PHYSICAL REVIEW A, VOLUME 65, 034303

Ammonia-based quantum computer

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(Received 16 July 2001; published 8 February 2002)

We propose a scheme for quantum computation using two eigenstates of ammonia or similar molecules. Individual ammonia molecules are confined inside fullerenes and used as two-level qubit systems. Interaction between these ammonia qubits takes place via the electric dipole moments, and in particular we show how a controlled-NOT gate could be implemented. After computation the qubit is measured with a single-electron electrometer sensitive enough to differentiate between the dipole moments of different states. We also discuss a possible implementation based on a quantum cellular automaton.

DOI: 10.1103/PhysRevA.65.034303 PACS number(s): 03.67.Lx, 85.65.+h, 61.48.+c

It is widely believed that reliable, useful quantum computers must be manufactured in the solid state. Many of these proposed implementations use artificially created quantum systems to generate the two basis states required for each qubit [1–3]. An advantage is that the system can be (eventually) designed to meet certain requirements for parameters such as energy-level spacing or qubit-qubit interaction energy, but a disadvantage is that some variation in the properties of the qubits must be tolerated. Here, we suggest a scheme involving ammonia molecules as the identical qubits.

The ammonia molecule is a well-known two-level system [4]. The pyramidal symmetry of the molecule means that there are two states of equal energy, with the nitrogen either above or below the plane of the three hydrogens. These two states are connected by a tunnel barrier of height 0.25 eV [5], often called the inversion barrier. The presence of tunneling means that the above, $|u\rangle$, and below, $|d\rangle$, states are not the eigenstates, which are instead the superposition states $|0\rangle$ and $|1\rangle$:

$$|0\rangle=\frac{|u\rangle+|d\rangle}{\sqrt{2}}, \tag{1}$$

$$|1\rangle=\frac{|u\rangle-|d\rangle}{\sqrt{2}}. \tag{2}$$

The difference in the energy eigenvalues of this system is 98.6 μeV, and this transition is exploited in the ammonia maser, which operates at a frequency 23.8 GHz [6].

It is important to note that not all molecules with such pyramidal geometry show these delocalized eigenstates. If the decoherence time is shorter than the tunneling time, then the $|u\rangle$ and $|d\rangle$ states become localized. Examples of such pyramidal molecules showing this localized behavior are arseine and phosphine [5,7]. In these cases there is no energy level splitting: the two eigenstates, $|u\rangle$ and $|d\rangle$ are degenerate. Another example of a molecule that does exhibit delocalized eigenstates is the cyanamide (NH_2CN) [8]. In this case the tunnel barrier has a lower height of 0.058 eV, leading to a higher energy-level splitting, and also a relatively high dipole moment of 0.95 D.

To be a practical system for quantum computation, each ammonia molecule must be somehow isolated and treated as an individual qubit. We suggest confining each ammonia molecule inside a fullerene to allow tagging of the ammonia. In a similar way the nuclear spin of nitrogen confined in a fullerene is used in a proposed variant of the Kane model [9]. This hybrid system, known as an endofullerene [10] has the dual advantage of the identical nature of the qubits combined with the ability, by changing the geometry and spacing, to tune the strength of the interactions. It also has the advantage that although each qubit can be made from identical molecules, each one is sufficiently large to allow manipulation, for example using relatively well-controlled scanning probe microscopy (SPM) or chemical techniques.

For useful quantum computation, the ability to set up an arbitrary superposition of the two basis states is required, written in general as

$$|\Psi\rangle=\alpha|0\rangle\pm\beta|1\rangle, \tag{3}$$

where α and β are both complex coefficients. An arbitrary ratio of these coefficients can be achieved when a resonant (23.8 GHz) electric field is applied for the appropriate time. When the resonant electric field is applied, the molecule undergoes Rabi oscillations between the two eigenstates with a frequency related to the amplitude of the radiation F and dipole matrix element of the transition μ_e,

$$\omega=\frac{\mu_e|F|}{2\hbar}. \tag{4}$$

The phase of the complex coefficients is altered by changing the voltage on a gate localized on one of the ammonia molecules for a certain time. For such a two-level system the vector on the Bloch sphere is rotating: by changing the energy splitting this angular frequency changes, allowing a phase shift to be introduced in the rotating frame.

The most common example of a desired superposition is in the Hadamard transformation

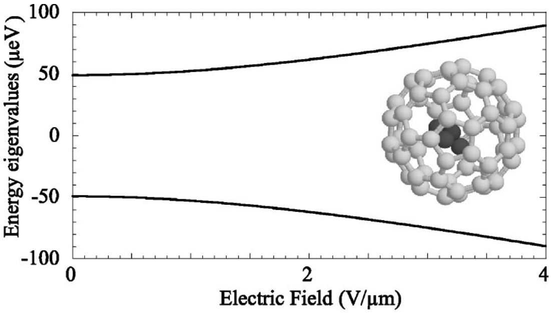

FIG. 1. In controlling the voltage on one of the electrometers the energy splitting of one qubit is changed relative to the other by more than the bandwidth of the microwave source. Typically, the Q factor is greater than 10^5, although it can be much higher. This implies that at least a 0.1% change in the energy gap of one of the qubits is required. This is realizable with a field of 0.34 V/μm, which is easily applied. The inset shows schematically an endohedral ammonia molecule, NH_3C_{60}.

$$U_H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \tag{5}$$

$$U_H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}. \tag{6}$$

If a microwave synthesizer is used as the source then the time to carry out this operation would be, depending on the exact power of the source, about 1 ns to 100 ns. This time scale is achievable using conventional electronics, with for example a p-i-n diode controlling the microwave source. By comparison the pulse length for a π rotation in a version of the maser is 100 μs [11].

The ammonia molecules can be separately addressed by applying a local electric field to individually tune the energy-level splitting for each molecule. A global microwave pulse can then be applied to the system in resonance with a specific ammonia molecule, or other molecules in the same condition. In this way a superposition state may be set up for any one of the ammonia molecules in the system.

In the presence of an applied dc electric field F, the energy splitting between the eigenstates is given by (Fig. 1)

$$\Delta E = \sqrt{(\mu_e F)^2 + E_0^2}. \tag{7}$$

A two-qubit gate, such as the controlled-NOT (c-NOT), can be implemented using the interaction between the electric dipole moments of the ammonia molecules. This interaction has the effect of splitting the energy levels. For two adjacent qubits, the energy levels for qubit B are split from two to four due to the presence of qubit A (Fig. 2). In contrast to some of the other schemes for quantum computation, this interaction is always on, the gate coming from a Rabi pulse at $\omega_{c\text{-NOT}}$. The fact that this interaction is always on is a big advantage, avoiding the necessity of high-speed electronics to switch the interaction: instead a suitable Rabi pulse can relatively easily be generated.

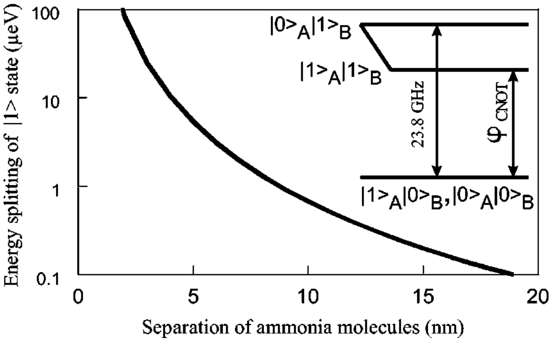

FIG. 2. Diagram showing the energy-level splitting of an ammonia molecule A due to the presence of adjacent ammonia B. A desirable, 1%, splitting of about 1 μeV corresponds to a separation of 9 nm (approximately the resolution of fabrication by electron-beam lithography). The inset shows the energy-level diagram, the splitting corresponding to that of the $|1\rangle_B$ levels.

The strength of the splitting needs to fulfil the same criterion as the energy shift from an external gate: a 0.1% shift at least being required. The degree of energy-level splitting due to a nearest neighbor will depend on the spatial separation of the two ammonia molecules. Ignoring the screening effects of the fullerene, Fig. 2 shows the $|1\rangle_B$ splitting with qubit separation for two separated ammonia molecules. This is calculated using a dipole-dipole interaction for two non-static dipoles oscillating in phase with each other. Phase coupling is seen in the ammonia dimer, with splitting between the antisymmetric and symmetric inversion modes [12]. The effect of this, coupled with the local control using gates of the individual molecules, is that the state of the ammonia molecules can be set up coherently or in a fixed phase relationship.

The c-NOT gate might be realized as follows:

(1) The system is cooled to the ground state using a dilution refrigerator, at a temperature of ~20 mK.

(2) Electric field applied to molecule A, Rabi pulse applied at ω_A to set up desired state of A. Rabi pulse applied at ω_B to set up desired state of B. Electric field removed from molecule A and B.

(3) A π pulse applied at a frequency $\omega_{c\text{-NOT}}$. This is the pulse that performs the c-NOT gate.

(4) States of both A and B measured using single-electron electrometers.

The net result of these operations is a c-NOT gate in which molecule A is the control qubit, and B the target, with unitary transformation

$$U_{c\text{-NOT}}|0\rangle_A|0\rangle_B = |0\rangle_A|0\rangle_B, \tag{8}$$

$$U_{c\text{-NOT}}|0\rangle_A|1\rangle_B = |0\rangle_A|1\rangle_B, \tag{9}$$

$$U_{c\text{-NOT}}|1\rangle_A|0\rangle_B = |1\rangle_A|1\rangle_B, \tag{10}$$

$$U_{c\text{-NOT}}|1\rangle_A|1\rangle_B = |1\rangle_A|0\rangle_B. \tag{11}$$

Considering the case of a two-qubit system, we suggest a geometry that would allow two separately addressable fullerenes (Fig. 3). The two fullerenes are placed on a Si

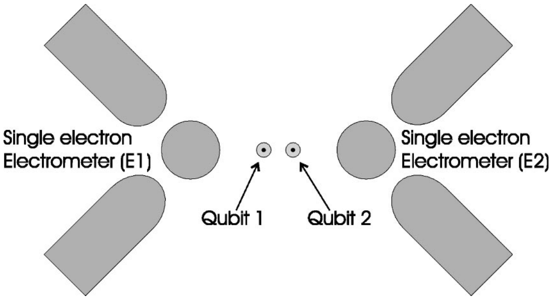

FIG. 3. Schematic illustration of a two-qubit geometry with two single-electron electrometers and a gate. The gate should not be confused with the J gate in the Kane model: it doesn't turn the interaction on and off but, together with a the floating electrometers, tunes the individual qubits.

substrate between two single-electron electrometers. These electrometers, typically fabricated by electron-beam lithography, are quantum dots in which the source-drain current is highly sensitive to the surrounding charge distribution. The dipole moment of the ammonia molecule induces a polarization charge on the dot, causing a measurable change in the current. Electrometers with sensitivity greater than 10^{-6} electrons/$\sqrt{\mathrm{Hz}}$ have been both fabricated and measured [13,14]. These electrometers can also be floated and used as the gates $E1$ and $E2$ (Fig. 3).

The two eigenstates of the ammonia molecule have polarizabilities of equal magnitude but opposite direction and it is these that are used in measurement. In the same way that an electric field is applied to separate out the eigenstates in the maser, an electric field applied to the ammonia molecule causes an induced dipole moment whose direction is dependent on the eigenstate of the molecule [4]. This field can come from the field of the electrometer itself, or from another gate.

In scaling up to a larger system, it is clear that this method of addressing qubits using gates becomes difficult. Other geometries can be devized that allow integration of more qubits. The use of carbon nanotubes as electrodes offers the possibility of gates of size comparable to the endofullerene molecules themselves, thus enabling single molecules to be individually addressed. Single nanotubes can be manipulated into position using an SPM, and then linked to metal contacts using electron-beam lithography. Fields of up to about 10^6 V/m can be sufficient to cause a modest perturbation in the energy-level splitting (Fig. 1) before field emission becomes a problem [15].

It might be expected that the fullerene acts as a miniature Faraday cage, screening out both time dependent and static E fields. In order to estimate the screening, we look at the polarizability of the fullerene. Calculating the field from this induced dipole moment in a static electric field we find that for C-60 in a static field the screening is approximately 20% [16]. Fullerenes can be placed inside nanotubes [17,18], with perhaps other fullerene spacers to achieve a uniform distance between cells.

Decoherence is a central issue in quantum computation, the challenge being to carry out the computation before the qubits decohere (entangle with the environment). The most practical measure of decoherence time is the number of operations possible before decoherence occurs.

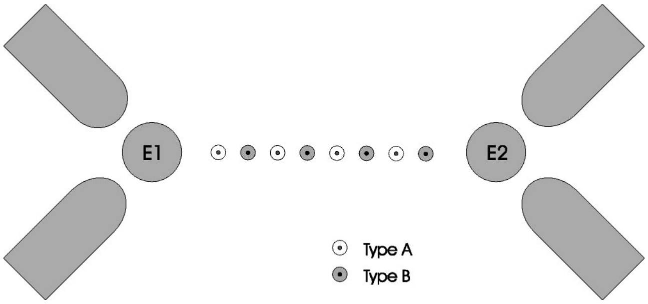

FIG. 4. Diagram showing how the confined ammonia molecules could be used in a cellular automaton approach.

The factors that are likely to contribute to the decoherence in the proposed system are the time-dependent field from the electrometers as they are being switched on, and the fluctuations in any applied gate voltages [19].

Another approach to quantum computation with fullerene confined ammonia molecules is to construct a cellular automaton (Fig. 4). From a decoherence point of view, this has the advantage that fewer gates and electrometers are required, thus reducing possible sources of decoherence. A system based on this principle comprising two types of cell has been proposed [20].

The requirements for this quantum cellular automaton approach are that a global pulse causes the operations, that the final state is measurable, that the interactions between nearest neighbors dominate, and that it is possible to set the system up into the ground state. In the proposed quantum cellular automata there are two different types of cell that can be separately addressed because of their different energy-level spacing.

There are several ways in which the two types of cell can be achieved. One possibility is to use gates to detune the ammonia molecules. Another method is to insert a different species into the fullerene, perhaps deuterated ammonia that has the same dipole moment as the ammonia but a smaller energy splitting [7]. Additionally, one could add a group exohederally to the fullerene to change its polarizability, and therefore the field the ammonia inside experiences for an applied field. Or, using this principle, two species of fullerene could be used to the same effect. In each one of these approaches, the applied pulses are the global microwave pulses and measurement again uses a single-electron electrometer.

We have presented a scheme that makes use of advances in nanotechnology to implement a flexible and realizable quantum computer. The transition exploited for the qubit, the two eigenstates of ammonia, was instrumental in developing the laser: perhaps it can do the same for solid-state quantum computation.

The authors would like to thank Simon Benjamin for useful discussions and comments.

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