Quantum computation with graphene nanoribbon

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Abstract. We propose a scheme to implement quantum computation in graphene nanoribbon (GNR). It is shown that an electron or hole can be naturally localized in each zigzag region for a GNR with a sequence of Z-shaped structures, without using confined gates. A one-dimensional graphene quantum dot chain is formed in such a GNR, where an electron or hole spin can be used as a qubit. The coupling interaction between neighboring qubits is found to be of the always-on Heisenberg type. By exploiting the bang–bang control strategy and the decoherence-free subspaces encoding method, universal quantum gates are argued to be realizable with the present techniques.

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1. Introduction

Electron spin is a promising candidate for realization of a practical quantum information processor [1]. The coherent manipulation of electron spins in GaAs quantum dots has been successfully realized [2, 3]. However, because of interaction with the environment, the decoherence time is often measured in nanoseconds in GaAs quantum dots [2, 4, 5]. Even when applying a complex technique to prepare the nuclear state, the dephasing time for the spin qubit is approximately 1 µs [6]. Decoherence is one of the greatest obstacles to a quantum computer for GaAs quantum dots. Because of the completely eliminated hyperfine interactions in graphene, there is great potential for electron spin qubits in a nuclear-spin-free quantum world [7]. It is highly desirable to propose an efficient architecture made with graphene nanostructures to implement quantum information processing (QIP) [8]. Recently, there was a striking advance in experimental production of a special graphene nanostructure, known as graphene nanoribbon (GNR), with well-defined zigzag or armchair edge structures [9, 10]. Taking advantage of QIP with graphene, and stimulated by the rapid experimental progress in the production of GNR, here we propose a scalable quantum information architecture based on a series of GNR quantum dots system.

Owing to the special band structure of graphene [11], its low-energy quasi-particles behave as Dirac fermions, and the Klein tunneling and Chiral effect make it non-trivial to form good quantum dots (localized electron states) in graphene. There are several ways in which one could localize electrons (holes) in graphene; by using suitable transverse states in GNR [7, 12], by electrical confinement in bilayer graphene [13], or by using the topological structure [14]. In the present paper, we propose as an alternative approach that the localized states can exist in the zigzag region of a GNR with a sequence of Z-shaped structures. Compared with previous works to form localized states, the proposed architecture confines electrons without exploiting confined gates, which greatly decreases the complexity of the circuits and the additional uncontrollable noise. The localized electron (hole) spin states can be used, as the physical qubit and the interaction between qubits is found to be of the always-on Heisenberg form. Moreover, for a practical quantum computer to operate, it is essential to properly manage decoherence. An important technique for doing this is the use of quantum bang–bang (BB) control strategy and the decoherence-free subspaces (DFS) encoding method, both of which are traditionally discussed in the context of atomic, molecular and optical setup [15]–[19]. In this paper, these ideas are introduced to construct an effective quantum information circuit in this new graphene nanostructure.

2. Graphene nanoribbon (GNR) quantum dot chain

Our graphene quantum system is presented in figure 1(d). The proposed GNR consists of an array of Z-shaped structures. Each Z-shaped structure includes a central region with a zigzag edge connecting to two regions with armchair edges. Using the π orbital tight-binding (TB) approximation, the Hamiltonian of our GNR system has the form $H_0 = \sum_{ij} \tau_{ij} |i\rangle\langle j|$, where the hopping matrix element $\tau_{ij} = -\tau$ if the orbits $|i\rangle$ and $|j\rangle$ are nearest neighbors on the honeycomb lattice, otherwise $\tau_{ij} = 0$ [20, 21]. The density of state (DOS) and the spectrum of the zigzag region in this GNR system can be obtained by direct diagonalization with periodic boundary conditions. In figure 1(a), we show the calculated energy levels and find that there are several localized states with electron–hole symmetry around the zero energy point. Hence,
Figure 1. Schematic of the proposed architecture of GNR for quantum computation. (a) The DOS of the GNR is calculated by nearest-neighbor TB approximation and third nearest-neighbor TB approximation with the second and third neighbor interaction energies $\gamma_1 = -0.12 \text{ eV}$ and $\gamma_2 = -0.068 \text{ eV}$. (b) The spatial distribution of local probability density of GNR with two Z-shaped structures, and $N = 7$, $L = 4$, $D = 6$ for $E = \pm 0.3 \text{ eV}$ discrete states. (c) Each zigzag region of the GNR confines one electron. The physical qubit is encoded into the spin of the confined electron. (d) The proposed architecture for quantum computation. The cyan ribbon indicates the micromagnet integrated on top of the GNR structure to apply a slanting magnetic field. The GNR and micromagnet are isolated by an insulating layer. Each zigzag region has a nearby gate to generate an ac electrical field and implement localized BB pulses. The nearby gates are not outlined for clarity. Here special methods are introduced to implement QIP on this GNR system. Physical qubits 1 and 2 form logical qubit $L_1$; physical qubits 3 and 4 form logical qubit $L_2$; physical qubits 5 and 6 form logical qubit $L_3$. $G^x$, $G^y$ and $G^z$ are the BB operation sets of $L_1$, $L_2$ and $L_3$, respectively.

we can have one localized electron or hole in the zigzag region by adjusting the Fermi level through the individual top gates. Actually, in the calculations we find that the spectrum of GNR depends very much on its geometry. There are no confined states in the zigzag regions when
Figure 2. The ground-state energies $E_0$ and energy gaps $E_1$ of the Z-shaped GNR quantum dot chain device depend on different widths of nanoribbon $N$ (unit cells) and different lengths of quantum dot region $L$ (unit cells).

the width of this GNR $N = 3m - 1$ or $N = 2m$ (unit cells), as shown in figure 2. Here $m$ is an integer. On the other hand, when $N$ is 7 (unit cells) and the lengths of the zigzag region $L$ are 3, 4, 5, 6, 7 (unit cells), or $N = 9$, $L = 3, 4$, both the ground-state energies $E_0$ and energy gaps $E_1$ are above 0.1 eV. Therefore, we can confine electrons (holes) to form quantum dots even at room temperature. Furthermore, considering higher-order hopping terms, we calculated the DOS and the spectrum using a third nearest-neighbor TB model instead of the nearest-neighbor TB model with the second and third neighbor interaction energies $\gamma_1 = -0.12$ eV and $\gamma_2 = -0.068$ eV [22, 23]. As shown in figures 1(a) and 2, higher order hopping terms destroy the electron–hole symmetry, but do not destroy the confined states in each zigzag region.

Figure 1(b) shows the spatial distribution of local probability density of a typical GNR with two Z-shaped structures, and $N = 7$, $L = 4$, $D = 6$ for $E_0 = \pm 0.3$ eV discrete states. Each zigzag region (quantum dot) confines one electron, and the quantum dots are coupled by the exchange coupling $J_1$. We obtain $J_1$ by calculating the exchange coupling $J_1 = 4t^2/U$ according to the Hubbard approximation. Here $U$ is onsite Coulomb energy and $t = E_0 \int \phi_1(r)\phi_2(r) d\vec{r}$ is the tunnelling matrix element between two neighboring quantum dots, and $\phi_1(\vec{r})$ and $\phi_2(\vec{r})$ are the wavefunctions of two neighboring dots. Obviously, the exchange coupling $J_1$ is determined by the geometry of the nanoribbon. For each $N$ and $L$, $J_1$ depends on the distance between two neighboring dots $D$ (unit cells), as shown in figure 3. For $N = 7$, $L = 4$, $D = 18$, $J_1 = 8 \mu$eV, $J_1/J_2 = 10^5$, where $J_2$ is the exchange coupling between next nearest-neighboring quantum dots, this exchange coupling between non-nearest-neighbor dots can be safely neglected. For clarity, in the reminder of the paper we focus on the GNR structure with these parameters.

To carry out quantum computation, the spin of the localized electron or hole can be used as the physical qubit, and the GNR with a sequence of Z-shaped structures forms a one-dimensional qubit chain as shown in figure 1(d). In this paper, we neglected the magnetic effect of the GNR edge [24]. The neighboring qubits in this chain have an always-on Heisenberg interaction $H = J_1 S_1 \cdot S_2$. Here $S_1$ and $S_2$ are the spin operators of the neighboring localized electron (hole). For a sequence of Z-shaped structure GNR with the parameters $N = 7, L = 4$
Figure 3. The coupling energy $J_1$ of two nearest-neighboring dots depends on the distance between two dots $D$ (unit cells) for different size of quantum dot region.

and $D = 18$, the Hamiltonian of the system can be expressed as

$$H_I = \sum_{\langle i, j \rangle} J_{i,j} (\sigma^x_i \otimes \sigma^x_j + \sigma^y_i \otimes \sigma^y_j + \sigma^z_i \otimes \sigma^z_j),$$

where $\sigma^{x,y,z}_{i,j}$ are the spin Pauli operators of the localized electron (hole) in the quantum dots, and $\langle i, j \rangle$ represent two nearest-neighbor dots.

3. Choice of encoded states

Achieving noise control is indispensable for practical QIP. While a variety of strategies have been devised to meet this challenge, no single method can compensate for a completely arbitrary noise process. Rather, constructing a reliable QIP scheme depends on the errors that happen. First, to avoid entanglement of the spin qubits with the environment, we can apply a BB operation $U_z = \exp(-i\sigma_z \pi/2)$ to each quantum dot region. These rotation operations can be implemented through the electrically driven single-electron spin resonance by localized ac electrical field pulses if ferromagnetic strips are integrated on top of the graphene quantum dots, which has been successfully realized in a GaAs/AlGaAs quantum dot experiment recently \[25\].

Next, to counteract the phase decoherence, we can use DFS encoding \[26\]–[28]. For a simple DFS encoding, two physical qubits can encode a logical qubit:

$$|0\rangle_L = |\uparrow_1 \downarrow_2\rangle, \quad |1\rangle_L = |\downarrow_1 \uparrow_2\rangle.$$  

(2)

As shown in figure 1(c), localized electron spins in the two neighboring zigzag regions can be used to form a logical qubit.

Furthermore, in order to protect quantum information in the logical qubits, we must decouple the always-on Heisenberg interaction between two physical qubits within a
logical qubit and the interaction between two neighboring logical qubits. Here a special encoding method and a non-synchronous BB pulse operation are exploited to eliminate these interactions [19]. The proposed architecture is a GNR quantum dot chain, which forms a periodic structure \( L_1L_2L_3L_1L_2L_3 \ldots \) with three logical qubits as a unit, as shown in figure 1(d). \( L_1 \) represents a logical qubit encoded as equation (2). \( L_2 \) is a logical qubit encoded as

\[
|0\rangle_{L_2} = \frac{1}{2}(|\uparrow\rangle_3 + |\downarrow\rangle_3)(|\uparrow\rangle_4 - |\downarrow\rangle_4),
\]

\[
|1\rangle_{L_2} = \frac{1}{2}(|\uparrow\rangle_3 - |\downarrow\rangle_3)(|\uparrow\rangle_4 + |\downarrow\rangle_4).
\]

\( L_3 \) is a logical qubit encoded as

\[
|0\rangle_{L_3} = \frac{1}{2}(|\uparrow\rangle_5 + i|\downarrow\rangle_5)(|\uparrow\rangle_6 - i|\downarrow\rangle_6),
\]

\[
|1\rangle_{L_3} = \frac{1}{2}(|\uparrow\rangle_5 - i|\downarrow\rangle_5)(|\uparrow\rangle_6 + i|\downarrow\rangle_6).
\]

With this periodic architecture, we have to apply non-synchronous BB pulse operations, respectively, to \( L_1, L_2, L_3 \) from the operation set \( G^z = \{I, U_z, R_z\}, G^x = \{I, U_x, R_x\}, G^y = \{I, U_y, R_y\} \), where \( U_z = -\sigma_z^x \otimes \sigma_z^x, R_z = -iU_z^c \otimes \sigma_z^x, U_x = -\sigma_z^x \otimes \sigma_z^x, R_x = -iU_x^c \otimes \sigma_z^x, U_y = -\sigma_z^x \otimes \sigma_z^x \) and \( R_y = -iU_y^c \otimes \sigma_z^x \). Thus, we obtain a quantum computation system with entirely decoupled logical qubits.

4. Single- and two-qubit gates

Now we show how to effect the universal quantum gates of the logical qubits defined above. Logical operations \( \tilde{X} \) and \( \tilde{Z} \) can generate all the SU(2) transformations of a logical qubit. For logical qubit \( L_1 \), \( \tilde{X} = \frac{1}{2}(\sigma_z^x + \sigma_y^x) \), \( \tilde{Z} = \frac{1}{2}(\sigma_z^z) \). The \( \tilde{X} \) gate can be easily achieved by adjusting the localized ac electrical field pulses of both qubits 1 and 2 to be synchronous. The operation time is \( \Delta t = \hbar \pi / 4J = 0.2 \) ns, for \( N = 7, L = 4 \) and \( D = 18 \). The \( \tilde{Z} \) gate can be achieved by localized electrical field pulses on the two physical qubits. The operation time of the \( \tilde{Z} \) gate can be on the nanosecond scale when a slanting magnetic field with large field gradient is applied onto each quantum dot region [25]. The fidelity of the \( \tilde{X} \) gate can be affected by the electron–phonon coupling and the charge noise in the substrate and back gates. Because the nuclear field changes the evolution of the spin states, the fidelity of the \( \tilde{Z} \) gate is dominated by the nuclear field in substrate [3]. The fidelity of the \( \tilde{Z} \) gate can be very high because of the small nuclear field in the graphene system.

We can construct a CNOT gate between two neighboring logical qubits, for example \( L_1 \) and \( L_2 \), by W gate \( W = e^{i\theta Z \otimes I} \) conjugating Hadamard operation. It is known that the W gate is equivalent to a controlled rotation about the z-axis: \( W = e^{i\theta Z \otimes I} = |0\rangle \langle 0| \otimes I + |1\rangle \langle 1| \otimes e^{i\theta Z} \) [29]. By performing a Hadamard transformation on the two physical qubits of the second logical qubit \( L_2 \) and changing the BB control pulse to be the same as \( L_1 \), we can recouple the two neighboring logical qubits and implement the W gate of logical qubits of \( L_1 \) and \( L_2 \). For the present graphene quantum dot chain with \( N = 7, L = 4 \) and \( D = 18 \), the total operation time of a CNOT gate can be implemented at the nanosecond scale. Similar to the above discussion for the \( \tilde{X} \) and \( \tilde{Z} \) operation, the dominating decoherence sources affecting the fidelity of the CNOT gate in the present protocol are the electron–phonon interaction, the charge noise and the nuclear field in substrate.

Assuming the abundance of \(^{13}C\) is about 1% as in the natural carbon material, the decoherence time has been predicted to be more than 10 \( \mu s \) in the graphene quantum dot [7, 30].
This decoherence time is four orders longer than the gate operation time of the present scheme. This combined DFS and BB control method is a useful approach for coherent controlling spin qubits on graphene.

5. Conclusion

In summary, we have proposed a scalable scheme of quantum computation based on GNR with a sequence of Z-shaped structures with high efficiency and fidelity. The qubit is encoded in electron or hole spin states, which is naturally localized in the zigzag region of GNR without confined gates. The neighboring qubits are found to have an always-on Heisenberg interaction and the quantum information in qubits can be protected from decoherence induced by the environment, and undesired disturbance induced by the inherent qubit–qubit interaction, by BB control and DFS strategies. Because of recent achievements in the production of GNR, this approach may be implementable within the present techniques, and offers a new possibility for QIP on graphene.

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