

Qubit Entanglement from a Bipartite Atomic System in a Carbon Nanotube

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ABSTRACT

We study a scheme for the entanglement of two two-level atoms based on the previously developed photon Green function formalism for quantizing an electromagnetic field in the presence of a carbon nanotube. We show that the (resonator-like) cylindrical nanotube environment can result in a significant degree of quantum-bit entanglement of the bipartite atomic subsystem.

Keywords: carbon nanotubes, strong atom-field coupling, atomic qubit entanglement

1 INTRODUCTION

In spite of impressive experimental demonstrations of basic quantum information effects in a number of different mesoscopic systems, such as quantum dots in semiconductor microcavities, cold ions in traps, nuclear spin systems, atoms in optical resonators, Josephson junctions, etc., their concrete implementation is still at the proof-of-principle stage [1]. It seems difficult at present to identify a specific low-dimensional physical system which could possibly at some point demonstrate technologically relevant implementations. The development of materials that may host quantum coherent states with long coherence lifetimes is a critical research problem for the nearest future. There is a need for the fabrication and characterization of quantum bits (qubits) with coherence lifetimes at least three-four orders of magnitude longer than it takes to perform a bit flip. Equally important would be the demonstration of quantum information transfer between two quantum bits arbitrarily separated in the material. This would involve entangling operations, followed by the nearest neighbor interaction over short distances and quantum information transfer over longer distances. It is thus of vital importance to pursue a variety of different strategies and approaches towards physically implementing novel non-trivial applications in modern nanotechnology.

Carbon nanotubes (CNs) are graphene sheets rolled-up into cylinders of approximately one nanometer in diameter. Extensive work carried out worldwide in recent years has revealed intriguing physical properties of these novel molecular scale wires [2]. Nanotubes have been

shown to be useful for miniaturized electronic, mechanical, electromechanical, chemical and scanning probe devices and as materials for macroscopic composites [2], [3]. Important is that their intrinsic properties may be substantially modified in a controllable way by doping with extrinsic impurity atoms, molecules and compounds [4], [5]. Recent successful experiments on the encapsulation of single atoms into single-walled CNs [5] and the progress in the growth techniques of centimeter-long small-diameter single-walled CNs [6], stimulate the study of dynamical quantum processes in atomically doped CN systems.

We have recently shown that the relative density of photonic states (DOS) near the CN effectively increases due to additional surface photonic modes coupled to CN electronic quasiparticle excitations [7]. This causes the atom-vacuum-field coupling constant [determined by the distance-dependent (local) photonic DOS] to be very sensitive to the atom-CN-surface distance. At small enough distances, the system may exhibit strong atom-field coupling — a highly desired property for quantum information science [8], [9], giving rise to rearrangement (“dressing”) of atomic levels and formation of atomic quasi-1D cavity polaritons [10], [11]. The latter ones are similar to quasi-0D excitonic polaritons in quantum dots in semiconductor nanocavities [12], that are currently being considered a possible way to produce the excitonic qubit entanglement [13]. We have recently analyzed the possibilities for experimental observation of atomic quasi-1D polaritons in optical absorption experiments with small-diameter atomically doped CNs [14], and have partly addressed the problem of their stability by investigating the atom-nanotube van der Waals interactions [11], [15]. Here, we show that under strong atom-field coupling the resonator-like cylindrical nanotube environment can result in a significant degree of qubit entanglement of the bipartite atomic subsystem.

2 BASIC EQUATIONS

We consider two identical two-level atoms, A and B , positioned at their respective equivalent places $\mathbf{r}_{A,B}$ inside an infinitely long achiral single-wall CN. Both atoms interact with a quantum electromagnetic field via their electric dipole transitions of frequency ω_A . Their dipole

moments, $\mathbf{d}_{A,B} = d_z \mathbf{e}_z$, are assumed to be directed along the CN axis (assigned by the unit vector \mathbf{e}_z) which is chosen to be the z -quantization axis of the system. The contribution of the transverse dipole moment orientations is suppressed because of the strong depolarization of the transverse field in an isolated CN (the so-called dipole antenna effect reported recently in Ref. [16]). We also assume that the atoms are sufficiently far from each other, so that the interatomic Coulomb interaction can be ignored. The total secondly quantized Hamiltonian of the bipartite atomic system is then given by [11], [15]

$$\begin{aligned} \hat{H} = & \int_0^\infty d\omega \hbar\omega \int d\mathbf{R} \hat{f}^\dagger(\mathbf{R}, \omega) \hat{f}(\mathbf{R}, \omega) + \sum_{i=A,B} \frac{\hbar\tilde{\omega}_i}{2} \hat{\sigma}_{iz} \\ & + \sum_{i=A,B} \int_0^\infty d\omega \int d\mathbf{R} [g^{(+)}(\mathbf{r}_i, \mathbf{R}, \omega) \hat{\sigma}_i^\dagger \\ & - g^{(-)}(\mathbf{r}_i, \mathbf{R}, \omega) \hat{\sigma}_i] \hat{f}(\mathbf{R}, \omega) + \text{h.c.}, \end{aligned} \quad (1)$$

with the three items representing the *medium-assisted* (modified by the presence of the CN) electromagnetic field, the two-level atoms, and their interaction with the medium-assisted field, respectively. The operators $\hat{f}^\dagger(\mathbf{R}, \omega)$ and $\hat{f}(\mathbf{R}, \omega)$ are the scalar bosonic field operators defined on the surface of the CN (\mathbf{R} is the radius-vector of an arbitrary point of the CN surface). They play the role of fundamental dynamical variables of the field subsystem and satisfy the standard bosonic commutation relations. The Pauli operators, $\hat{\sigma}_i = |L\rangle\langle u_i|$, $\hat{\sigma}_i^\dagger = |u_i\rangle\langle L|$ and $\hat{\sigma}_{iz} = |u_i\rangle\langle u_i| - |L\rangle\langle L|$ with $i = A$ or B , describe the atomic subsystem and electric dipole transitions between its two states, upper $|u_i\rangle$ with either of the two atoms in its upper state and lower $|L\rangle$ with both atoms in their lower states, separated by the transition frequency ω_A . This (bare) frequency is modified by the diamagnetic ($\sim \mathbf{A}^2$) atom-field interaction yielding the new *renormalized* transition frequency $\tilde{\omega}_i = \omega_A [1 - 2/(\hbar\omega_A)^2 \int_0^\infty d\omega \int d\mathbf{R} |g^\perp(\mathbf{r}_i, \mathbf{R}, \omega)|^2]$ in the second term of the Hamiltonian. The dipole atom-field interaction matrix elements are given by $g^{(\pm)} = g^\perp \pm (\omega/\omega_A) g^\parallel$ where $g^{\perp(\parallel)} = -i(4\omega_A/c^2) \sqrt{\pi\hbar\omega} \text{Re} \sigma_{zz}(\omega) d_z^{\perp(\parallel)} G_{zz}(\mathbf{r}_i, \mathbf{R}, \omega)$ with $d_z^{\perp(\parallel)} G_{zz}(\mathbf{r}_i, \mathbf{R}, \omega)$ being the zz -component of the transverse (longitudinal) Green tensor (with respect to the first variable) of the electromagnetic subsystem and $\sigma_{zz}(\omega)$ representing the CN surface axial conductivity. The matrix elements $g^{\perp(\parallel)}$ have the property of $\int d\mathbf{R} |g^{\perp(\parallel)}(\mathbf{r}_i, \mathbf{R}, \omega)|^2 = (\hbar^2/2\pi) (\omega_A/\omega)^2 \Gamma_0(\omega) \xi^{\perp(\parallel)}(\mathbf{r}_i, \omega)$ with $\xi^{\perp(\parallel)}(\mathbf{r}_i, \omega) = \text{Im}^{\perp(\parallel)} G_{zz}^{\perp(\parallel)}(\mathbf{r}_i, \mathbf{r}_i, \omega) / \text{Im} G_{zz}^0(\omega)$ being the transverse (longitudinal) local photonic DOS functions and $\Gamma_0(\omega) = 8\pi\omega^2 d_z^2 \text{Im} G_{zz}^0(\omega) / 3\hbar c^2$ representing the atomic spontaneous decay rate in vacuum where $\text{Im} G_{zz}^0(\omega) = \omega/6\pi c$ is the vacuum imaginary Green tensor zz -component. The Hamiltonian (1) involves only two standard approximations. They are the electric dipole approximation and the two-level approximation.

The rotating wave approximation commonly used is not applied, and the diamagnetic term of the atom-field interaction is not neglected (as opposed to, e.g., Refs. [7], [10]). The whole system of the two two-level atoms dipole-coupled to the quantized medium-assisted field of the carbon nanotube is thus described in terms of only two intrinsic physical characteristics of the field subsystem — the transverse and longitudinal local photonic DOS functions.

For single-quantum excitations, the time-dependent wave function of the whole system can be written as

$$\begin{aligned} |\psi(t)\rangle = & \sum_{i=A,B} C_{u_i}(t) e^{-i(\tilde{\omega}_i - \bar{\omega})t} |u_i\rangle | \{0\} \rangle \\ & + \int_0^\infty d\omega \int d\mathbf{R} C_L(\mathbf{R}, \omega, t) e^{-i(\omega - \bar{\omega})t} |L\rangle |1(\mathbf{R}, \omega)\rangle, \end{aligned} \quad (2)$$

where $\bar{\omega} = \sum_{i=A,B} \tilde{\omega}_i/2$, $| \{0\} \rangle$ is the vacuum state of the field subsystem, $| \{1(\mathbf{R}, \omega)\} \rangle$ is its excited state with the field being in the single-quantum Fock state, and C_{u_i} and C_L are the respective probability amplitudes of the upper states and the lower state of the system. For the following it is convenient to introduce the new variables $C_\pm(t) = [C_{u_A}(t) \pm C_{u_B}(t)]/\sqrt{2}$ that are the expansion coefficients of the wave function (2) in terms of the maximally entangled 2-qubit atomic states $| \pm \rangle = (|u_A\rangle \pm |u_B\rangle)/\sqrt{2}$. In view of Eqs. (1) and (2), the time-dependent Schrödinger equation yields then

$$\dot{C}_\pm(\tau) = \int_0^\tau d\tau' K_\pm(\tau - \tau') C_\pm(\tau') + f_\pm(\tau), \quad (3)$$

where

$$\begin{aligned} K_\pm(\tau - \tau') = & - \int_0^\infty dx \frac{\tilde{\Gamma}_0(x)}{2\pi} \xi^\pm(\mathbf{r}_A, \mathbf{r}_B, x) \\ & \times e^{-i(x - \bar{x}_A)(\tau - \tau')}, \\ \xi^\pm(\mathbf{r}_A, \mathbf{r}_B, x) = & \frac{x^2}{x^2} [\xi^\perp(\mathbf{r}_A, x) \pm \xi^\perp(\mathbf{r}_B, x)] \\ & + \xi^\parallel(\mathbf{r}_A, x) \pm \xi^\parallel(\mathbf{r}_B, x), \\ f_\pm(\tau) = & - \frac{1}{\sqrt{2}} \int_{-\Delta\tau}^0 d\tau' K_\pm(\tau - \tau') C_{u_A}(\tau'), \end{aligned}$$

and we have, for convenience, introduced the dimensionless variables $\tilde{\Gamma}_0 = \hbar\Gamma_0/2\gamma_0$, $x = \hbar\omega/2\gamma_0$, and $\tau = 2\gamma_0 t/\hbar$ with $\gamma_0 = 2.7$ eV being the carbon nearest neighbor hopping integral appearing in the CN surface axial conductivity σ_{zz} . The functions $f_\pm(\tau)$ are only unequal to zero when the two atoms are initially in their ground states, with the initial excitation residing in the nanotube. Eq. (3) assumes that this situation is realized by starting the measurement time after the time interval $\Delta\tau$, that is necessary for the atom A to decay completely into the nanotube photonic modes, has elapsed.

The entanglement of two quantum bits occurs when the 2-qubit wave function cannot be represented as a

3 RESULTS

product of the two 1-qubit states in any basis. To determine this quantity in our particular case, we follow the recipe based on the "spin flip" transformation and valid for an arbitrary number of qubits (see Ref. [17] for details). First, we define the reduced density matrix $\hat{\rho}_{AB}(\tau) = |\psi_{AB}(\tau)\rangle\langle\psi_{AB}(\tau)| = \text{Tr}_{field}|\psi(\tau)\rangle\langle\psi(\tau)|$ describing the bipartite atomic subsystem in terms of the wave function (2) of the whole system. Next, we introduce the "concurrence" $C(\psi_{AB}) = |\langle\psi_{AB}|\tilde{\psi}_{AB}\rangle|$, where $|\tilde{\psi}_{AB}\rangle = \hat{\sigma}_y^A \hat{\sigma}_y^B |\psi_{AB}^*\rangle$ with $\hat{\sigma}_y^{A(B)}$ being the Pauli matrix that represent the "spin flip" transformation in the atom $A(B)$ single-qubit space. This, after some algebra, becomes

$$C[\psi_{AB}(\tau)] = |C_+^2(\tau) - C_-^2(\tau)| \quad (4)$$

with $C_{\pm}(\tau)$ given by the integral equation (3). Finally, the degree of entanglement ("entanglement of formation" [17]) $E(\psi_{AB})$ of the 2-qubit atomic state $|\psi_{AB}\rangle$ is given by

$$E[\psi_{AB}(\tau)] = h\left(\frac{1 + \sqrt{1 - C[\psi_{AB}(\tau)]^2}}{2}\right),$$

$$h(y) = -y \log_2 y - (1 - y) \log_2 (1 - y). \quad (5)$$

Obviously, the entanglement of formation (5) can only be found numerically, in general, in view of the fact that the coefficients $C_{\pm}(\tau)$ in the concurrence (4) are given by the integral equation (3). This, however, offers very little physical insight into the problem of the two atomic qubits entanglement under different atom-field coupling. Therefore, we choose a simple analytical approach valid for those atomic transition frequencies \tilde{x}_A which are located in the vicinity of the resonance frequencies x_r of the combined DOS functions $\xi^{\pm}(\mathbf{r}_A, \mathbf{r}_B, x)$ (determined, obviously, by resonances of $\xi^{\pm(\text{II})}(\mathbf{r}_A, x)$ at least for not too large inter-atom separations). Within this approach, $\xi^{\pm}(x \sim x_r)$ are approximated by the Lorentzians of the same half-width-at-half-maxima δx_r , thus making it possible to solve the integral equation for C_{\pm} analytically to obtain [10], [11]

$$C_{\pm}(\tau) \approx A_{\pm} e^{-\frac{1}{2}(\delta x_r - \sqrt{\delta x_r^2 - X_{\pm}^2})\tau} + B_{\pm} e^{-\frac{1}{2}(\delta x_r + \sqrt{\delta x_r^2 - X_{\pm}^2})\tau} \quad (6)$$

with A_{\pm} (B_{\pm}) being the constants of integration to be determined appropriately depending on the initial conditions, and

$$X_{\pm} = \sqrt{2\delta x_r \tilde{\Gamma}_0(\tilde{x}_A)\xi^{\pm}(\mathbf{r}_A, \mathbf{r}_B, \tilde{x}_A)}.$$

This solution is valid for $\tilde{x}_A \approx x_r$ whatever the atom-field coupling strength is, yielding the exponential decay, $C_{\pm}(\tau) \sim \exp[-\tilde{\Gamma}_{\pm}(\tilde{x}_A)\tau/2]$ with the rate $\tilde{\Gamma}_{\pm} = \tilde{\Gamma}_0\xi^{\pm}$, in the weak coupling regime where $(X_{\pm}/\delta x_r)^2 \ll 1$, and the decay via damped Rabi oscillations, $C_{\pm}(\tau) \sim \exp(-\delta x_r\tau/2) \cos(X_{\pm}\tau/2)$, in the strong coupling regime where $(X_{\pm}/\delta x_r)^2 \gg 1$.

To compute the entanglement of formation (5) via the concurrence (4) with coefficients (6), one needs to know the combined local photonic DOS functions $\xi^{\pm}(\mathbf{r}_A, \mathbf{r}_B, \tilde{x}_A)$. These are determined by $\xi^{\pm(\text{II})}$ whose frequency behavior is determined by the CN surface axial conductivity σ_{zz} . The latter one was calculated in the relaxation-time approximation (relaxation time 3×10^{-12} s [1]) at temperature 300 K. The functions ξ^{\pm} were calculated thereafter as described in Refs. [11], [15] for the simplest case where both of the atoms are positioned in the center of the nanotube. The vacuum spontaneous decay rate was estimated from the expression $\tilde{\Gamma}_0(x) = \alpha^3 x$ ($\alpha = 1/137$ is the fine-structure constant) valid for atomic systems with Coulomb interaction [18].

Figure 1 (a) presents, as an example, a typical frequency behavior of the transverse local photonic DOS $\xi^{\pm}(\mathbf{r}_A = 0, x)$ in the infrared and visible frequency range $x < 0.4$ for the atom inside 'zigzag' CNs of increasing radius. Sharp DOS resonances are clearly seen, thus justifying our approximate 'single-resonance' approach chosen to analyze the 2-qubit entanglement in atomically doped CNs. The peaks are much sharper for metallic CNs ($m = 3q$, $q = 1, 2, \dots$) than for semiconducting ($m \neq 3q$) in agreement with the fact that this frequency range is being dominated by the classical Drude-type conductivity which is larger in metallic CNs than in semiconducting ones [7]. In the following, we therefore analyze the metallic (9,0) CN more deeply. Figure 1 (b) shows the dependence of ξ^{\pm} on the inter-atom separation Δ_{AB} for the frequency fixed at $x = 0.32$ [peak position of ξ^{\pm} in Fig. 1 (a)] for the two atoms in the center of the CN. One can see that as Δ_{AB} is increasing, the values of ξ^+ and ξ^- can be substantially different from each other in a periodic manner, thereby making the mixing coefficients (6) different and thus, according to Eqs. (4) and (5), resulting in the entanglement of the two spatially separated atomic qubits. Figure 1 (c) presents the calculated time dynamics of the entanglement of formation of the 2-qubit atomic state with the two atoms positioned in the center of the CN and separated from each other by the distance $\Delta_{AB} = 2.1R_{cn} \approx 7.4 \text{ \AA}$ [shown by the vertical dash-dotted line in Fig. 1 (b); roughly corresponds to doping of 1 atom per 4 carbon rings] under different initial excitation conditions of the bipartite atomic subsystem. The entanglement is seen to reach sizable amounts for large enough times when either a maximally entangled 2-qubit state is initially excited [curves $C_{\pm}(0) = 1$], or the initial excitation resides in the nanotube [curve $C_+(0) = C_-(0) = 0$]. The latter is less trivial, but is clear since the initial excitation may only be distributed equally among the equivalent atoms as time goes, thus resulting in a better entanglement of atomic qubits than, say, that obtained by exciting initially only one of the atoms [curve $C_A(0) = 1$]. Note

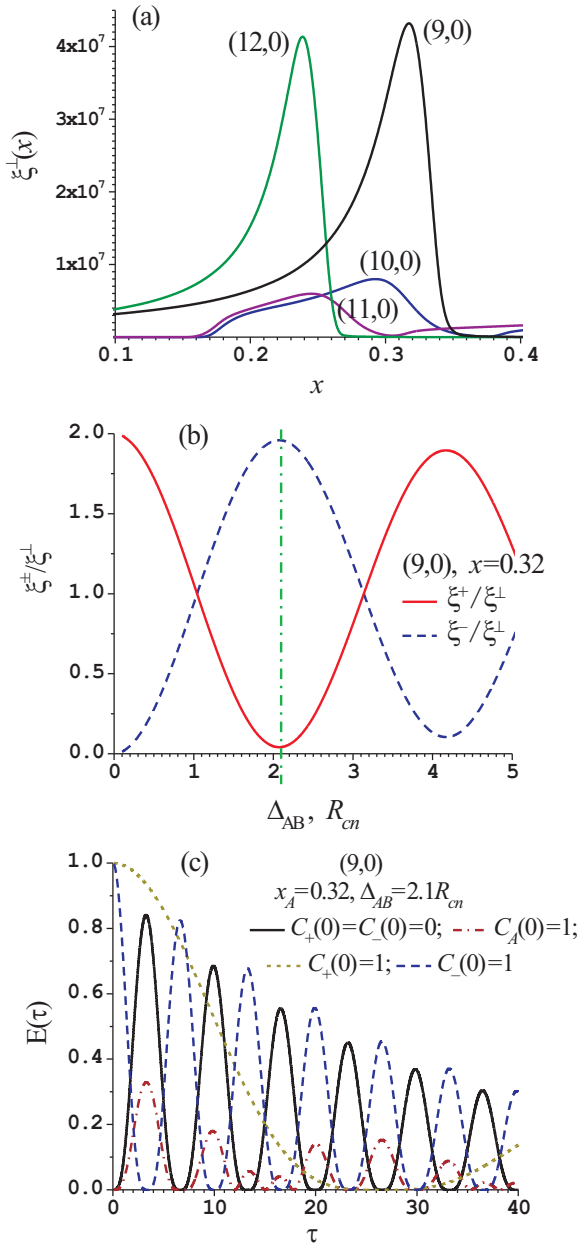


Figure 1: (a) Frequency dependencies of the transverse local DOS functions $\xi^\pm(\mathbf{r}_A, x)$ for the two-level atom positioned in the center of the 'zigzag' nanotubes. (b) Two-particle local DOS functions ξ^\pm taken at the peak frequency of ξ^\pm [Fig. 1 (a)], as functions of the inter-atom separation Δ_{AB} for the two atoms in the center of the (9,0) CN. (c) Time dependencies of the entanglement of formation $E(\tau)$ of the 2-qubit atomic state for the two atoms positioned in the center of the (9,0) CN and separated from each other by the distance $\Delta_{AB} = 2.1R_{cn} \approx 7.4 \text{ \AA}$ [shown by the vertical dash-dotted line in Fig. 1 (b)], for different initial excitation conditions of the atomic subsystem.

that the atoms can in principle be separated by longer distances with roughly the same entanglement because of the periodic behavior of the functions ξ^\pm [Fig. 1 (b)].

4 CONCLUSION

Based on the previously developed Green function formalism for quantizing an electromagnetic field close to a CN, we have studied the scheme for entangling two two-level atoms strongly coupled to the resonator-like nanotube environment. Our approach captures the dominant features of all atom-field coupling regimes. We predict sizable amounts of the 2-qubit atomic entanglement for sufficiently long times. Our scheme can be further generalized to the multi-atom entanglement via the nearest neighbor pairwise quantum correlations, thus challenging novel applications of atomically doped carbon nanotubes in quantum information science.

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