Scalable Quantum Computing based on Spin Qubits in CNT QD

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We study experimentally demonstrated single-electron $^{12}\text{C}$ CNT QD with significant spin-orbit interaction as a scalable quantum computer candidate. Both electron spin and orbital angular momentum can serve as a logical qubit for quantum processing. We introduce macroscopic quantum memory for the system in a form of injected either magnetic or spin carrying atomic ensemble into the nanotube. CNT provides with a stable atomic trap in finite temperature and with one-dimensional nuclear spin lattice in an external magnetic field. The electron is coupled to the atomic ensemble through either magnetic or hyperfine interaction. Easy electron and nuclear spin read-out procedure for this system is possible.

I. INTRODUCTION

The spin degrees of freedom are promising stationary qubit candidates useful for quantum information processing, quantum computation and quantum memory $^{[1, 2, 3, 4, 5]}$. Ease in accessibility and possibility of coupling to light $^{[7, 8]}$ makes the electronic spin suitable for quantum gating. Due to long coherence times of order of seconds $^{[2]}$, the nuclear qubit is likely to perform as a quantum memory.

Since the two seminal papers on solid state based quantum computer by Kane $^{[9]}$ and Loss and DiVincenzo $^{[10]}$, the theoretical and experimental effort has been pursued to realize a physical system which will unify the electronic and nuclear spins and where the spin - spin interactions will be controllable $^{[11, 12]}$. This is difficult because the interaction responsible for coupling, and thus information transfer between the electronic and nuclear spins, should be strong enough in order to perform quantum operations effectively. However, it is not possible to turn the interaction off after the operation is completed and thus the coupling will result in rapid spin relaxation and decoherence $^{[13]}$. Also unavoidable random nuclear field fluctuations influence the electron $^{[14]}$.

Carbon nanotube quantum dots (CNT QD) constitute an excellent physical system where mutual interactions between one-dimensional spin structures towards applications in quantum computation can be studied. Recently it was theoretically shown that relatively weak hyperfine interactions in $^{13}\text{C}$ (nuclear spin $I = 1/2$) enriched CNT QD lead to the nuclear and electronic self-stabilizing spin ordered phases in finite temperatures $^{[15]}$ while keeping the electron decoherence time of order of microseconds $^{[16]}$. Experimentally, in $^{13}\text{C}$ CNT double QDs the influence of controllable nuclear spin environment on few-electron spins state, the strength of hyperfine interaction as well as relaxation and dephasing times were determined $^{[17, 18]}$.

In this paper we study experimentally demonstrated single-electron $^{12}\text{C}$ CNT QD with significant spin-orbit interaction $^{[19]}$ as a scalable quantum computer candidate obeying all the DiVincenzo requirements $^{[20]}$. In this system both electron spin and orbital angular momentum can serve as a qubit for processing. Anomalous spin relaxation times for this system were found $^{[21]}$. Since $^{12}\text{C}$ atom does not carry nuclear spin, we provide macroscopic quantum memory for the system in a form of injected either magnetic or spin carrying atomic ensemble into the nanotube. Thus, the electron is coupled to the atomic ensemble through either hyperfine or magnetic interaction. After information recording onto the atomic ensemble the electron can be off loaded to turn the electron-nuclear interactions off. Easy electron spin read-out procedure for this system is possible.

Originally, encapsulation of molecules and other nano-objects in CNT was extensively studied towards high energy storage and its controllable realise (see e.g. $^{[22, 23]}$). However, up to our best knowledge it has never been investigated towards a neutral atomic trap and macroscopic quantum memory applications. Carbon nanotube provides with stable atomic trap in finite temperature (preventing from possible molecular phase formulation)

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as well as with one-dimensional nuclear spin lattice in an external magnetic field.

Similar idea to our was explored for intercalated fullerens. Single nitrogen ($^{14}$N, $^{15}$N) or phosphorus ($^{31}$P) atoms injected into a $C_{60}$ molecule would serve as a quantum memory [24, 25, 26]. However, for these schemes the read-out protocol turned out to be very challenging. Moreover, our scheme involves macroscopic atomic ensemble, thus enhancing the efficiency of interaction with a single electron and enabling coupling to light and memory read-out via Faraday effect.

This paper is organized as follows. In section II we briefly identify the energy eigenstates of the $^{12}$C CNT QD and possible logical qubit realizations. Next, we discuss the implementations of single- and two-qubits rotations necessary for gating. We discuss the idea of atomic trap for one-dimensional nuclear spin lattice inside the CNT and continue towards its applications as a quantum memory. Finally, we conclude.

II. SCALABLE QC CANDIDATE

Recently, a single-electron carbon nanotube quantum dot (CNT QD) with a significant spin-orbit interaction in regime of mK temperatures has been reported [13]. The electron was loaded onto a small-band gap 'quasi-metallic' single wall nanotube (SWNT) and an external magnetic field $B$ along the nanotube (zed direction) was applied. The field constitutes a quantization axis for the electron's spin and orbital angular momentum degrees of freedom, see Fig. 1. The spin $S_z$ projection is oriented either parallelly $|\uparrow\rangle$ or anti-parallelly $|\downarrow\rangle$ to the field direction. The electron circumvents clockwise $|\uparrow\rangle$ or anti-clockwise $|\downarrow\rangle$ the CNT. The measured energy spectrum versus the magnetic field and a gate voltage $V_g$ shows four possible system quantum states ($\alpha$, $\gamma$, $\beta$, $\delta$). They become pairwise energetically degenerate for some specific values of the external parameters, see Fig. 2. The states are two-dimensional product states $|\alpha\rangle = |1/2\rangle_S |\uparrow\rangle_L$, $|\beta\rangle = |1/2\rangle_S |\downarrow\rangle_L$, $|\gamma\rangle = |-1/2\rangle_S |\uparrow\rangle_L$, $|\delta\rangle = |-1/2\rangle_S |\downarrow\rangle_L$, where $S$ and $L$ stand for spin and angular momentum Hilbert space respectively. For $B = 0$ and $V_g = V_{g0}$ ($V_g = V_{g+}$) the states $\alpha$ and $\gamma$ ($\beta$ and $\delta$) acquire the same energy. Therefore, the system is naturally described by their superpositions, the Kramers doublets being the maximally entangled Bell states at the same time

$$
|\Omega_1\rangle = |1/2\rangle_S |\uparrow\rangle_L + e^{i\varphi_1} |1/2\rangle_S |\downarrow\rangle_L, \quad (1)
$$

$$
|\Omega_2\rangle = |1/2\rangle_S |\downarrow\rangle_L + e^{i\varphi_2} |1/2\rangle_S |\uparrow\rangle_L, \quad (2)
$$

where $\varphi_i$ are relative phases. The energy splitting between them results from the spin-orbit coupling and is equal to $\Delta_{SO} = 0.4$ [19]. For $B = B_+$ ($B = B_-$) and $V_g = V_{g0}$ the states $\alpha$ and $\delta$ (and $\beta$ and $\gamma$) are almost degenerate with a small splitting $\Delta_{KK'} = 65 \mu eV$ emerging from the Dirac cones anti-mixing. Nevertheless, it is possible to couple $\gamma$ and $\beta$ ($\alpha$ and $\delta$) in a non-resonant transition and describe the system by a product state of the form

$$
|\omega_1\rangle = |-1/2\rangle_S (|\uparrow\rangle_L + e^{i\varphi_3} |\downarrow\rangle_L), \quad (3)
$$

$$
|\omega_2\rangle = |1/2\rangle_S (|\downarrow\rangle_L + e^{i\varphi_4} |\uparrow\rangle_L). \quad (4)
$$

please note, that angular momentum part of the state is given by its eigenstates superposition.

Both electron's degrees of freedom, spin and angular momentum $L_z$ (valley degree of freedom), can be used for encoding logical qubits with experimentally feasible one- and two-qubit rotations since they are easily accessible for the external operations. Tunneling spectroscopy realized by rising and lowering the Fermi level provides a read-out scheme for spin state [19].

A. System Hamiltonian

Due to barrier potential in CNT QD electron's longitudinal momentum component $k_\parallel$ is quantized. The nanotube periodic boundary conditions enforce quantization of perpendicular $k_{\perp}$ component as well. Assuming the lowest electron momentum excitation and $k_\parallel = 0$ what corresponds to the experimental situation [13] (for a metallic zig-zag CNT) we identify the orbital angular momentum quantum number to be $\ell = 1$. The eigenstates

![FIG. 1: A single-electron CNT QD in external magnetic field. Spin (yellow arrow) and orbital angular momentum (blue arrow) can be parallel or antiparallel.](image1)

![FIG. 2: Electronic states in CNT QD in presence of an external magnetic field.](image2)
of $\hat{L}_z$ component correspond to its eigenvalues $m_l$ in the following way $|\uparrow\rangle_L = |m_l = 1\rangle_L$, $|\downarrow\rangle_L = |m_l = -1\rangle_L$, where $m_l \leq |L|$. Next, we introduce the total angular momentum quantum number $J = 1/2, 3/2$. This values of $J$ correspond to spin hybridization $^{10}
abla$.

Since the smallest diameter of a stable carbon nanotube is 0.6–0.7 nm, the system can be simulated as a hydrogen-like structure with an electron being 14 times further from the nucleus or as a Rydberg-like atom with an electron on a nanoshell. In this case a Hamiltonian of the system reads

$$H = \frac{1}{2m^2 c^2} \int \frac{dV(r)}{r} \hat{L}_z \cdot \hat{S}_z - \frac{eB}{2m} \left( \hat{L}_z + 2\hat{S}_z \right).$$

The states $\alpha$ and $\gamma$ are the energy eigenstates

$$\alpha = \left| J=3/2, m_J=3/2 \right>, \quad \gamma = \left| J=3/2, m_J=-3/2 \right>, $$

whereas the other two are not

$$\delta = \left( |J=3/2, m_J=-1/2 \rangle - \sqrt{2} |J=1/2, m_J=-1/2 \rangle \right) / \sqrt{3},$$

$$\beta = \left( |J=3/2, m_J=1/2 \rangle + \sqrt{2} |J=1/2, m_J=1/2 \rangle \right) / \sqrt{3}.$$  

B. Logical qubit in $\vec{B} = 0$ regime

Let us define the logical qubit as the energy eigenstates $|1\rangle = \alpha$ and $|0\rangle = \gamma$. One-qubit rotation requires creating superposition of the form $\alpha + e^{i\varphi} \gamma$ for an arbitrary phase value $\varphi$. This is possible by applying magnetic field kick. For $\vec{B}! = 0$ the states $\alpha$ and $\gamma$ correspond to different energy eigenstates $E_\alpha$ and $E_\gamma$, and therefore evolve with different phases $\alpha + e^{i\varphi} e^{-i(E_\alpha - E_\gamma)t/\hbar} \gamma$.

C. Logical qubit in $\vec{B} = B_+ \text{ regime}$

Let us encode the logical qubit in orbital angular momentum $|1\rangle = \gamma$ and $|0\rangle = \beta$. Since the states are not fully energetically degenerate, one-qubit rotations have to induced by a near resonant transition. Simple algebra $\gamma = \frac{1}{2}(\beta + \bar{\gamma}) + \frac{1}{2}(\gamma - \bar{\beta})$ shows that state $\gamma$ addressed by a microwave pulse with $\nu = 65 \text{ GHz}$ evolves to

$$\frac{1}{2}(\gamma + \bar{\gamma}) + \frac{1}{2} e^{i\Delta t}(\gamma - \bar{\gamma}) = \cos(\Delta t) \gamma + \sin(\Delta t) \beta. \quad (6)$$

D. Coupling between two CNT QDs

Two-qubit rotations can be realized using either magnetic dipole interaction

$$H = -\frac{\mu_0}{2\pi} \frac{1}{r^3} (\hat{L}_{z1} \cdot \hat{L}_{z2}) \quad (7)$$

present when the two CNT are located one after another (see Fig. 5) or a Heisenberg spin-spin exchange interaction when two electrons are brought close to each other.

III. 1D NUCLEAR SPIN LATTICE TRAP

A numerical analysis of a potential energy for a system consisting of a single empty SWCNT and gas of hydrogen, nitrogen and phosphorus atoms in $T = 0K$ and in finite temperature $T > 0K$ was performed. The results showed self-induced intercalation of the atoms into the nanotube due to the van der Waals interactions. We employed HyperChem program and performed our calculations using Molecular Mechanics MM+ method for $T = 0K$ and Molecular Dynamics with step size $10^{-4}\text{ps}$ and runtime 1ps for $0 < T < 100K$. Due to the symmetric and periodic structure of the nanotube, the atoms form a string located on the nanotube axis with almost equal spacing between them of approximately 3Å for hydrogen atoms and 3.5Å nitrogen atoms. Moreover, the trapping energy is strong enough to prevent from forming molecular phase of the H and N atoms. Thus, the nanotube provides with a stable atomic trap. If the atoms carry spin, in an external magnetic field they form a 1D nuclear spin lattice. The calculations were obtained for the following nanotubes with similar diameters (around 0.7nm): CNT(5,5) (armchair), CNT(9,0) (zig-zag), CNT(8,2) (chiral). The CNT were filled with 8 atoms. In order to avoid the edge effects CNTs were longer than chain of atoms. The depth of the trapping potential at all atomic positions was the same since the atoms when slightly increasing temperature acquired the same thermal oscillations frequency remained still trapped. Any off-axial position of the chain was self-corrected into the axial location.

Our results remain in agreement with other findings reported in literature. For example, the stability conditions of the carbon chains inside CNT as a function of CNT diameter were studied in $^{12}\nabla$. The binding energy was found to be of order of 0.1eV. The stretching mode frequency for the chain inside CNT was lower than this of the isolated chain as was of order of $2000\text{cm}^{-1}$.

A. Application towards quantum memory

If the spin carrying or magnetic atomic ensemble was injected into the $^{12}\text{C}$ CNT QD, in external magnetic field the system could mimic quantum computer with long lived quantum memory (see Fig. 4). Since carbon C$^{12}$

FIG. 3: Two-qubit coupling architecture for single-electron CNT QDs.
FIG. 4: A single wall carbon nanotube provides with a stable atomic trap.

has no nuclear spin, the system allows for exploiting hyperfine interaction between the macroscopic nuclear spin $\hat{I}$ lattice inside the CNT and the electron

$$H = -\frac{\mu_0}{4\pi} \frac{2\mu_B g_I g_B}{\hbar^2} \frac{1}{r^3} \left( \hat{I} \cdot \hat{L} + 3(\hat{I} \cdot \hat{n})(\hat{S} \cdot \hat{n}) - \hat{I} \cdot \hat{S} \right).$$

(8)

Also angular momentum coupling could be realized if the atoms were magnetic. Read-out scheme for quantum memory is possible via Faraday effect.

IV. CONCLUSIONS

We have discussed a single-electron $^{12}$C CNT QD as a candidate for a scalable quantum computer. This system has already been realized experimentally. It is possible to define logical qubits for the electron degrees of freedom and perform their rotations. Nuclear quantum memory could be added to the system if additionally spin carrying or magnetic atoms were injected into the CNT. Intercalation of CNT of any chirality is already a standard procedure within current technology.

The source of relaxation and decoherence effects for this enriched system remains an open question. They can result from Coulomb interactions or coupling between the electron and CNT phonons [21].

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