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Buckyball quantum computer: realization of a quantum gate

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Abstract. We have studied a system composed by two endohedral fullerene molecules. We have found that this system can be used as good candidate for the realization of quantum gates. Each of these molecules encapsules an atom carrying a spin, therefore they interact through the spin dipole interaction. We show that a phase gate can be realized if we apply static and time dependent magnetic fields on each encased spin. We have evaluated the operational time of a π-phase gate, which is of the order of ns. We made a comparison between the theoretical estimation of the gate time and the experimental decoherence time for each spin. The comparison shows that the spin relaxation time is much larger than the π-gate operational time. Therefore, this indicates that, during the decoherence time, it is possible to perform some thousands of quantum computational operations. Moreover, through the study of concurrence, we get very good results for the entanglement degree of the two-qubit system. This finding opens a new avenue for the realization of quantum computers.

PACS. 03.67.-a Quantum information – 03.67.Lx Quantum computation – 61.48.+c Fullerenes and fullerene-related materials

1 Introduction

During recent years there is a strong progress in modeling physical realizations of a quantum computer. Many quantum physical systems have been investigated for the realization of quantum gates. The most remarkable studies were related to systems associated to Quantum Optics Ion Traps, to Quantum Electrodynamics in Optical Cavities and to Nuclear Magnetic Resonance. All these experiments are aimed to realize a quantum gate. The first type of experiments is based on trapping ions in electromagnetic traps, where the ions, which encode the qubit in the charge degrees of freedom, are subjected to the mutual electrostatic interaction and to a state selective displacement generated by an external state dependent force [1–4]. Cavity quantum electrodynamics (QED) techniques are based on the coherent interaction of a qubit, generally represented by an atom or semiconductor dot system, with a single mode or a few modes of the electromagnetic field inside a cavity. Depending on the particular system, the qubit can be represented by the polarization states of a single photon or by two excited states of an atom. Although cavity QED experiments are very promising, they have been accomplished for few qubits [5–8]. In the third experiment, nuclear spins represent qubits. These spins can be manipulated using nuclear magnetic resonance techniques, and through the study of the quantum behavior of spins, quantum operations are realized. However, the number of spins which can be collected in a system is very limited, and this forbids the building up of a scalable quantum computer [9–12]. From the study of such systems, we learn that the decoherence phenomenon is the main issue which prevents the realization of quantum gates.

Here we will focus on a physical systems, which will be able to produce a realistic quantum gate. The basic elements of our system are fullerene molecules with encapsulated atoms or ions, which are called *buckyballs* or *endohedral fullerenes*. Each of the trapped atoms carries a spin. This spin, associated with electronic degrees of freedom, encodes the qubit. It has been shown [13], that these endohedral systems provide a long lifetime for the trapped spins and that the fullerene molecules represent a good sheltering environment for the very sensible spins trapped inside. These endohedral systems are typically characterized by two relaxation times. The first is T_1, which is due to the interactions between a spin and the surrounding environment. The second one is T_2 and it is due to the dipolar interaction between the qubit encoding spin and the surrounding endohedral spins randomly distributed in the sample. While T_1 is dependent on temperature, T_2 is practically independent of it. The experimental measure of the two relaxation times shows that T_1 increases with decreasing temperature from about 100 μs at $T = 300$ K to several seconds below $T = 5$ K, and that the value of the other relaxation time, T_2, remains constant, that

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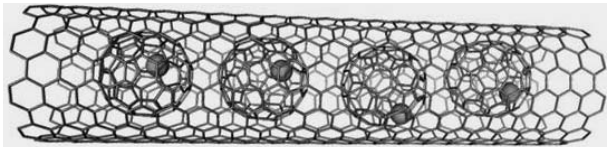

Fig. 1. The schematic picture of the peapod: a nanotube filled with four endohedrals.

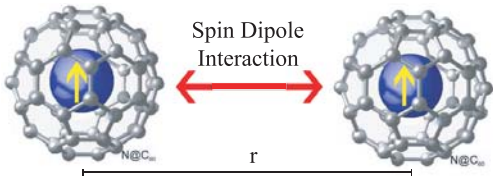

Fig. 2. Our system: two interacting buckyballs.

is $T_2 \simeq 20\ \mu$s [14,15]. In comparison with T_2 the value of T_1 is very large, therefore the system decoherence is determined by the spin-spin relaxation processes. It is supposed that the value of T_2 can be increased, if it will be possible to design a careful experimental architecture, which could screen the interaction of the spins with the surrounding magnetic moments. It should be possible to reduce the relaxation time of the system due to the random spin-spin interactions, if we consider a system composed by arrays of endohedrals encapsulated in a nanotube [16], this system is also called as *peapod*, see Figure 1, or considering buckyballs embedded on a substrate. These should be reliable systems for the realization of quantum gates. In such architectures the decoherence time for each encapsulated spin should be longer.

Quantum computing through the study of doped fullerene systems has been investigated in many works [17–21]. Although we have followed many ideas suggested in these previous papers, we consider a different approach for the realization of quantum gates.

Our study is focused on a system composed by two buckyballs. Our aim is the realization of a quantum π-*gate*, which is a generalization of the *phase gate*, this will be treated in Section 3. To perform the π-gate, we need to know the time evolution of the coefficients of the standard computational basis states over which we expand the wave function of our system. The two particle phases are evaluated through the numerical solution of the Schrödinger equation, see Sections 5–6. We have used two approaches: a time independent Hamiltonian, see Section 5, and a time dependent one, see Section 6. The main result of our study is the gate time, that is the time required by the system in order to perform the π-gate. The values obtained are around $\tau \simeq 1 \times 10^{-8}$ s, which is a few orders smaller than the shortest relaxation time, T_2. From the comparison of the gate time, τ, to the relaxation time, T_2, we get that it is theoretically possible to realize some thousands of basic gate operations before the system decoheres. We have also checked the reliability of our gate through the analysis of the *concurrence* of the two-qubit state, see Section 4. The best value for the concurrence is obtained in the case of a time dependent Hamiltonian, while the gate time is nearly the same in both cases.

2 Physical features of the system

The system under consideration is composed by two interacting buckyballs, see Figure 2. Several experimental and theoretical studies on buckyballs [13,17,22–25], show that many different types of atoms can be encased in fullerenes molecules. However, in most of the studied endohedral fullerenes, there is a charge transfer from the encapsulated atom to the fullerene cage, with a resulting considerable alteration of the electronic properties of the cage. This is not the case for group V encased atoms. These atoms reside just at the center of the fullerene molecule, therefore there is no hybrididazion of the electron cloud of the encased atom and there is no Coulomb interaction with the fullerene cage. In particular, the most promising endohedral molecule should be the $N@C_{60}$, which is characterized by many interesting chemical-physical properties. Following references [13,17,25], experiments and theoretical calculations suggest that there is a repulsive exchange interaction between the fullerene and the electronic cloud of the encapsulated atom. The electrons in the cloud of the encased nitrogen are tighter bound than in a free nitrogen atom, which allow the encased nitrogen to be less reactive even at room temperature. These results, together with the location of the nitrogen atom in the central site, suggest that in $N@C_{60}$ the nitrogen can be considered as an independent particle, with all the properties of the free atom. Since any charge interaction is screened, the fullerene cage does not take any part in the interaction process and it can be considered just as a trap for the nitrogen atom. Therefore, the only physical quantity of interest is the spin of the trapped particle. A nitrogen atom can be effectively described as a 3/2-spin particle. This spin is associated with the electronic degrees of freedom. Taking into account also the nuclear spin, which is 1/2 for the $N@C_{60}$, the number of relevant degrees of freedom will be not increased [26]. We will consider a more simple model assuming that the encased atoms are described as 1/2-spin particles. In absence of any mutual interaction and without any applied magnetic field, the energy levels associated with these spin particles are degenerate. If we apply a static magnetic field, this degeneracy is lifted. As a result, due to the Zeeman effect, a two level system arises for each 1/2-spin particle. Each of these two levels encodes the qubit. The spin-up component, $m_s = +1/2$, encodes the computational basis state $|1\rangle$, and the spin-down component, $m_s = -1/2$, represents the state $|0\rangle$.

3 Gate operation: the phase gate

Quantum computers operate with the use of *Quantum Gates*. Quantum gates are defined as fundamental quantum computational operations. They are presented as unitary transformations, which act on the quantum states,

which describe the qubits. Therefore a quantum computer must operate with the use of many quantum gates. The simplest gates are the single-qubit gates. Since our system is composed by two qubits, we will consider a two-qubit quantum gate. One of the most important quantum gates is the *Universal Two-Qubit Quantum Gate* [12], which is called the CNOT-gate. The CNOT operation is defined by the following four by four unitary matrix

$$U_{\mathrm{CNOT}} = \begin{pmatrix} 1\,0\,0\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,1 \\ 0\,0\,1\,0 \end{pmatrix}, \tag{1}$$

and its action over the computational basis states reads:

$$\begin{aligned} |00\rangle &\rightarrow |00\rangle; \\ |01\rangle &\rightarrow |01\rangle; \\ |10\rangle &\rightarrow |11\rangle; \\ |11\rangle &\rightarrow |10\rangle. \end{aligned} \tag{2}$$

The CNOT gate is given by the composition of a single-qubit Hadamard gate followed by a two-qubit π-gate, finally followed by another single-qubit Hadamard gate. The representation of the Hadamard gate in the Bloch sphere is a $\pi/2$ rotation about the y-axis, followed by a reflection of the x-y plane. In this paper we will focus on the realization of the two-qubit π-gate. It is a particular choice of the general *phase gate*, represented by the following matrix

$$G = \begin{pmatrix} 1\,0\,0\,\;0 \\ 0\,1\,0\,\;0 \\ 0\,0\,1\,\;0 \\ 0\,0\,0\,e^{\imath\vartheta} \end{pmatrix}, \tag{3}$$

and its action on the computational basis states is the following:

$$|00\rangle \rightarrow |00\rangle \tag{4}$$

$$|01\rangle \rightarrow |01\rangle \tag{5}$$

$$|10\rangle \rightarrow |10\rangle \tag{6}$$

$$|11\rangle \rightarrow e^{\imath\vartheta}|11\rangle. \tag{7}$$

When $\vartheta = \pm\pi$, the resulting quantum gate is called a π-*gate*. In general, the time evolution of the four states of the standard computational basis can be described as follows:

$$\begin{aligned} |00\rangle &\rightarrow e^{i\phi_{00}}|00\rangle \\ |01\rangle &\rightarrow e^{i\phi_{01}}|01\rangle \\ |10\rangle &\rightarrow e^{i\phi_{10}}|10\rangle \\ |11\rangle &\rightarrow e^{i\phi_{11}}|11\rangle. \end{aligned} \tag{8}$$

In order to obtain the action of the ideal quantum phase gate, equations (4–7), see reference [4], we have to apply the following local operator:

$$\hat{S} = \hat{S}_1 \otimes \hat{S}_2, \tag{9}$$

where

$$\hat{S}_1 = |0\rangle_1\langle 0|e^{\imath s_1^0} + |1\rangle_1\langle 1|e^{\imath s_1^1} \tag{10}$$

$$\hat{S}_2 = |0\rangle_2\langle 0|e^{\imath s_2^0} + |1\rangle_2\langle 1|e^{\imath s_2^1} \tag{11}$$

and the phases s_1^0, s_1^1, s_2^0, s_2^1 are defined as follows:

$$s_1^0 = -\phi_{00}/2 \tag{12}$$

$$s_1^1 = -\phi_{10} + \phi_{00}/2 \tag{13}$$

$$s_2^0 = -\phi_{00}/2 \tag{14}$$

$$s_2^1 = -\phi_{01} + \phi_{00}/2. \tag{15}$$

After a straightforward calculation we obtain the desirable phase:

$$\vartheta = \phi_{11} - \phi_{10} - \phi_{01} + \phi_{00}. \tag{16}$$

In our system, in order to realize a π-gate, we need to know the time evolution of the wave function. The time evolved wave function, expanded on the standard computational basis, is given by the following equation:

$$|\psi(t)\rangle = c_1(t)|00\rangle + c_2(t)|01\rangle + c_3(t)|10\rangle + c_4(t)|11\rangle. \tag{17}$$

Each coefficient $c_i(t)$, $i = 1, ..., 4$, is a complex number, whose phase, arranged as in equation (16), is used for the realization of the π-gate.

4 Concurrence

When we consider a 1/2-spin particle as the encoding system for the qubit, it may incur to a *spin-flip* process. This phenomenon consists in the swapping between the spin-up and spin-down components

$$|0\rangle \rightarrow |1\rangle, \tag{18}$$

$$|1\rangle \rightarrow |0\rangle. \tag{19}$$

If we consider the two-qubit state, known as *EPR pair*,

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}, \tag{20}$$

we can see that it is unaffected by the spin-flip of both qubits. This state, for this feature, is called maximally *entangled*. Therefore, we can define the *entanglement* as the property of quantum states, which shows if the state is good for carrying quantum information. The most entangled a quantum state is, the most reliable it is for transferring quantum information. In our study we have considered the *concurrence*, see reference [27], as a measure of the entanglement of the state describing the two-qubit system. A *pure* state of two particles is called entangled if it cannot be factorisable, that is it cannot be written as the direct product of the states describing each particle. A *mixed* state is entangled if it cannot be represented as a mixture of factorisable pure states. In this section we will refer to the *entanglement of formation*, which quantifies the resources needed for the creation of an entangled state. For a complete treatment about the entanglement of

formation of pure and mixed states see references [28,29]. The entanglement of formation of a quantum state can be evaluated through the concurrence [27]. Since the state describing our system is a pure state, the degree of entanglement of our system can be quantified through the definition of the concurrence for a pure state [27], which is defined by

$$C(\psi) = |\langle\psi|\tilde{\psi}\rangle|, \tag{21}$$

where $|\tilde{\psi}\rangle$ is the spin-flipped state of system. The spin-flip transformation, which for a 1/2-spin particle is the standard time reversal transformation [30], is defined as follows

$$|\tilde{\psi}\rangle = \hat{\sigma}_y|\psi^*\rangle, \tag{22}$$

where $\hat{\sigma}_y$ is the Pauli y-matrix and $|\psi^*\rangle$ is the complex conjugate of $|\psi\rangle$. The entanglement, see [27], is defined as a function of concurrence, through the following equation

$$E(\psi) = f(C(\psi)), \tag{23}$$

where function $f(C(\psi))$ is given by

$$f(C(\psi)) = h\left(\frac{1+\sqrt{1-C(\psi)^2}}{2}\right), \tag{24}$$

$$h(x) = -x\log_2 x - (1-x)\log_2(1-x), \tag{25}$$

where

$$x = \frac{1+\sqrt{1-C(\psi)^2}}{2}. \tag{26}$$

Function $h(x)$ can be seen as the entropy, which measures the physical resources needed to store information [12]. Function $f(C(\psi))$ increases monotonically from 0 to 1 as $C(\psi)$ ranges from 0 to 1. Therefore, the concurrence can be considered as a measure of the entanglement.

The state describing our two-qubit system, written as a superposition of the standard two-qubit computational basis states, is given by

$$|\psi\rangle = c_1|00\rangle + c_2|01\rangle + c_3|10\rangle + c_4|11\rangle. \tag{27}$$

Following equation (22), the spin-flip transformation over the state (27) gives

$$|\tilde{\psi}\rangle = -c_1^*|00\rangle + c_2^*|01\rangle + c_3^*|10\rangle - c_4^*|11\rangle. \tag{28}$$

Finally, we obtain the concurrence of our system, see equation (21), by performing the state product between states (27) and (28). The normalized concurrence of the system is given by the following equation

$$C(\psi) = \frac{2|c_2^*c_3^* - c_1^*c_4^*|}{|c_1|^2+|c_2|^2+|c_3|^2+|c_4|^2}. \tag{29}$$

The result obtained in equation (29) will be used to evaluate the concurrence, i.e. the degree of entanglement of our two-qubit system, arising during the time evolution which leads to the π-gate. When the concurrence related to a wave function reaches its maximum value, the state is maximally entangled. Therefore, at the end of the gate operation we require that the concurrence of the wave function of the system reaches a value close to its maximum.

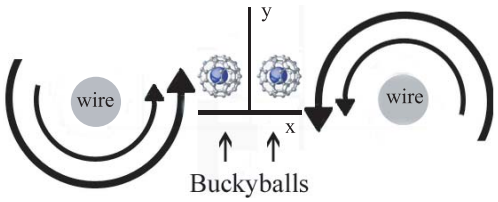

Fig. 3. Schematic arrangement of the physical apparatus for the realization of a magnetic field gradient.

5 Phase gate: time independent case

5.1 Preliminary set-up

Our system is composed by two spins, which interact with a static magnetic field. Applying a static magnetic field oriented in the z-direction, for the Zeeman effect, we get the splitting of the spin z-component into the spin-up and spin-down components. The energy difference between the two levels give the resonance frequency of the particle. However, when we apply a static magnetic field on the whole sample, all the particles will have the same resonance frequency. To perform manipulations on each buckyball, we need to be able to distinguish each of them. This setup leads to the most relevant experimental disadvantage for systems composed by arrays of buckyballs, which is the difficulty in the individual addressing of each qubit particle. This problem can be overcome with the use of external field gradients, which can shift the electronic resonance frequency of the qubit-encoding spins [18,20]. Magnetic field gradients can be generated by considering wires through which flows current. If we place two parallel wires outside our two buckyball system, it is generated an additional magnetic field in the space between the wires, Figure 3. Following a paper by Groth et al. [31], with the help of atom chip technology, wires with a high current density can be built. The magnetic field amplitude generated by the two wires is given by

$$B_g = \frac{\mu_0}{2\pi} I\left(\frac{1}{x+\rho+d/2} + \frac{1}{x-\rho-d/2}\right), \tag{30}$$

where I is the current intensity, d is the distance between the two wires, ρ is the radius of each wire and x is the distance of a buckyball with respect to the origin of the axes. With the choice $I = 0.6$ A, $d = 1$ μm and $\rho = 1$ μm, through a numerical computation, we obtain the magnetic field distribution shown in Figure 4. We could not consider a current greater than $I = 0.6$ A because the wires would face a too high heating process, and eventually they could be destroyed. On the other hand, we could not consider currents smaller than 10^{-1} A, because the arising magnetic field gradient would be too small for each buckyball. In this case, the resonance frequencies related to the buckyballs would differ for only few MHz, which could be a too small gap to be realized by a frequency resonator.

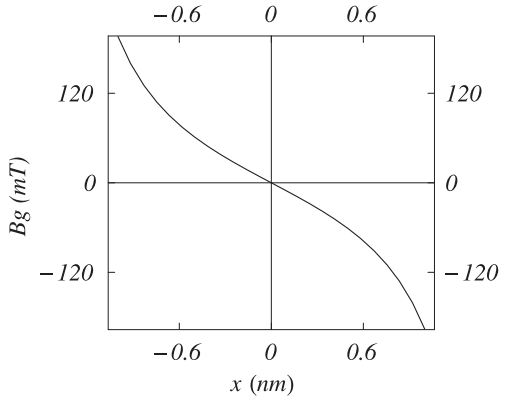

Fig. 4. Magnetic field generated by two 1 μm-radius wires at a distance $d = 1$ μm, which carry a current $I = 0.6$ A. The two buckyballs are placed at a symmetrical distance x with respect to the origin of the axes.

5.2 Realization of the phase gate

Choosing a static magnetic field in the z-direction, the Hamiltonian of the system is given by the following equation ($\hbar = 1$)

$$H = J_0\hat{\sigma}_1 \cdot \hat{\sigma}_2 + g(r)[\hat{\sigma}_1 \cdot \hat{\sigma}_2 - 3(\hat{\sigma}_1 \cdot \mathbf{n})(\hat{\sigma}_2 \cdot \mathbf{n})] - \mu_B[((B_{z_1} + B_{g_1})\hat{\sigma}_{z_1}) \otimes I_2 + I_1 \otimes ((B_{z_2} + B_{g_2})\hat{\sigma}_{z_2})], \quad (31)$$

where J_0 is the exchange spin-spin interaction coupling constant, $\hat{\sigma}_1$ and $\hat{\sigma}_2$ are the Pauli spin matrices, $g(r) = \gamma_1\gamma_2\frac{\mu_0\mu_B^2}{8\pi r^3}$, where μ_0 is the diamagnetic constant, μ_B is the Bohr magneton and r is the distance between the two trapped atoms, $\mathbf{n}$ is the unit vector in the direction of the line which joins the centers of the two encased atoms, $B_{z_1} = B_{z_2}$ is the static magnetic field in the z-direction, B_{g_1} and B_{g_2} are the additional magnetic fields due to the field gradient. We make an assumption, considering the trapped particles as electrons. Therefore the gyromagnetic ratio $\gamma \simeq 2$, and $g(r) = \frac{\mu_0\mu_B^2}{2\pi r^3}$. Through the study of fullerenes' spectra in ESR (Electron Spin Resonance) experiments, and also through theoretical studies, it has been shown [13,32,17], that the exchange interaction is very small. Therefore, in equation (31), we can neglect the exchange term proportional to J_0, leaving the spin dipole-dipole interaction as the leading term of the mutual interaction between the two endohedrals. Choosing the direction of vector $\mathbf{n}$ parallel to the x axis, the dipole-dipole interaction term is simplified as follows

$$\hat{D} = g(r)(\hat{\sigma}_{z_1}\hat{\sigma}_{z_2} + \hat{\sigma}_{y_1}\hat{\sigma}_{y_2} - 2\hat{\sigma}_{x_1}\hat{\sigma}_{x_2}). \quad (32)$$

The Hamiltonian matrix form is given by the following matrix

$$\begin{pmatrix} g(r)+m_1 & 0 & 0 & -3g(r) \\ 0 & -g(r)+m_2 & -g(r) & 0 \\ 0 & -g(r) & -g(r)-m_2 & 0 \\ -3g(r) & 0 & 0 & g(r)-m_1 \end{pmatrix}, \quad (33)$$

where

$$m_1 = -\mu_B(B_{z_1} + B_{g_1} + B_{z_2} + B_{g_2}) \quad (34)$$

and

$$m_2 = -\mu_B(B_{z_1} + B_{g_1} - B_{z_2} - B_{g_2}), \quad (35)$$

are the static magnetic field terms. Solving the Schrödinger equation

$$\imath\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle, \quad (36)$$

where the wave function is a superposition of the standard two-qubit computational basis, given by equation (17), we get the four differential equation system

$$\dot{c}_1(t) = -\imath[(g(r) + m_1)c_1(t) - 3g(r)c_4(t)]; \quad (37)$$
$$\dot{c}_2(t) = -\imath[(-g(r) + m_2)c_2(t) - g(r)c_3(t)]; \quad (38)$$
$$\dot{c}_3(t) = -\imath[-g(r)c_2(t) + (-g(r) - m_2)c_3(t)]; \quad (39)$$
$$\dot{c}_4(t) = -\imath[-3g(r)c_1(t) + (g(r) - m_1)c_4(t)], \quad (40)$$

which allows us to evaluate the phases acquired by each computational basis state during the time evolution. Applying equation (16) to the present time evolved phases, we get the desirable π-gate

$$\vartheta = Arg(c_1(t)) - Arg(c_2(t)) - Arg(c_3(t)) + Arg(c_4(t)) = \pm\pi, \quad (41)$$

where $Arg(c_i(t))$, $i = 1, ..., 4$, which correspond to phases ϕ_{jl}, $j, l = 0, 1$, in equation (16), are the phases of coefficients $c_i(t)$ of equation (17). We have numerically solved the differential equation system (37–40), with the use of a Mathematica programme. The numerical quantities used for the numerical calculations are $r = 1.14$ nm, $B_{z1} = B_{z2} = 10 \times 10^{-2}$ T, $B_{g_1} = 6.08 \times 10^{-5}$ T and $B_{g_2} = -6.08 \times 10^{-5}$ T, which give the resonance frequencies $\omega_1 = 1.7599 \times 10^{10}$ Hz and $\omega_2 = 1.7577 \times 10^{10}$ Hz. The time evolution of the phase ϑ is shown in Figure 5. The gate time, which corresponds to the case $\vartheta = -\pi$ is $\tau \simeq 9.1 \times 10^{-9}$ s. This result has been found for a chosen set of initial conditions $c_i(0)$, $i = 1, ..., 4$. However, we did many trials for different numerical values of the set $c_i(0)$, $i = 1, ..., 4$. In all these cases, phase ϑ shows a linear behavior and the resulting gate times are all in the same range, which is of the order of 10^{-8} s. If the set of initial conditions is real, the starting value of phase ϑ is always equal to zero. If the set of initial conditions is complex, the starting value of ϑ is in the range $[-\pi, +\pi]$, but it can always be rescaled to zero. The numerical value of the distance between the two buckyballs, r, is a fixed value, which depends on the substrate where the buckyballs reside. The amplitude of the static magnetic field has been found by considering the allowed experimental limits for its realization. The chosen value for this amplitude has been found by checking the response of the system, i.e. the gate time, after some trials. Therefore, we can say that the phase gate time depends on the distance between the two buckyballs and on the amplitude of the static magnetic field, but it is independent of the choice of the initial values $c_i(0)$, $i = 1, ..., 4$.

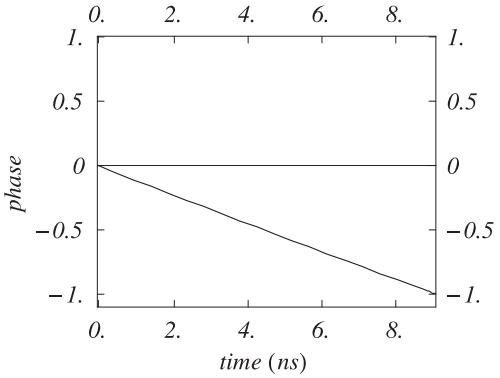

Fig. 5. Time evolution of the phase $\vartheta(t)$ in $\pi-$units, when static magnetic fields oriented in the z direction are applied on two buckyballs separated by a distance $r = 1.14$ nm. The total magnetic field applied on each particle is $B_{z_i} + B_{g_i}$, $i = 1, 2$. In this case we have chosen $B_{z_1} = B_{z_2} = 10 \times 10^{-2}$ T, $B_{g_1} = 6.08 \times 10^{-5}$ T and $B_{g_2} = -6.08 \times 10^{-5}$ T. The value $\vartheta = -\pi$ is reached at the time $\tau \simeq 9.1 \times 10^{-9}$ s.

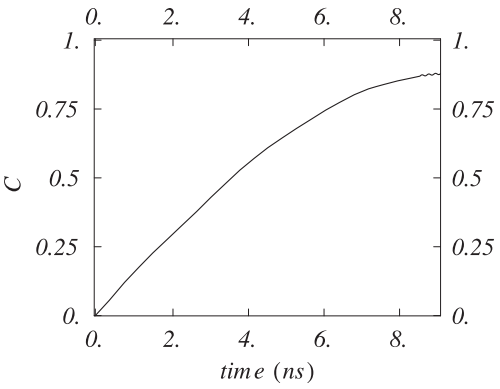

Fig. 6. Time evolution of the concurrence, $C(\psi)$. In this case the two buckyballs, separated by a distance $r = 1.14$ nm, are subjected to static magnetic fields in the z-direction, whose amplitude is $B_{z_i} + B_{g_i}$, $i = 1, 2$. The numerical values chosen for these amplitudes are $B_{z_1} = B_{z_2} = 10 \times 10^{-2}$ T, $B_{g_1} = 6.08 \times 10^{-5}$ T and $B_{g_2} = -6.08 \times 10^{-5}$ T.

If we compare the gate-time, τ, to the shortest decoherence time, $T_2 \simeq 20$ μm, we can deduce that it will be theoretically possible to realize about thousands gate operations before the system relaxes.

To know the fidelity of the gate and the reliability of the results, we need to evaluate the concurrence during the time evolution. With the use of a Mathematica programme we have plotted the time evolution of the concurrence, equation (29), from $t = 0$ s to the gate time $t = \tau$, see Figure 6. Analyzing picture (6), we can see that the concurrence shows a smooth behavior. It monotonically ranges from zero and its maximum is reached at time $t = \tau$, with the respective value $C(\psi(\tau)) = 0.88$. Even if the maximum concurrence does not coincides with the ideal value 1, it is near to this value and the system shows an acceptable degree of entanglement. It is convenient to investigate other system configurations, in order to check if it is possible to improve the concurrence. In

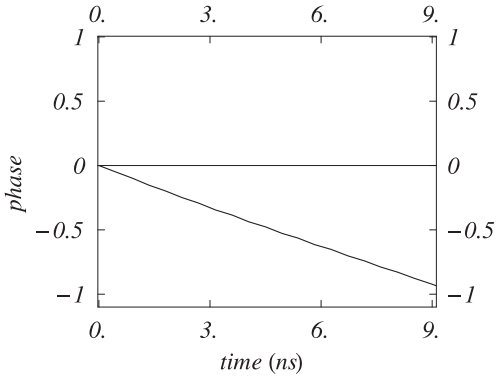

Fig. 7. Time evolution of the phase $\vartheta(t)$ in $\pi-$units, with the respective gate time $\tau \simeq 9.8 \times 10^{-9}$ s. Here the two buckyballs are separated by a distance $r = 1.14$ nm and are subjected to static and time dependent magnetic fields. The total applied magnetic field on each particle is $\boldsymbol{B}(t) = (B_{l_i} \cos\omega_i t, B_{l_i} \cos\omega_i t, (B_{z_i} + B_{g_i}))$, $i = 1, 2$. In the calculations we chose $B_{z_1} = B_{z_2} = 10 \times 10^{-2}$ T, $B_{g_1} = 6.08 \times 10^{-5}$ T, $B_{g_2} = -6.08 \times 10^{-5}$ T, $B_{l_1} = B_{l_2} = 5 \times 10^{-4}$ T, $\omega_1 = 1.7599 \times 10^{10}$ Hz and $\omega_2 = 1.7577 \times 10^{10}$ Hz.

the next section we will analyze the case of an additional magnetic field, oscillating in time in the x-y plane.

6 Phase gate: time dependent case

In this section, we apply to our system an additional time dependent magnetic field. To induce the transitions between the two Zeeman energy levels, we need to apply an oscillating magnetic field in the x-y plane with angular frequency, ω, equal to the spin resonance frequency. In the case of a transverse linear oscillating magnetic field, the total applied magnetic field is given by

$$\mathbf{B}(t) = (B_l \cos\omega t, B_l \cos\omega t, (B_z + B_g)). \qquad (42)$$

The Hamiltonian of the system reads

$$\begin{aligned} H = {} & g(r)(\sigma_{z_1}\sigma_{z_2} + \sigma_{y_1}\sigma_{y_2} - 2\sigma_{x_1}\sigma_{x_2}) \\ & - \mu_B(B_{z_1} + B_{g_1})\sigma_{z_1} \otimes I_2 \\ & - \mu_B(B_{z_2} + B_{g_2}) I_1 \otimes \sigma_{z_2} \\ & - \mu_B B_{l_1}(\sigma_{x_1}\cos\omega_1 t + \sigma_{y_1}\cos\omega_1 t) \otimes I_2 \\ & + I_1 \otimes (-\mu_B B_{l_2}(\sigma_{x_2}\cos\omega_2 t + \sigma_{y_2}\cos\omega_2 t)). \end{aligned} \qquad (43)$$

Like in the time independent case, solving the Schrödinger equation, we get a four differential equation system, whose solution give the time evolution of the phase for each computational basis state. Arranging the phases as prescribed in equation (16), we have obtained the π-gate shown in Figure 7, and the numerical value of the gate time is $\tau \simeq 9.8 \times 10^{-9}$ s. In the numerical computation we have used the additional quantity $B_{l_1} = B_{l_2} = 5 \times 10^{-4}$ T. Also in this case, comparing the gate time, τ, to the decoherence time T_2, we observe that it will be possible to perform about thousands gate operations before the system relaxes. The relevant result in the treatment of

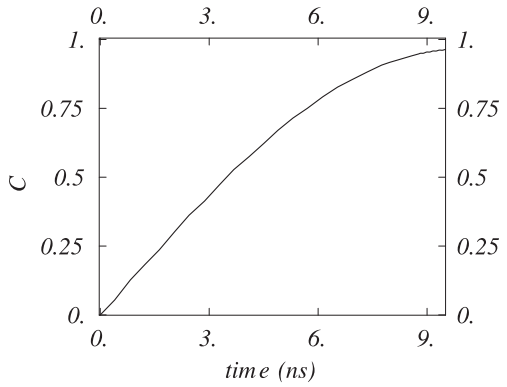

Fig. 8. Time evolution of the concurrence, $C(\psi)$. In this case, the total magnetic field applied on each buckyball is $\mathbf{B}(t) = (B_{l_i} \cos\omega_i t, B_{l_i} \cos\omega_i t, (B_{z_i} + B_{g_i}))$, $i = 1, 2$. The choice of the numerical values is $B_{z_1} = B_{z_2} = 10 \times 10^{-2}$ T, $B_{g_1} = 6.08 \times 10^{-5}$ T, $B_{g_2} = -6.08 \times 10^{-5}$ T, $B_{l_1} = B_{l_2} = 5 \times 10^{-4}$ T, $\omega_1 = 1.7599 \times 10^{10}$ Hz and $\omega_2 = 1.7577 \times 10^{10}$ Hz.

the time dependent case is the concurrence. In Figure 8, it is represented the time evolution of the concurrence, $C(\psi(t))$, which has been numerically evaluated with a Mathematica programme. It shows a monotonic behavior and its maximum, evaluated at time $t = \tau$, corresponds to $C(\psi(\tau)) = 0.96$. Therefore, an additional linearly polarized oscillating field in the x-y plane allows the system to be characterized by a better concurrence degree.

7 Conclusions

To model quantum gates we considered a system composed by two endohedral fullerene molecules, subjected to external magnetic fields. We assume that each molecule may be treated as a 1/2-spin particle, where the spin is associated to the encapsulated atoms. In the magnetic field the spin degeneracy of the spin up and down components is lifted and it arises the Zeeman splitting. As the result, there two two-level system are arising. Each of these two-level systems corresponds to a single qubit. If the applied static magnetic field to the whole sample is homogeneous, each of these qubits will be characterized by the same resonance frequency. This leads to the difficulty in the individual addressing of each single qubit. To overcome this problem, we have to apply inhomogeneous magnetic fields. In this paper we have used a magnetic field generated by two metallic wires. Each wire is carrying a current, therefore the magnetic field is decreasing with the distance from a wire. In the proposed configuration of two parallel wires, there arises a gradient of the magnetic field when we are moving from a wire to the other one. If we place two buckyballs in the space between these two wires, they will be subjected to the gradient of this field, and therefore the associated resonance frequencies of the related two-level system are different. In this paper we have performed a quantum π-phase gate. To realize this particular quantum gate we have estimated the phase of each computational basis state, see equation (16). The leading mutual interaction between the two qubits is the spin dipole-dipole interaction. First we studied the time evolution of our system taking into account this mutual interaction between the qubits and considering the qubits subjected to static magnetic fields only. Then we applied to the system also time dependent magnetic fields. The wave function of the system is given by the superposition of the four computational basis states, see equation (17). The time evolution of the coefficients of each computational basis state is determined via the solution of the Schrödinger equation. With the use of these coefficients and of equation (41), we can evaluate the operational gate time for the π-phase gate. Its numerical value is $\tau \simeq 9.1 \times 10^{-9}$ s for the time independent case, and $\tau \simeq 9.8 \times 10^{-9}$ s for the time dependent one. Comparing the gate time, τ, to the shortest relaxation time, T_2, we have observed that in both cases it will be possible to perform about thousands quantum gate operations before the system decoheres. This is our main result. As far as we are aware, this result indicates that our system could be the most favorable for the realization of a quantum gate. Obviously, for realistic models of quantum computers, the ratio of the decoherence time and the operational time must be very large, otherwise the system relaxes before the completing of the quantum computation. The goal of any quantum computational proposal is the entanglement of the state of the system under consideration. At this purpose, we have studied the concurrence, see Section 4. The concurrence gives information about the entanglement of the state, therefore it is related to the reliability of the gate operation. A maximally entangled state is left unchanged under a spin-flip operation and its concurrence is maximum. In our system, at the end of the gate operation, the value of the concurrence is $C \simeq 0.88$ in the time independent case, and $C \simeq 0.96$ in the time dependent one. Both values are acceptable because they are both related to a very good degree of entanglement for the state describing our system. We can conclude that the best configuration for our system is the time dependent one. It is characterized by a very small operational time, in comparison to the relaxation times, and by the best concurrence.

Many features claim the buckyball systems as good candidates for performing quantum gates. Not only they are characterized by very long decoherence times, but also they can be maneuvered very easily. This feature allows the realization of experimental quantum devices, which form scalable architectures. For example, buckyballs can be embedded in silicon surfaces or arranged in arrays encased in a nanotube (peapod). Moreover, in such systems we suppose that the value of the relaxation time T_2, due to random spin dipole-dipole interactions, could be reduced.

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