Readout scheme of the fullerene-based quantum computer by a single electron transistor

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Abstract

We propose a potential scheme, based on the achieved technique of single electron transistor (SET), to implement the readout of electronic spin state inside a doped $C_{60}$ fullerene by means of the magnetic dipole-dipole coupling and spin filters. In the presence of an external magnetic field, we show how to perform the spin state detection by transforming the information contained in the spin state into the tunneling current. The robustness of our scheme against sources of error is discussed.

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Spin based solid-state quantum computing has drawn much attention recently due to the possibility of building large-scale quantum processors [1]. Besides the challenge of elaborately manipulating individual qubits - encoded into single spin states - within small regions, a serious obstacle is to read out the information contained in each of these qubits. This readout is both necessary to measure the state of the completed computation and required to perform quantum error correction.

To our knowledge, there have been some proposals for single spin detection. The conversion of single spin states into charge states is the main idea in this respect [2, 3]. Our scheme is also based on this idea. Experimentally Scanning-Tunneling-Microscope electron spin resonance (ESR), has demonstrated single molecule ESR spectroscopy of iron impurities in Silicon [4]. However theoretical work remains to clarify for the best description of the effects [5], although experimental work in this respect is still in rapid progress [6]. Micro-Squids is a technique capable of distinguishing large spin difference ($\Delta m_S \sim 30$) [7]. Magnetic Resonance Force Microscopy, which utilizes a cantilever oscillation driven by spins oscillating in resonance spin, is hopeful to be an efficient single spin detector [8], although it has not yet reached single spin sensitivity. Recently, a single $C_{60}$ molecule has been used as a single electron transistor (SET) through electro-mechanical coupling [9]. It may be possible to use this quantum electromechanical system as a single spin detector in the presence of an external magnetic field.

Our work is focused on the detection of the electronic spin states of the dopant atom inside a fullerene $C_{60}$, an essential ingredient in the performance of quantum computing based on the endohedral fullerenes $N@C_{60}$ or $P@C_{60}$ [10, 11, 12]. In many of these fullerene-based designs, the qubits are encoded in nuclear spins. The quantum gating, based on coupling the nuclear spins via the Hyperfine interaction to the electrons and then coupling the electrons via a magnetic dipole interaction, is done by using NMR (i.e., nuclear magnetic resonance) and ESR pulse sequences. It has been checked in detail in [12], that this fullerene-based quantum computing meets the requirement for a quantum computer, except the lack of an effective readout technique. Since the nuclear spin is less sensitive to the external environment, our detection of single spin state would be carried out on the electronic spin state. As the swap between the nuclear spin and the electronic spin is available, the detection of an electronic spin state is an efficient way to execute the readout of a fullerene-based quantum computer.
As shown in [12], quantum information can be encoded in electronic spin states of $|\pm 1/2\rangle$ (called 'inner qubits') or $|\pm 3/2\rangle$ (called 'outer qubits'), and quantum gating can be carried out independently with inner qubits or outer qubits. Therefore what we want to detect is whether the inner qubit is in $|1/2\rangle$ or $|-1/2\rangle$, or whether the outer qubit is in $|3/2\rangle$ or $|-3/2\rangle$.

The endohedral fullerene systems are significantly different from the systems in [2, 3], in that the electrons of the dopant atoms of $C_{60}$ cannot escape the cage while preserving their spin state. Thus many of the readout techniques under development elsewhere [2, 3], will not suit endohedral fullerenes. So the first thing we have to do is to convert the electronic spin state information contained within the endohedral fullerene to an outside mobile electronic spin. We can then detect the outside spin state by transforming the spin-based information into current-based information via spin-filters.

As shown in Fig. 1, our readout device is very similar to a SET, which includes source, island and drain, and the voltages between two of them drive the electrons to jump on or off the island. However, different from [9], in our scheme, we have two built-in spin filters located in the source and drain respectively, which block the spin-up electrons, but only let the spin-down electrons pass [13]. So we have a source which could provide down-polarized current, and the click of the detector implies the arrival of a down-polarized electron. Moreover, we do not consider the vibrational motion of the fullerene. We suppose that the variation of the vibration of the fullerene is only related to the arrival and departure, instead of the spin degrees of freedom, of the mobile electron. The validity of this assumption will be discussed later. Furthermore, the Coulomb Blockade regime is employed [14], which means the $C_{60}$ on the island cannot be charged by more than one extra electron, while an electron can jump on to the island only when the island is electron empty, i.e. after any electron residing on the $C_{60}$ has jumped off.

The key idea of our scheme is to carry out a conditional gating between the motive electronic spin (shortly called 'outside spin') and the stationary endohedral electronic spin (shortly called 'inside spin'). An essential ingredient in our scheme is the microwave controlled entangling of the inside spin and the outside spin. The principle is quite similar to the situation presented in [13], where the the electron transport through a quantum dot entangles Hyperfine-coupled nuclear spins via a spin flip interaction. Since the spin information will be transferred from the inside spin to the outside one, we are able to get the knowledge
of the inside spin from the current constituted by the mobile electrons. We will show that the outside spin interacts with the inside spin via a magnetic dipole-dipole coupling, and using this we can carry out conditional gating between the stationary and mobile spins.

Let us consider the singly charged island. As each of the carbon atoms of the $C_{60}$ molecule are identical, we have no idea which atom absorbs that electron. As a result, the charge can be considered to distribute uniformly on the surface of the fullerene. When an external magnetic field is applied, the net spin effect of the jumping - on electron is equivalent to that of an electron with the same spin state positioned at the core of the fullerene. Therefore, when this charged fullerene is moved close to a fullerene with dopant atoms, the outside spin (on the empty $C_{60}$), will interact with the inside spin (in the doped $C_{60}$), by magnetic dipole-dipole coupling between the geometric centers of the two fullerenes. The strength of this coupling is proportional to $(r/nm)^{-3}$, and is 50 MHz in the case of 1 nm of inter-spin distance [10].

Consider the system with these two coupled fullerenes, the Hamiltonian, in units of $\hbar = 1$, is

$$H_0 = g\mu_B B_1 \sigma^z_1 \otimes I_2 + g\mu_B B_2 I_1 \otimes \sigma^z_2 + J \sigma^z_1 \otimes \sigma^z_2.$$  \hspace{1cm} (1)

where the subscripts 1 and 2 correspond to inside and outside spins, respectively. $J$ is the dipole-dipole coupling strength between the two spins. We suppose that $\nu_1 = g\mu_B B_1/2$, and $\nu_2 = g\mu_B B_2/2$. As in [11, 12], we suppose $J < |\nu_2 - \nu_1|$ (weak coupling limit) and thereby we can neglect the terms non-commuting with the Zeeman terms. We have the eigenenergies $\epsilon^\pm_\pm = \pm 3\nu_1 + (\nu_2 \pm 3J/4)$, $\epsilon^\pm_\pm = \pm \nu_1 + (\nu_2 \pm J/4)$, $\epsilon^3_\pm = \pm \nu_1 - (\nu_2 \pm J/4)$, and $\epsilon^4_\pm = \pm 3\nu_1 - (\nu_2 \pm 3J/4)$, within the Hilbert space spanned by $|\pm 3/2, \pm 1/2\rangle$, and $|\pm 1/2, \pm 1/2\rangle$.

To read out the state of the inside spin by means of the current made of mobile electrons we have to carry out two-qubit gating by ESR between the inside and outside spins. Since the outside spin is very sensitive to decoherence, our gating time should be shorter than the decoherence time of the outside spin. As the outside spins are well polarized and their interaction with the inside spin is controlled the outside spins do not constitute a source of decoherence. Potential sources of decoherence would be magnetic dipole interactions with unknown spin centers, both electronic and nuclear etc. As in [12], we consider the ideal case when $T_2 \sim T_1$ for the electrons (in the case of zero spin density). Due to the cage effect of the fullerene, $T_1^{in}$ of the inside spin is longer than 1 sec [16], whereas $T_1^{out}$ of the outside
spin may be much shorter. Anyway $T_{1\text{out}}$ is much longer than $T_{2\text{out}}$, which is generally $T_{1\text{out}} \sim 100\ T_{2\text{out}}$. We suppose that $T_{2\text{out}}$ is long enough to avoid the related homogeneous broadening affecting our scheme. On the other hand, to implement ESR with microwave pulses, we have to avoid degenerate transitions. To this end, we introduce a magnetic field gradient with $\partial B/\partial z \geq 4 \times 10^6\ T/m$, which separates the resonance frequencies of $| \pm 1/2 \rangle$ by $\delta = 2(\nu_2 - \nu_1) \geq 127\ MHz$. In Table I, we list the ESR transition frequencies. We can classify those transition frequencies which have (have no) $\delta$ dependence as those which leave the inside spin unaltered (altered). This observation will play a crucial role in the following.

Suppose that $\nu_1$ and $\nu_2$ are of the order of GHz, and the system under consideration is in the Coulomb Blockade regime. We define the dwell times $t$ of the mobile electron to be the duration of each electron residing on to the island, and suppose we can tune $t \sim 150\ ns$. As part of any previous quantum computation, we will know whether the qubit has been encoded into the inner or outer endohedral electron qubit levels, i.e. $| \pm 1/2 \rangle$ or $| \pm 3/2 \rangle$. Based on this knowledge, our detection scheme can be described as follows: For the case of outer qubits, we send one ESR pulse every $150\ ns$ with the frequency of $2\nu_1 + 2\delta + 3J/2$ for a certain period, say, $10^{-2}\ sec$. If no current is found behind the spin filter in the drain, the inside spin is in the $| 3/2 \rangle$ state, otherwise, it is in the $| -3/2 \rangle$ state. Similarly, for the inner qubits case, we send one ESR pulse every $150\ ns$ with the frequency of $2\nu_1 + 2\delta + J/2$. If after irradiation for a short period there is no current found behind the spin filter in the drain, the inside spin must be in the $| 1/2 \rangle$ state, otherwise, it is in the $| -1/2 \rangle$ state.

The operation of our scheme relies on four quantities. First of all, we need to know the strength of the magnetic dipole-dipole coupling $J$, which determines the frequency of the ESR pulse. This can be determined through interrogative ESR pulse operations. Secondly, the dwell time of the mobile electrons on the island should be controlled so that we can have good quality two-spin gating by ESR pulses under the Coulomb Blockade regime. Thirdly, the linewidth of ESR pulses should be narrower than $J$. Fourthly, the spin filters located in the source and drain must work well to ensure that only down-polarized electrons are transmitted.

However, the tunneling of the mobile electrons is intrinsically stochastic, which can be described by normal distribution. Experimentally by adjusting the voltages and the electron density of the source, we can have a mean dwell time $t_0$. For simplicity we define $\alpha = \sigma/t_0$ where $\sigma$ is the deviation of the normal distribution. Considering this deviation, when we
perform a spin flip of a down-polarized mobile electron, the time evolution would instead yield $-i \cos(\alpha \pi/2)|\uparrow\rangle \mp \sin(\alpha \pi/2)|\downarrow\rangle$ corresponding to dwell time $t_0(1 \pm \alpha)$ respectively.

Let us estimate the implementation of our scheme under the influence of noise sources. Based on the fact that the inside spin is much more stable than the outside spins, we consider following Hamiltonian $H = \tilde{H}_0 + H_1 + H_2$, with

$$\tilde{H}_0 = H_0 + H_b^s + H_d^s, \quad (2)$$

where $H_1 = \Omega_e(e^{-i\omega_e t}\sigma_2^+ + e^{i\omega_e t}\sigma_2^-)$ and $H_2 = (\Gamma_s\sigma_2^+ + \Gamma_\uparrow\sigma_2^-) + \Gamma_{ps}\sigma_2^z$, with $\sigma^k_2 (k = z, +, -)$ being Pauli operators for the outside spin. $s = l, r$ correspond to source and drain respectively. $H_b^s$ and $H_d^s$ are baths associated with spin flip and dephasing of the outside spins respectively. $\omega_e$ is the frequency of ESR. $\Gamma_s$ and $\Gamma_{ps}$ are the couplings to the outside spins which yield spin flip and dephasing respectively. If the pulse is resonant with one of the transition frequencies of the outside spins (in Table 1), we suppose $\Omega_e = \Omega_0$. For non-resonant case, we consider $\Omega_e = 0$ (i.e. no interaction) due to the large detuning. In this case, given a perfectly polarized current produced in the source, since the nonresonant ESR does not flip the outside spin, the outside spin should still remain well polarized after the mobile electron jumps off the island. As a result, we consider $\Gamma_{ps}$ to be zero. This kind of problems have been well studied [17], from which we know that the high quality measurement in the detector can be achieved within the time period $1/|\Gamma_r|^2$.

Our interest is more focused on the case of $\Omega_e = \Omega_0$. In the readout stage with inside and outside spins being initially well polarized, except the short period of interaction under the ESR pulse, there is no entanglement between the inside and outside spins. Assuming a perfectly down-polarized source, since we cannot exactly control the dwell time of the mobile electrons on the island, the resulting imperfect ESR generated spin flip due to the time deviations $\sigma$, generates a superposition state which is more sensitive to decoherence. This is the main source of error. To gain more physical insight in this case, we will only consider the state of the mobile electron after the irradiation by the ESR pulses, with the initial state being $|\psi_\pm\rangle = -i \cos(\alpha \pi/2)|\uparrow\rangle \mp \sin(\alpha \pi/2)|\downarrow\rangle$. In the Coulomb Blockade regime we examine the subsequent decoherence of the mobile electron following the master equation [18],

$$\frac{d\rho_2}{dt} = \frac{\gamma_0}{2}(2\sigma^-_2\rho_2\sigma^+_2 - \sigma^+_2\sigma^-_2\rho_2 - \rho_2\sigma^+_2\sigma^-_2) - \gamma_p[\sigma_2^z, [\sigma_2^z, \rho_2]], \quad (3)$$

where $\rho_2$ is the density operator of the outside spin. $\gamma_0$, and $\gamma_p$, are decoherence rates
regarding $T_{1}^{\text{out}}$, and $T_{2}^{\text{out}}$ respectively. To avoid indistinguishability in the spectrum due to homogeous broadening regarding $T_{2}^{\text{out}}$, we suppose $1/\gamma_p = 25$ ns. Straightforward calculation shows in Fig. 2 that the cross terms $\rho_{2\uparrow\downarrow}$ (or $\rho_{2\downarrow\uparrow}$), related to $\cos(\alpha\pi/2)\sin(\alpha\pi/2)$, will decohere to zero quickly. As long as $\alpha$ is small enough, the initial spin flip signature will remain as the population in $|\uparrow\rangle$ will still be much larger than that of $|\downarrow\rangle$ even after a time evolution for 1000 ns. This signature is translated to a current signature - a macroscopic quantity, and the small error occurring in individual electron flips will not significantly affect our scheme as long as $\alpha$ is not too large. In above mentioned case (i.e., Eq. (3)), the detected current will be somewhat weaker than the perfect case ($\alpha = 0$). By considering the contrast of the current, however, we can still recognize the correct spin signature from the brightness of the current. Therefore, our scheme is robust due to this projective strong measurement.

Although we considered a perfect polarized current in above treatment, there most likely will be some small leakage of undesired electrons out of the spin filters. In this case, any up-polarized component mixing in the down-polarized current would evolve under resonant irradiation of ESR pulses with the frequency $2\nu_1 + J/2$, (see Table I). Employing a magnetic field gradient to break the degenerate transitions (i.e. a non-zero $\delta$), makes such evolution non-resonant under the above scheme. In other words, with this magnetic field gradient, our scheme is robust to the non-ideal spin-polarized current. However, strictly speaking, even for the case of very small undesired spin-polarized current, the full numerical study of Eq. (2) is necessary. We will investigate this point in detail elsewhere.

On the other hand, our scheme also works for the imperfectly spherical fullerene case, in which additional anisotropy terms, such as $(\sigma_i^z)^2$ and $(\sigma_i^z)^4$ ($i = 1, 2$), should be considered in Eq. (1). This can be easily checked by straightforward calculation that those additional terms only change the bottom six frequencies in Table 1, instead of the top four ones.

So far, our discussion has been based on the assumption that the spin degrees of freedom of the mobile electron is independent of the vibration of the fullerene. This is true in the case of a spatially constant magnetic field. In the case of a magnetic field with spatial gradients, however, we should consider the effects of this magnetic gradient due to its interaction with the inside and outside spins assuming the fullerene is bound harmonically in space. It yields a shift of position $\Delta z = (2g\mu_B/k)\partial B/\partial z$, with $k = 70$ N/m, being the force constant of the binding harmonic oscillator force. We get $\Delta z = 2.1 \times 10^{-7}$ pm, which is negligible.
compared to the distance variation $\delta = 4$ pm caused by the Coulomb interaction upon the arrival of the extra electron on the fullerene. Therefore our assumption of non spin-vibration coupling is reasonable and valid.

If we suppose $t_0 = 150$ ns, then we have to emit ESR pulses sequently with each pulse length of 140 ns. To have a flip operation on the outside spin, $\Omega_0$ should be 36 MHz. This kind of ESR pulses, with linewidth much narrower than $J$, have been achieved experimentally [22].

Technically, the spin filters can be built from ferromagnetic materials [23], or semiconductor quantum dots [3], which can block up-polarized electrons with high fidelity. Experimental demonstrations of the generation of spin polarized current with high quality has been achieved by [21]. Moreover, the required magnetic field gradients is readily available with current technique [24], and the gate performance by ESR rectangular pulses can be improved by the sophisticated composed rotation method [25]. Therefore, to reliably carry out our scheme, on the one hand, we need a long dwell time with the deviation as small as possible. On the other hand, the longer decoherence time (e.g. $T_{2}^{out} > 25$ ns) of the outside spin is highly expected.

In conclusion, we have proposed a potential scheme for the readout of single spin state inside a fullerene. By strictly controlling the tunneling of the electron and implementing ESR pulses, based on a SET device, we can reliably convert a spin state signature into a current signature, which is readable and can be detected robustly. Since SET technology is developing rapidly, our scheme offers a promising way for the readout of fullerene based quantum computation.

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time of bulk two-dimensional electron gas is 150 ns. So by considering the difference between bound and unbound electrons, we here give this value based on the fact that the homogeous broadening should be smaller than the transition frequency difference $J$ shown in Table I.

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**Table I.** The resonant transition frequencies in various cases, where the first four rows are the transition frequencies of the outside spin with respect to a certain inside spin, while the final six rows list the transition frequencies of the inside spin with respect to a certain outside spin.

| Inside Spin | Outside Spin | Transition Frequency |
|-------------|--------------|----------------------|
| $|3/2\rangle$ | $|1/2\rangle \leftrightarrow | -1/2\rangle$ | $2\nu_1 + 2\delta + 3J/2$ |
| $|1/2\rangle$ | $|1/2\rangle \leftrightarrow | -1/2\rangle$ | $2\nu_1 + 2\delta + J/2$ |
| $| -1/2\rangle$ | $|1/2\rangle \leftrightarrow | -1/2\rangle$ | $2\nu_1 + 2\delta - J/2$ |
| $| -3/2\rangle$ | $|1/2\rangle \leftrightarrow | -1/2\rangle$ | $2\nu_1 + 2\delta - 3J/2$ |
| $|3/2\rangle \leftrightarrow |1/2\rangle$ | $|1/2\rangle$ | $2\nu_1 + J/2$ |
| $|1/2\rangle \leftrightarrow | -1/2\rangle$ | $|1/2\rangle$ | $2\nu_1 + J/2$ |
| $| -1/2\rangle \leftrightarrow | -3/2\rangle$ | $|1/2\rangle$ | $2\nu_1 + J/2$ |
| $|3/2\rangle \leftrightarrow |1/2\rangle$ | $| -1/2\rangle$ | $2\nu_1 - J/2$ |
| $|1/2\rangle \leftrightarrow | -1/2\rangle$ | $| -1/2\rangle$ | $2\nu_1 - J/2$ |
| $| -1/2\rangle \leftrightarrow | -3/2\rangle$ | $| -1/2\rangle$ | $2\nu_1 - J/2$ |
FIG. 1: Schematic diagram of our readout scheme, where the fullerene with inside spin is to be detected, and the spin-readout device consists of source, island, drain, two built-in spin filters and a detector. The unfilled circles denote the electrons whose spins have been flipped by ESR pulses. The spin filter blocks spin-up electrons and only lets spin-down electrons pass. As a result, we have down-polarized current in the source, and the click of the detector means the presence of the filled circle electrons in the drain.
FIG. 2: Time evolution of the density matrix elements for the case of $\omega_e = \omega_0$ with the initial state $-i \cos(\alpha \pi/2) |\uparrow\rangle \mp i \sin(\alpha \pi/2) |\downarrow\rangle$, where $1/\gamma_p = 25$ ns, the solid and dashed curves represent $\alpha = 0.1$ and $\alpha = 0.2$ respectively. $P_1$, $P_2$ and $P_3$ correspond to $\rho_{2\uparrow\uparrow}$, $\rho_{2\uparrow\downarrow}$ (or $\rho_{2\downarrow\uparrow}$) and $\rho_{2\downarrow\downarrow}$, respectively.