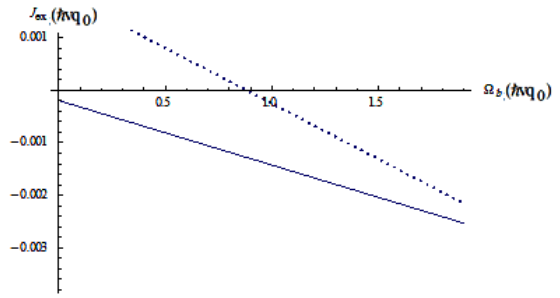

Fig. 6. The exchange coupling J_{ex} $(\hbar v q_0)$ as a function of barrier height Ω_b $(\hbar v q_0)$ at l= 3 q_0^{-1}, q_0=1/20 $(nm)^{-1}$ and d=1.5 q_0^{-1} (solid line), d=3 q_0^{-1} (dot line)

4. Conclusions

We have examined the value of J_{ex} of different parameters such as barrier height Ω_b between double quantum dot, and barrier thickness d to study the effect of each one on J_{ex}. We find that the value of exchange interaction changed with this parameter. Also, our result shows that the variation of J_{ex} with Ω_b is accompanied by a transition of the state from singlet into triplet state. We concentrate on this truth to conclude that; the transmission of the qubit accompany by the transfer of information.

Further, since the operation of the gate depends on switching time compared to

coherence time, for graphene the coherence time is about ≈80μs [21] is 10^4 longer than the switching time. In other words: the qubit can work stably. Since the source of de-coherence time like spin-orbit interaction, and hyperfine interaction is neglect in graphene, so we found that the graphene qubit is better than that of GaAs.

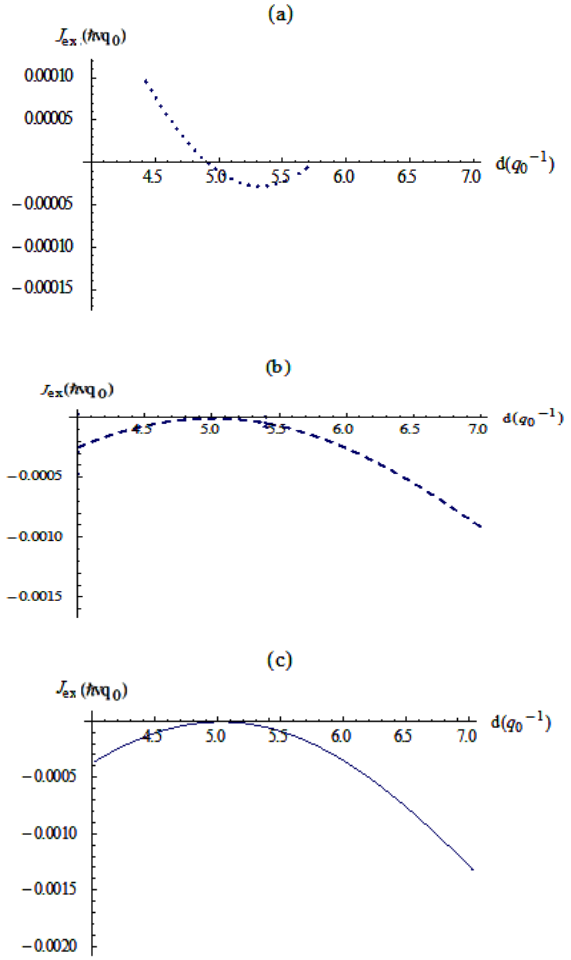

Fig. 7. The exchange coupling $\boldsymbol{J_{ex}}$ $(\hbar v q_0)$ as a function of inter- dot distance d (q_0^{-1}) at l= 5 q_0^{-1}, q_0=1/20 $(nm)^{-1}$ (a) for Ω_b=0 $\hbar v q_0$ (b) Ω_b=1.3 $\hbar v q_0$ and (c) for Ω_b=1.95 $\hbar v q_0$.

References

[1] Ponomarenko LA, Schedin F, Katsnelson MI, Yang R, Hill EW, Novoselov KS, Geim AK. Chaotic Dirac billiard in graphene quantum dots. Science 2008; 320 (5874): 356-358. doi: 10.1126/science.1154663.

[2] Jie-Sen Li, Zhi-Bing Li, Dao-Xin Yao. Quantum computation with two dimentional graphene quantum dots. Chinese Physics B 2012; 21: 1. dio: 10.1088/1674-1056/21/1/017302.

[3] DiVincenzo DP, Bacon D, Kempe J, Burkard G, Whaley KB. Universal quantum computation with the exchange interaction. Nature 2000; 408:339–342. doi: 10.1038/35042541.

[4] Wang WL, Yazyev OV, Meng S, Kaxiras E. Topological Frustration in Graphene Nanoflakes: Magnetic Order and Spin Logic Devices. Phys.Rev.Lett. 2009; 102 : 157201. doi: 10.1103/PhysRevLett.102.157201.

[5] Deutsch D. Quantum theory, the Church-Turing principle and the universal quantum computer. Proc. R. Soc. Lond. A 1985; 400 : 97. doi: 10.1098/rspa.1985.0070

[6] Loss D, DiVincenzo DP. Quantum computation with quantum dots. Phys.Rev.A 1998; 57:120. https://doi.org/10.1103/PhysRevA.57.120.

[7] Kotov VN, Uchoa B, Pereira VM, Guinea F, Castro Neto AH. Electron–Electron Interactions in Graphene: Current Status and Perspectives. Rev. Mod. Phys. 2012; 84 : 1067. doi: 10.1103/RevModPhys.84.1067.

[8] Guttinger J. Graphene Quantum Dots. ETH ZURICH 2011. https://www.research collection.ethz.ch.

[9] Chiu KL, Xu Yang. Single-electron transport in graphene-like nanostructures. Elsevier 2017; 669: 1-42. doi: 10.1016/j.physrep.2016.12.002.

[10] Droth M, Burkard G. Spintronics with graphene quantum dots. Phys.Status Solidi 2016; 10(1) : 75-90. doi: 10.1002/pssr.201510182.

[11] Bertrand B, Hermelin S, Takada S, Yamamoto M, Tarucha S, Ludwig A, Wieck AD, Bäuerle C, Meunier T. Fast spin information transfer between distant quantum dots using individual electrons. Nature Nanotechnology 2016; 11: 672–676. doi: 10.1038/nnano.2016.82.

[12] Katsnelson MI, Novoselov KS, Geim AK. Klein paradox in graphene. Nature Phys. 2006; 2 : 620–625. doi: 10.1038/nphys384.

[13] Chen H-Yi, Apalkov V, Chakraborty T. Fock-Darwin States of Dirac Electrons in Graphene-Based Artificial Atoms. Phys. Rev. Lett. 2007; 98: 186803. doi: 10.1103/PhysRevLett.98. 186803.

[14] Trauzettel B, Bulaev DV, Loss D, Burkard G. Spin qubits in graphene quantum dots. Nature Physics 2007; 3 : 192. doi: 10.1038/nphys544.

[15] Espinosa-Ortega T, Luk'yanchuk IA, and Rubo YG. Magnetic properties of graphene quantum dots. Phys. Rev. B 2013; 87: 205434. doi: 10.1103/PhysRevB.87.205434.

[16] G¨u AD¸ cl¨u, Potasz P, Korkusinski M, Hawrylak P. Graphene Quantum Dots. Springer 2014. doi: 10.1007/978-3-662-44611-9.

[17] Tetsuka H, Nagoya A, Fukusumi T, Matsui T. Molecularly Designed, Nitrogen-Functionalized Graphene Quantum Dots for Optoelectronic Devices. Adv. Mater. 2016; 28 : 4632–4638. doi: 10.1002/adma.201600058.

[18] Burkard G, Loss D, DiVincenzo DP. Phys. Rev. B 1999 ; 59 : 2070. https://doi.org/10.1103/PhysRevB.59.2070.

[19] Lin Z-R, Guo G-P, Tu T, Ma Q, Guo G-C. Quantum Computation with Graphene Nanostructure. Physics and Applications of Graphene - Theory, Sergey Mikhailov, IntechOpen; 2011. doi: 10.5772/15097.

[20] Fuchs J-N. Dirac fermions in graphene and analogues: magnetic field and topological properties ; 2013. arXiv:1306.0380 [cond-mat.mes-hall].

[21] Kloeffel C, Loss D. Prospects for Spin-Based Quantum Computing in Quantum Dots. Annual Review of Condensed Matter Physics 2013; 4 : 51–81. https://doi.org/10.1146/annurev - conmatphys - 030212-184248.

نقطة كمية مزدوجة من كيوبت شريط الجرافين للحصول على معلومات الكم

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الموجز

تسببت المشاكل التي واجهتنا في انظمة اشباه الموصلات للعمل ككيوبت كالتفاعل مع الحركة المغزلية للنواه وتفاعل الحركة المغزلية مع الحركة الدورانية على استخدام تلك النقطة الكمومية من الجرافين ككيوبت. هنا نقترح نموذجا للكميات الكمومية المزدوجة من شريط الجرافين معتمد على التفاعل مع الهيروجين لانتاج دراسة نظرية للحاسوب الكمومى. باستخدام معادلة ديراك ونهج التبادل لهيزنبرج ،تم تحديد التفاعل التبادلى ودراسة تأثير كلا من ارتفاع حاجز الجهد ، وسماكة الحاجز على التفاعل التبادلى. اظهرت نتائجنا اعتماد كبير للتفاعل التبادلى على هذه العوامل. أيضا، يمكننا استخدام هذا التأثير لتمثيل كيفية نقل المعلومات ، وهو امر مهم لتشغيل البوابة الكمية للحاسوب الكمومى.