Communications: Entanglement switch for dipole arrays

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We propose a new entanglement switch of qubits consisting of electric dipoles oriented along or against an external electric field and coupled by the electric dipole-dipole interaction. The pairwise entanglement can be tuned and controlled by the ratio of the Rabi frequency and the dipole-dipole coupling strength. Tuning the entanglement can be achieved for one, two, and three-dimensional arrangements of the qubits. The feasibility of building such an entanglement switch is also discussed. © 2010 American Institute of Physics. [doi:10.1063/1.3366522]

Entanglement is a quantum mechanical property that describes a correlation between quantum mechanical systems. It has no classical analog and has been lying in the heart of the foundation of quantum mechanics. The desire to understand, tune, and manipulate quantum entanglement is of fundamental importance in the field of quantum information and computation.1–4 Recently, we studied a set of localized spins controlling cold polar molecules make them an excellent candidate for quantum computation.9–12 Trapped polar molecules was proposed as a novel physical realization of a quantum computer by a number of authors.12–20 In this paper, we propose a new entanglement switch of qubits consisting of the electric dipole moment of diatomic polar molecules, oriented along or against an external electric field and coupled by the electric dipole-dipole interaction.

Recent progress in methods for producing, trapping, and controlling cold polar molecules make them an excellent candidate for quantum computation.9–12 Trapped polar molecules was proposed as a novel physical realization of a quantum computer by a number of authors.12–20 In this proposal, the qubits are the molecular electric dipole moments which can only orient along (|0⟩) or against (|1⟩) the external electric field. Each qubit is one polar molecule with equal spacing along the axis. For such a system, tuning and controlling the entanglement between the dipoles is of great importance.

The Hamiltonian of N-trapped dipoles in an external electric field reads

$$H = \hbar \sum_{i=1}^{N} \omega_i \hat{S}_i^z + \hbar \sum_{i \neq j}^{N} \Omega_{ij} \hat{S}_i^z \hat{S}_j^z,$$

where $\hat{S}_i^+$ and $\hat{S}_i^z$ represent dipole excitation and de-excitation, respectively. $\omega_i$ is the transition frequency of the dipole on site $i$, which is a function of dipole moment and external electric fields at site $i$.

$$\hbar \omega_i = |\vec{d} \cdot \vec{E}|,$$

where $\vec{d}$ is the electric dipole moment which we assume the same for each site. $\Omega_{ij}$ is the dipole coupling constant between sites $i$ and $j$, which is determined by the strength of dipole moment, the direction of the external electric field and the lattice constant of the dipole array.

$$\hbar \Omega_{ij} = |\vec{d}|^2(1 - 3 \cos^2 \theta) / |\vec{r}_{ij}|^3,$$

where $\theta$ is the angle between $\vec{r}_{ij}$ and external electric field.

We will expand the Hamiltonian in pure standard basis, $\{|00\}, |01\}, |10\}, |11\}$, and all the eigenstates will be obtained by diagonalizing the Hamiltonian matrix. For example, for $N=2$, we obtained the following four eigenvectors:

$$\Psi_1 = |00\rangle, \quad |\Psi_2 = (1/\sqrt{2})(|01\rangle - |10\rangle), \quad |\Psi_3 = (1/\sqrt{2} \times (|01\rangle + |10\rangle), \quad |\Psi_4 = |11\rangle$$

with corresponding eigenvalues: $E_1 = 0$, $E_2 = \omega - \Omega$, $E_3 = \omega + \Omega$, $E_4 = 2\omega$. For the ratio $\omega/\Omega < 1$, $\Psi_2$ is fully entangled ground state. However, for $\omega/\Omega > 1$ the nonentangled state $\Psi_1$ is the ground state. Thus, we have a curve crossing at $\omega/\Omega = 1$.

The concept of entanglement of formation is related to the amount of entanglement needed to prepare the state $\rho_{22}$, where $\rho$ is the density matrix. It was shown by Wooters that concurrence is a good measure of entanglement.23 The concurrence $C$ is given by

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}. $$

For a general state of two qubits, $\lambda_i$’s are the eigenvalues, in decreasing order, of the Hermitian matrix $R = \sqrt{\rho \rho^\dagger \rho}$ where $\rho$ is the density matrix and $\rho^\dagger$ is the spin-flipped state defined as

$$\bar{\rho} = (\sigma_z \otimes \sigma_z) \rho^\dagger (\sigma_z \otimes \sigma_z),$$

where the $\rho^\dagger$ is the complex conjugate of $\rho$ and is taken in the standard basis, which for a pair of two level particles is $\{|00\}, |01\}, |10\}, |11\}$. 

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In order to calculate thermal entanglement, we need the temperature dependent density matrix and the density matrix for a system in equilibrium at a temperature \( T \) reads:

\[
\rho = e^{-\beta H/Z},
\]

\[
Z = \text{Tr}(e^{-\beta H}).
\]

In this case, the partition function is

\[
Z = \sum_i g_i e^{-\beta \lambda_i},
\]

where \( \lambda_i \) is the \( i \)th eigenvalue and \( g_i \) is the degeneracy. And the corresponding density matrix can be written

\[
\rho(T) = \frac{1}{Z} \sum_{i,j} \langle \Phi_i | e^{-\beta H} | \Phi_j \rangle.
\]

where \( | \Phi_i \rangle \) is the \( i \)th eigenfunction. For pairwise thermal entanglement, we can get reduced density matrix as a function of temperature in the same way, which leads to temperature dependent entanglement.

In Fig. 1 we show the tuning of the pairwise entanglement, measured by concurrence, of one-dimensional arrangements of the dipoles as one varies the ratio \( \omega/\Omega \) at different temperatures for \( N=9 \) dipoles. Here we took all transition frequencies to be the same, \( \omega_j = \omega \), and the nearest neighbor dipole-dipole interaction to be the same, \( \Omega_{j,j+1} = \Omega_{j,j-1} = \Omega \). All other dipole-dipole coupling constants \( \Omega_{j,j \neq \pm 1} \) can be expressed in terms of \( \Omega \). Thus, we have two parameters to vary, the ratio \( \omega/\Omega \) and temperature \( kT \). At \( kT \approx 0 \) one has a constant entanglement over a long ratio \( \omega/\Omega \) and sharp transitions or jumps to lower values at other values of \( \omega/\Omega \). It is worth mentioning that for \( \omega/\Omega < 0.64 \), entanglement is only between dipoles 1 and 2. For \( 0.64 < \omega/\Omega < 1.14 \) dipole one becomes entangled also with dipole 3 and with other dipoles until we reach \( \omega/\Omega \approx 1.74 \), above this value the concurrence is zero between all sites. As one increases the temperature, the curve becomes smoother as mixing occurs with higher states. Calculations for \( N=3,4,\ldots,8 \) gave similar behavior of tuning and controlling entanglement as for the case \( N=9 \). To show how the populations changes at the transition point, we present in Fig. 2 the coefficients of the wave function for \( N=4 \) before and after the transition point \( \omega/\Omega = 0.64 \). When \( \omega/\Omega < 0.64 \), the ground state wave
function is $|\Psi\rangle = (0.19|↓↑↓↑⟩-0.51|↓↑↑↓⟩+0.45|↑↑↑↓⟩-0.51|↑↑↓↑⟩+0.19|↓↑↓↑⟩)$, however, when $\omega/\Omega > 0.64$, the ground state wave function becomes $|\Psi\rangle = (0.36|↓↓↓↑⟩-0.61|↓↑↓↑⟩+0.61|↑↓↓↑⟩-0.36|↑↑↓↑⟩)$. Figures 3 and 4 show a similar phenomena for two and three-dimensional arrangements of the dipoles. The pairwise entanglement decreases as one increases the dimensionality of the system and the temperature.

There have been rapid advances made recently in cooling, trapping and manipulating atomic (Rydberg) and molecular dipoles. For example, a wide variety of ground state polar molecules with large electric dipole moments (several debyes, where $1\, \text{D} = 10^{-30}\, \text{Cm}$) have been cooled to ultracold ($\sim\text{mK}$ or below) regime, some even near quantum degeneracy. These developments provide exciting opportunities to experimentally realize the entanglement switch described above, which requires tuning $\omega/\Omega$ around 1, and cooling the dipoles to temperatures ($T$) corresponding to a fraction of the dipole-dipole interaction energy ($\Omega$). For a dipole moment ($\mu$) of few debyes, and a typical experimental electric field ($\sim 10^5 \, \text{V/m}$, required for the dipole moment to actually manifest itself), dipole-dipole separation ($d$) on the order of 10 nm is required for $\omega/\Omega \sim 1$. Such $d$ is much shorter than what can be achieved in typical optical lattices (as envisaged in Ref. 12 which corresponds to the regime of $\omega/\Omega \gg 1$), but can be realized with arrays of nanoscale plasmon-enhanced electric/electro-optical traps recently proposed (where extremely tight, few-nanometer confinement, and trap frequencies exceeding 100 MHz are shown to be possible). At such short $d$, the dipole-dipole interaction $\Omega = \mu^2/4\pi\varepsilon_0 d^3$ is on the order of 0.1 K. Cooling to a small fraction of such a temperature scale is easily within the current experimental technology. Furthermore, $\omega/\Omega$ can be tuned experimentally by the electrical field, and/or by $d$ (e.g., by varying the microtrap configuration).

In summary, we presented a new way to construct an entanglement switch in an optical lattice and discussed the experimental feasibility of building such switch. The realization of such a scheme will have a profound impact on the implementation of quantum gates in quantum computing with trapped polar molecules. The similar idea could in principle also be applied to other systems with electric dipoles, such as quantum dots and excitons in nanostructures.

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