Photon Enhanced Interaction and Entanglement in Semiconductor Position-Based Qubits

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Abstract: CMOS technologies facilitate the possibility of implementing quantum logic in silicon. In this work, we discuss a minimalistic modelling of entangled photon communication in semiconductor qubits. We demonstrate that electrostatic actuation is sufficient to construct and control desired potential energy profiles along a Si quantum dot (QD) structure allowing the formation of position-based qubits. We further discuss a basic mathematical formalism to define the position-based qubits and their evolution under the presence of external driving fields. Then, based on Jaynes–Cummings–Hubbard formalism, we expand the model to include the description of the position-based qubits involving four energy states coupled with a cavity. We proceed with showing an anti-correlation between the various quantum states. Moreover, we simulate an example of a quantum trajectory as a result of transitions between the quantum states and we plot the emitted/absorbed photos in the system with time. Lastly, we examine the system of two coupled position-based qubits via a waveguide. We demonstrate a mechanism to achieve a dynamic interchange of information between these qubits over larger distances, exploiting both an electrostatic actuation/control of qubits and their photon communication. We define the entanglement entropy between two qubits and we find that their quantum states are in principle entangled.

Keywords: entanglement; charge qubit; position-based semiconductor qubits; cryogenic technologies; semiconductor photon communication; Jaynes–Cummings–Hubbard formalism

1. Introduction

In a world where the quantum technology rapidly emerges, CMOS technologies seem to be attractive candidates for a successful widely spread realization of quantum computers. Recently, efforts have been reported towards the construction of quantum computers on a silicon chip [1–4]. When cooled down to cryogenic temperatures, CMOS allows constructing effective quantum potential energy profiles where particles can realize their nano-world properties. Such implementations can be based on spin-spin interaction or in the position of single and/or multiple fermions or even Majorana particles [5–10].

The manipulation of semiconductor qubits can be carried out in principle by the application of an electric/magnetic field. The control over semiconductor position-based qubits (also known in the literature as charge qubits) can be achieved by using only a static electric field, which is of interest in this work. It can be shown that one can move the charge between neighboring quantum dots (QD) by applying appropriate voltages across a given array of a quantum register/structure. The fine lithography of nanometer-scale CMOS allows the use of single-electron devices (SED) for the injection
and detection of single electrons, as well as their quantum transport through the quantum register. Correlated oscillations and signatures of entanglement of silicon-based qubits have been demonstrated in the literature, making the construction of quantum gates and algorithms possible [11–15].

At the same time, the possibility of integration of double-quantum-dots (DQDs) with microwave cavities was recently demonstrated, where an absorbed photon facilitates tunneling of electrons between QDs by means of pumping energy into the system. However, a reversed phenomenon is also possible, i.e., a photon emission due to the tunneling of particles in a quantum transport operation, where the DQDs are coupled through a cavity [16–21]. Previous experiments showed that the cavity photon emission can be enhanced as a result of entangled states between coupled atoms. It is also known that semiconductor quantum dots, acting as artificial atoms, can emit photons, opening a possibility to achieve communication between qubits within a chip. This photon exchange via a waveguide is expected to enhance the coupling between DQDs by introducing a superposition of many quantum paths [22–25]. By proper manipulation of the system and by exploiting its optical properties, one could control the transport of flying qubits and, as a result, the dynamic interchange of information.

In our previous work, we showed that it is possible to control and construct semiconductor position-based qubits in DQDs in nanometer-scale CMOS. We also showed that electrostatically coupled interacting DQDs are in principle entangled [26,27]. In this paper, motivated by the recent demonstrations of semiconductor-based photon communication, and expanding our previous work on modelling of position-based semiconductor qubits, we will focus on a minimalistic modelling of two-coupled DQDs in silicon interconnected with a waveguide.

To start, we illustrate that electrostatic actuation is sufficient for the construction of valid potential energy profiles. This allows the formation of position-based qubits in a DQD. We show how one can apply voltages and voltage pulses to manipulate the tunneling rates and energy levels in a quantum register.

We continue by describing a system of a position-based qubit exhibiting four energy levels, coupled with a cavity. We demonstrate photon emission and absorption through quantum paths by capturing the dynamics of the various quantum states of the system. Remarkably, anticorrelations of quantum states can be observed, even in a single-qubit system.

Finally, we expand our description to a system of two coupled position-based qubits via a waveguide. We define the Von Neumann entanglement entropy of the system, and then show that anticorrelation and entanglement between the quantum states of the two qubits can be achieved through an interchange of photons. The electrostatic actuation of the position-based qubits coupled through a cavity allows quantum communication via longer distances, opening the possibility of the formation of quantum gates between non-neighboring qubits.

The paper is organized as follows: Section 2 discusses the system under study. Section 3 introduces a brief description of the position-based qubit and the basic transitions between the quantum states that can take place in the system. Section 4 develops a minimalistic modelling based on the Jaynes–Cummings–Hubbard formalism. We examine selected case studies and present simulation results demonstrating photon absorption, emission and entanglement.

### 2. Statement of the Problem

The quantum structure under study is realized in a CMOS fully depleted silicon-on-insulator (FDSOI) technology. A transistor-like CMOS device is depicted in Figure 1a. When operating at cryogenic temperatures, such devices can be seen as artificial atoms, giving rise to a double-quantum-dot (DQD). DQDs can be arranged in series forming a quantum register of an arbitrary number of qubits. The quantum transport can be achieved electrostatically by manipulating the electrical potential, i.e., by applying appropriate DC and pulsed voltages at the gates. For a more detailed description of this system, an interested reader can refer to [26].
Figure 1. (a) Cross-section of an FDSOI transistor-like ‘quantum’ device, without the source/drain diffused regions. Details of the specific technology are omitted. As the device dimensions decrease, one can achieve quantum operation at cryogenic temperatures. Various layers of the device facilitate different properties which are essential to the resulting potential energy profile. (b) Each device can facilitate a double-quantum-dot (DQD). When interconnected via a waveguide, it can couple the entangled qubits. This can be achieved with the use of high-$\epsilon$ materials and proper isolation of the quantum core from the rest of the surrounding circuitry of a chip. (c) Top-view of a layout structure of two coupled DQDs interconnected via a waveguide. (d) 1D representation of two coupled (DQDs). Each DQD can facilitate a qubit. In the schematic, the two states of each qubit are denoted, as $|0\rangle_{A,B}$, corresponding to a particle in the left QD of system-A or system-B (of the corresponding potential energy profile of a device), and as $|1\rangle_{A,B}$, corresponding to a particle in the right QD. (e) 1D schematic representation of a potential energy profile formed by a chain of devices forming a series of QDs. The absorption of a photon can cause a transition to a higher energy level. Similarly, the emission of a photon can occur when a particle transitions from a higher energy level to a lower energy level.

In Figure 1b, the concept of coupling two qubits over longer distances, in the case electrostatic (Coulomb) interaction is negligible, is demonstrated. The coupling is expected to be achieved through a waveguide by means of a high-$\epsilon$ material layer. Figure 1c visualizes a top-view layout of two coupled DQDs with a waveguide. Each DQD realizes a qubit. In this work, we will focus on the modelling of a qubit coupled into a cavity and two coupled qubits coupled via a waveguide. As visualized in Figure 1d, each qubit has two states, denoted as $|0\rangle$ and $|1\rangle$. These are localized states which correspond to the presence of a particle in a given well of an electrostatically shaped potential energy profile. In other words, the quantum logic in such a system is based on the position of the particle in a given quantum register.

By manipulating the potential energy of a particle one can achieve photon emission and absorption. An example of the potential energy on the surface of silicon channel of a quantum register, as obtained from electrostatic finite-element-method (COMSOL) simulations, is shown in Figure 2a. At the beginning (and also at the end) of the chain, the first (and the last) device serves as a reconfigurable injector/detector. The injector, in this context, is typically a single-electron device responsible for injecting individual electrons into the quantum register. The detector is an analog circuit which can detect (by a weak or strong measurement, depending on a particular configuration) a presence of a single electron. In the schematic, “S” and “D” denote Source and Drain regions (i.e., highly doped silicon), while “$I_1-\cdots I_7$” denote imposers (gates). One can apply precisely controlled DC voltages and pulses to the source/drain and the imposers to achieve desired modes of operation.
Figure 2. (a) Finite element method (FEM) COMSOL simulations of the electrostatically shaped potential energy as a function of distance assuming carrier freezeout operation for a chain of six devices for a quantum register. Appropriate voltage configuration allows one to construct a desired potential energy profile of a desired mode of operation. In the figures, “S/D” denote the source/drain, while “I1–I7” denote the imposers (gates). It can be seen that the potential energy profile can be approximated by an equivalent square-potential energy profile. The position-based qubit can be defined in a region of two potential wells separated by a barrier. For example, as shown, a qubit can be defined between the imposers “I3–I5”. The double well can be approximated by a DQD. The smaller the dimensions of the structure the more accurate this approximation. (b) By manipulating $V_{GS}$ (gate-source) and $V_{DS}$ (drain-source) applied voltages, one can achieve various potential energy profiles. In the schematic, the potential well bottoms between the imposers “I3–I5” are raised, which is equivalent to a lowered energy barrier between them. With the use of such an electrostatic mechanism, one can manipulate the resulting tunneling probability between the wells. Such an alteration of a potential energy profile can be achieved in a specific implementation by keeping $V_{GS}$, $V_{DS}$ voltages constant and by applying pulses at the imposers at precisely controlled time instances, duration and magnitude. Depending on the magnitude of the pulse, one can pump enough energy into the system so the particle (assuming in the ground state) gets excited from the ground energy and jumps to a new energy level. These transitions between energy levels due to the perturbed driving field can cause photon emission, typically of the same energy as the perturbation. This mechanism is similar to the absorption of a photon from a cavity. In this case, if the photon’s energy is similar to the gap between the two energy levels in a potential well, the particle (assuming already in the ground state) can become excited to allow tunneling.

In such a geometry, with specifically voltages applied, barriers (or wells) are formed between (or under) the imposers. In principle, the resulting potential energy profile can be approximated by an equivalent square potential energy profile. The DQD, defined as an abstract approximation of a double-well, i.e., in this example in the region between any two imposers $I_3$–$I_5$, can represent a position-based qubit. This will be discussed in more detail in the next section.

It is also possible to slightly alter the potential energy profile with purely electrostatic actuation, i.e., by applying positive or negative voltage pulses of a specific width and magnitude at the gate(s). The outcome is schematically illustrated in Figure 2b, where the well bottoms between imposers “I3–I5” are raised, which is equivalent to a lowered barrier between the wells. With such an electrostatic mechanism, electron tunneling can be induced or prohibited (more accurately, the probability of tunneling can be increased or decreased). In other words, by lowering (raising) the
barrier, the probability of tunneling increases (decreases) drastically. Depending on the magnitude of perturbation, one can excite a particle by pumping energy into the system. From this point of view, an electrostatic driving field/perturbation can have a similar result as photon absorption (electromagnetic driving field) from a cavity. A tunneling electron will then emit photons of specific (discrete) energies related to the bounded energy levels of the constructed potential wells.

To sum up, as with the electrostatic actuation, photon absorption can also activate tunneling. Therefore, as discussed and demonstrated later in this paper, the coupling between DQDs via a waveguide allows the manipulation of qubits, exploiting both the electrostatic manipulation and photon exchange.

3. Position-Based Semiconductor Qubits in the Frame of Semiconductor Photon Communication

3.1. Rabi Flopping Frequency of a Position-Based Qubit

We start our analysis by considering the system of a CMOS double-quantum-dot (DQD). We assume initially that only the two lowest states can be populated. In this case, the system can be seen as a two-level system: the ground state, denoted as \( |g\rangle \), and the first excited state, denoted as \( |e\rangle \).

In this basis, the wave-function can be expressed as a superposition of the two eigen-functions:

\[
|\psi\rangle = c_g |\psi_g\rangle + c_e |\psi_e\rangle \tag{1}
\]

where \( c_g \) and \( c_e \) are the probability amplitudes of each energy state, with \( c_g^2 + c_e^2 = 1 \). The energy difference between the ground state, \( E_g \), and the first excited state, \( E_e \), defines the occupancy frequency, \( \omega_0 = (E_e - E_g)/\hbar \). When in relaxation, the system is expected to be in the ground state. However, one can excite the system by applying a driving field, which can be a square or a sinusoidal pulse of a given width. Assuming initially a small pertubative pulse, the system will be in a quantum superposition of the first two states, and it will display occupancy oscillations [26].

The Hamiltonian of the system can be written as:

\[
\hat{H} = \hat{H}_0 + \hat{H}_I \tag{2}
\]

where \( \hat{H}_0 \) is the Hamiltonian of the system in equilibrium, with \( \hat{H}_0 = \hat{p}^2/2m_e^* + U_0 \), \( \hat{H}_I = U_{BI} \cos \omega t \) is the interaction Hamiltonian and \( m_e^* \) is the effective electron mass. \( U_{BI} \) denotes the change to the initial potential energy profile, \( U_0 \), of the DQD system, when an arbitrary bias voltage waveform of frequency \( \omega \) is applied at the gates (The interaction Hamiltonian due to a single-mode cavity field of frequency \( \omega \) will have the same effect and can be represented qualitatively by the same expression). In the rotating wave approximation, the Rabi flopping frequency, \( \omega_R \), is [28]:

\[
\omega_R \equiv \frac{1}{2} \sqrt{(\omega - \omega_0)^2 + (U_{BI}/\hbar)^2} \tag{3}
\]

and

\[
c_e(t) = i \frac{U_{BI}}{\hbar \omega_R} \frac{e^{\delta t/2}}{\sin(\omega_R t/2)} \cos(\omega_R t/2) - i \frac{\delta}{\omega_R} \frac{e^{\delta t/2}}{\sin(\omega_R t/2)} \cos(\omega_R t/2) \tag{4}
\]

where \( \delta = \omega - \omega_0 \) is the detuning term. In this work, we are not interested in investigating the effects of detuning, therefore we assume \( \delta = 0 \). The transition probability, \( P_{g\rightarrow e} \equiv P_e(t) \), can be written as:

\[
P_e(t) = |C_e(t)|^2 = \frac{U_{BI}^2}{\omega_R^2} \sin^2(\omega_R t/2) \tag{5}
\]
3.2. Representation of the System in a Position Basis

Qualitatively, we can write the Hamiltonian in the tight binding approximation:

$$H = \begin{pmatrix} E_p & t_{s,0 \rightarrow 1} \\ t_{s,1 \rightarrow 0} & E_p \end{pmatrix}$$

(6)

where $t_{s,i \rightarrow j} = (i | \hat{\cal{H}} | j)$, $i \neq j = \{0,1\}$ are the tunneling (also known as hoping) terms in the tight-binding formalism which express the tunneling probability between the two neighboring quantum dots. Now, if we set $E_g = E - \Delta$ and $E_e = E + \Delta$, then $E_e - E_g = 2\Delta$ and $\omega_0 = \frac{2\Delta}{\hbar}$, so (6) can be written as [29,30]:

$$H = \begin{pmatrix} E & -\Delta \\ -\Delta & E \end{pmatrix}$$

(7)

with eigen-values $\lambda = E \pm \Delta$. The wave-function, in a position basis can be written as:

$$|\phi\rangle = c_0 |0\rangle + c_1 |1\rangle$$

(8)

where $c_0$ and $c_1$ are the occupancy coefficients in the Wannier-position basis $\{|0\rangle, |1\rangle\}$, with

$$|0\rangle (t=0) = \frac{1}{\sqrt{2}} (|\psi_{g}\rangle + |\psi_{e}\rangle)$$

$$|1\rangle (t=0) = \frac{1}{\sqrt{2}} (|\psi_{g}\rangle - |\psi_{e}\rangle)$$

(9)

The time evolution of the system, starting from state $|0\rangle (t=0)$ is:

$$|\phi(t)\rangle = \frac{1}{\sqrt{2}} (|\psi_{g}\rangle e^{-i(E-\Delta)t/\hbar} + |\psi_{e}\rangle e^{-i(E+\Delta)t/\hbar}) = \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) e^{-i(E-\Delta)t/\hbar} + \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) e^{-i(E+\Delta)t/\hbar} \right) = \frac{1}{\sqrt{2}} e^{-iEt/\hbar} \left( e^{i\Delta t/\hbar} (|0\rangle + |1\rangle) + (e^{-i\Delta t/\hbar} (|0\rangle - |1\rangle)) \right) = e^{-iEt/\hbar} \left( \cos\left(\frac{\Delta t}{\hbar}\right) |0\rangle + i \sin\left(\frac{\Delta t}{\hbar}\right) |1\rangle \right)$$

(10)

The above time-dependent oscillations have frequency probabilities:

$$P_{|0\rangle}(t) = |\langle 0 | 0 \rangle (t) |^2 = \cos^2\left(\frac{\Delta t}{\hbar}\right)$$

$$P_{|1\rangle}(t) = |\langle 1 | 1 \rangle (t) |^2 = \sin^2\left(\frac{\Delta t}{\hbar}\right)$$

(11)

Notice that we can write:

$$|\phi(t)\rangle = c_0 |0\rangle e^{i\omega_0 t} + c_1 |1\rangle e^{-i\omega_0 t}$$

(12)

4. Photon Emission Due to Transitions in a Semiconductor Position-Based Qubit—Description Based on a Jaynes–Cummings–Hubbard Formalism

4.1. Description of the System of Coupled Position-Based Qubit with a Cavity

In this section, we will expand the system of semiconductor position-based qubit by including a Jaynes–Cummings–Hubbard formalism for the full description of the system of a coupled qubit with a cavity. We will additionally assume four energy levels, and a square double-well potential energy approximation for the potential energy profile of the double quantum dot, as they are depicted in Figure 3. All the simulations in this study were performed assuming the potential energy profile and
energy levels of Figure 3. In this case, the four bound states of the system can be expressed in the position basis \(|0_g⟩|n⟩, |1_g⟩|n⟩, |0_e⟩|n+1⟩, |1_e⟩|n+1⟩\):

\[
|0_g⟩|n⟩ = \frac{1}{\sqrt{2}} \left( |ψ_0⟩|n⟩ + |ψ_1⟩|n⟩ \right), \quad |1_g⟩|n⟩ = \frac{1}{\sqrt{2}} \left( |ψ_0⟩|n⟩ - |ψ_1⟩|n⟩ \right)
\]

\[
|0_e⟩|n+1⟩ = \frac{1}{\sqrt{2}} \left( |ψ_2⟩|n+1⟩ + |ψ_3⟩|n+1⟩ \right), \quad |1_e⟩|n+1⟩ = \frac{1}{\sqrt{2}} \left( |ψ_2⟩|n+1⟩ - |ψ_3⟩|n+1⟩ \right)
\]

where the localized \(|0, 1⟩_g, e\) states are expressed as a superposition of \(|ψ_i⟩, i = 0, \ldots, 3\) eigen-states, and \(n \in \mathbb{N}\) denotes the number of photons. In this basis, the Hamiltonian of the system in spectral representation can be written as:

\[
\hat{H} = \sum_{i=0,1} \sum_{k=g,e} E_{p,k} |i_k⟩⟨i_k| + \sum_{i\neq j=0,1} t_{s,jk→i} |i_k⟩⟨j_k| + \sum_{i=0,1} t_{c,i} |i⟩⟨i⟩
\]

where \(E_p\) denotes the potential energy terms of each site, \(t_s\) denotes the hopping terms of the tunneling between neighbor quantum dots of the same energy level, \(|g⟩\) or \(|e⟩\), and \(t_c\) denotes the frequency of transitions between the lower \(|g⟩\) and upper \(|e⟩\) energy states of the same localized state, \(|0⟩\) or \(|1⟩\).

We should also note that we consider photon emission only in transitions from the ground energy split (the first two eigen-energies, \(E_0, E_1\)) to the excited energy split (eigen-energies \(E_2, E_3\)) without losing generality of our results. Then, from (14), the time-evolution of the system can be found from the time-dependent Schrödinger equation in a matrix representation:

\[
i\hbar \frac{dc_m}{dt} = \sum_n H_{mn} c_n
\]

where \(c_m\) are the probability amplitudes of each coefficient of the superposition of quantum states. For the given initial conditions, a solution of (15) will have the form:

\[
|ψ(t)⟩ = c_{0g}(t) |ψ_0⟩ + c_{1g}(t) |ψ_1⟩ + c_{1g}(t) |ψ_3⟩ + c_{1g}(t) |ψ_4⟩
\]

where in this notation, for example, amplitude \(c_{0g}\) corresponds to the ground localized state, \(|0_g⟩\), i.e., where “0” is the position (state \(|0⟩\)) and “g” is the energy level (state \(|g⟩\)). Then, the time evolution of the probability of the particle to be found, for example in the state \(|0_g⟩\), will be denoted as:

\[
P_{|0_g⟩}(t) = |c_{0g}(t)|^2
\]

or in general

\[
P_{|n⟩}(t) = |c_{nm}(t)|^2, \quad n = 0, 1 \quad m = g, e
\]
Figure 3. Potential energy profile as a piecwise approximation of a double-well with four energy-levels. This function is extracted from COMSOL electrostatic simulations, assuming carrier freezeout operation. The number of bound states in the double well depends on a particular voltage configuration applied at the gates. Therefore, it is possible to electrostatically control the energy gaps between the different energy levels. In addition, the energy levels of a given potential energy double well determine the allowed energies of photons that are possible to emit and absorb during the quantum operation between communicating qubits.

4.2. Simulation Results

The time evolution of the probabilities of different quantum states, as obtained from solving (15), is depicted in Figure 4. The probability of the states $|0_g\rangle$ and $|0_e\rangle$ is visualized in Figure 4a. The probabilities of the localized states $|0\rangle$ are, as expected, anti-correlated. Similarly, the probabilities $|1_g\rangle$ and $|1_e\rangle$ are also anti-correlated, as shown in Figure 4b. Therefore, the evolution of quantum states in terms of ground $|g\rangle$ and excited $|e\rangle$ energies exhibits an anti-correlation. Moreover, in Figure 4c one can see that the anti-correlation occurs also in the probabilities of the two localized states $|0_g\rangle$ and $|1_g\rangle$, of a quantum particle of the same ground level, $|g\rangle$, i.e., this is a positional anti-correlation. The same positional anti-correlation occurs between the two localized states, $|0_e\rangle$ and $|1_e\rangle$, but now of the same excited energy level, as depicted in Figure 4d.
Figure 4. (a) Evolution of the probability of the states $|0_g\rangle$ and $|0_e\rangle$. These states correspond to the same position (localized state $|0\rangle$) but different energy levels (ground state $|g\rangle$ and excited state $|e\rangle$). It is observed that they are anti-correlated. (b) Time Evolution of the probability of the states $|1_g\rangle$ and $|1_e\rangle$. Similarly, these states correspond to the same position (in this case the localized state $|1\rangle$). Energy anti-correlation is also observed in this case. (c) The time evolution of the probability of the states $|0_g\rangle$ and $|1_g\rangle$. These states correspond to the same ground energy level (energy state $|g\rangle$) but different position (localized states $|0\rangle$ and $|1\rangle$). Therefore, they are anti-correlated. (d) Time evolution of the probability of the states $|0_e\rangle$ and $|1_e\rangle$. These states correspond to the same excited energy level (in this case energy state $|e\rangle$) but different position (localized states $|0\rangle$ and $|1\rangle$). They are also anti-correlated.

Finally, to conclude the analysis of the system of a single qubit, an example of a typical quantum path following the time evolution of (15) is presented in Figure 5, where a photon is absorbed during a transition from a localized ground state $|g\rangle$ to a localized excited state $|e\rangle$, while a photon is emitted during a transition from the state $|e\rangle$ to the state $|g\rangle$. After obtaining the expressions for the evolution of various amplitude probabilities from (17), we follow the numerical approach of [23] to simulate the quantum path.
Figure 5. (a) Simulated quantum path as a result of transitions from the localized ground state $|g\rangle$, to the localized excited state $|e\rangle$. The transitions take place in a probabilistic manner, following the time evolution determined from the solution of (15). (b) Number of emitted/absorbed photons as a result of transitions between the ground $|g\rangle$ and the excited $|e\rangle$ states for the simulated quantum path. It is evident that transitions from the ground state $|g\rangle$ to the excited state $|e\rangle$ correspond to an absorption of a photon, while the transitions from the excited state $|e\rangle$ to the ground state $|g\rangle$ correspond to an emission of a photon.

### 4.3. Description of System of Two Entangled Coupled Position-Based Qubits with a Cavity

The system of two qubits, A and B, each one defined by a particle confined to its respective double-well, as shown in Figure 1d, can be expressed by the wavefunction:

$$|\Psi\rangle = \sum_{n_A=0}^1 \sum_{n_B=0}^1 c_{n_An_B} |n_A^A, n_B^B\rangle$$

where we again assume four quantum states for each particle. The Hamiltonian of the system can be written as:

$$H = H(B) \otimes I_4 + I_4 \otimes H(A)$$

where $H(A)$ and $H(B)$ are the Hamiltonians of the first particle (system-A) and second particle (system-B), respectively, of the form (14), and $I_4$ is a 4x4 identity matrix.

### 4.4. Maximally Entangled States and Entanglement Entropy

To investigate the entanglement and the dynamics of the system of two qubits, we will use the Von Neumann entanglement entropy $S_N$. The density operator is given by the expression:

$$\hat{\rho}_{AB} = |\psi\rangle \langle \psi|$$

Then, the Von Neumann entanglement entropy $S_N$ is defined as follows:

$$S_N = -\text{tr}(\hat{\rho}_A \ln \hat{\rho}_A) = -\text{tr}(\hat{\rho}_B \ln \hat{\rho}_B)$$

where, operators $\hat{\rho}_A$ and $\hat{\rho}_B$ are the reduced density operators, which can be found via the partial trace as

$$\hat{\rho}_A = \left(0^S_B \hat{\rho}_{AB} 0^B_S\right) + \left(0^e_B \hat{\rho}_{AB} 0^B_e\right) + \left(1^B_S \hat{\rho}_{AB} 1^B_S\right) + \left(1^e_B \hat{\rho}_{AB} 1^B_e\right)$$

$$\hat{\rho}_B = \left(0^A_S \hat{\rho}_{AB} 0^A_S\right) + \left(0^A_e \hat{\rho}_{AB} 0^A_e\right) + \left(1^A_S \hat{\rho}_{AB} 1^A_S\right) + \left(1^A_e \hat{\rho}_{AB} 1^A_e\right)$$

Let us now assume the maximally entangled Bell state [31]:

$$|\Phi_{AB}\rangle = \frac{1}{\sqrt{2}} \left( |0^A 0^B\rangle + |1^A 1^B\rangle \right)$$
which is defined generally between any two systems $A$ and $B$. Writing this state in the basis of our system with system-A (qubit #1) and system-B (qubit #2), we get:

$$|\Phi_{AB}\rangle = \frac{1}{\sqrt{2}} \left( |0^A_s0^B_s\rangle + |0^A_s0^B_g\rangle + |0^A_g0^B_s\rangle + |0^A_g0^B_g\rangle + |1^A_s1^B_s\rangle + |1^A_s1^B_g\rangle + |1^A_g1^B_s\rangle + |1^A_g1^B_g\rangle \right)$$

and

$$\hat{\rho}_A = tr_B (\langle \Phi_{AB}|\Phi_{AB}\rangle) = \frac{1}{2} I_4$$

In this case, from (22) $S_N = 2 \ln 2$.

In general, the maximum value of $S_N$ is $\ln N$, where $N$ is the number of states of one qubit. The system will be maximally entangled when all the probability amplitudes $c_m$, for $m = 1, 2, ... N$, reach the same value, $c_m = 1/N$ [32].

4.5. Simulation Results

Considering the system with the Hamiltonian (20) and by solving Equation (15), we obtain the amplitudes $c_{n,n_\rho}$ that describe the examined system. The evolution of the probability of the system to be found in a specific state will be given by expressions similar to (18)

$$P_{[n,n_\rho]}(t) = |c_{n,n_\rho}(t)|^2, \quad n_{A,B} = 0^A_s, 0^A_g, 1^A_s, 1^A_g$$

Then, the probability of finding each particle in a specific position and energy state will be given as a sum of combined probabilities since we assumed a combined wave-function to describe the system. In particular, we can write:

$$P_{[0^A_s]}(t) = |c_{0^A_s0^B_s}(t)|^2 + |c_{0^A_s0^B_g}(t)|^2 + |c_{0^A_g0^B_s}(t)|^2 + |c_{0^A_g0^B_g}(t)|^2$$

$$P_{[0^A_g]}(t) = |c_{0^A_s0^B_s}(t)|^2 + |c_{0^A_s0^B_g}(t)|^2 + |c_{0^A_g0^B_s}(t)|^2 + |c_{0^A_g0^B_g}(t)|^2$$

$$P_{[1^A_s]}(t) = |c_{1^A_s0^B_s}(t)|^2 + |c_{1^A_s0^B_g}(t)|^2 + |c_{1^A_g0^B_s}(t)|^2 + |c_{1^A_g0^B_g}(t)|^2$$

$$P_{[1^A_g]}(t) = |c_{1^A_s0^B_s}(t)|^2 + |c_{1^A_s0^B_g}(t)|^2 + |c_{1^A_g0^B_s}(t)|^2 + |c_{1^A_g0^B_g}(t)|^2$$

$$P_{[0^B_s]}(t) = |c_{0^A_s0^B_s}(t)|^2 + |c_{0^A_s0^B_g}(t)|^2 + |c_{0^A_g0^B_s}(t)|^2 + |c_{0^A_g0^B_g}(t)|^2$$

$$P_{[0^B_g]}(t) = |c_{0^A_s0^B_s}(t)|^2 + |c_{0^A_s0^B_g}(t)|^2 + |c_{0^A_g0^B_s}(t)|^2 + |c_{0^A_g0^B_g}(t)|^2$$

$$P_{[1^B_s]}(t) = |c_{1^A_s0^B_s}(t)|^2 + |c_{1^A_s0^B_g}(t)|^2 + |c_{1^A_g0^B_s}(t)|^2 + |c_{1^A_g0^B_g}(t)|^2$$

$$P_{[1^B_g]}(t) = |c_{1^A_s0^B_s}(t)|^2 + |c_{1^A_s0^B_g}(t)|^2 + |c_{1^A_g0^B_s}(t)|^2 + |c_{1^A_g0^B_g}(t)|^2$$

In Figure 6a, the probability as a function of time of the ground state of system-A, $P_{[0^A_s]} = P_{[0^A_s]}(t)$, is plotted together with that of the ground state of system-B, $P_{[0^B_s]} = P_{[0^B_s]}(t) + P_{[1^B_s]}(t)$. Remarkably, the energy states of the two qubits are anti-correlated. This result is significant since the coupling between the two qubits in this model is achieved through a photon communication. For instance, in Figure 7a, typical quantum paths of system-A and system-B are plotted. It can be seen that the quantum trajectories of the two systems are anti-correlated. This is also visible from Figure 7b, where the emitted and absorbed photons between the two systems are anti-correlated as well. When system-A emits a photon, system-B absorbs a photon, and vice versa.
Figure 6. (a) Evolution of probability as a function of time of the ground state of system-A, \( P_{|0\rangle} = P_{|0\rangle_A} (t) + P_{|1\rangle_A} (t) \), together with that of the ground state of system-B, \( P_{|0\rangle} = P_{|0\rangle_B} (t) + P_{|1\rangle_B} (t) \). Remarkably, the energy states of the two qubits are anti-correlated. (b) Evolution of the probability of the localized state \( |0\rangle \) of system-A, \( P_{|0\rangle} (t) = P_{|0A\rangle} (t) + P_{|0B\rangle} (t) \), together with the evolution of probability of the localized state \( |0\rangle \) of system-B, \( P_{|0\rangle} (t) = P_{|0A\rangle} (t) + P_{|0B\rangle} (t) \) as a function of time. In this case, the anti-correlation is not trivial, and the result will depend on initial conditions. This is expected, since we assumed that there is no electrostatic interaction between the two particles, i.e., the Coulomb force is negligible. Considering this, the position of each particle is not expected to be “strongly” affected by the position of the other, only their energy states.

Figure 7. (a) Quantum paths of system-A and system-B. The methodology to obtain these graphs is similar to the one discussed for the system of a single qubit. It can be seen that the quantum trajectories of the two systems are anti-correlated. In other words, when system-A is in the ground state \( |n+1, g\rangle \), system-B is in the excited state \( |n, e\rangle \). (b) The emitted and absorbed photons between the two systems are anti-correlated. When system-A emits a photon, system-B absorbs a photon, and vice versa.

However, we also plot in Figure 6(b) the evolution of the probability with time of the localized state \( |0\rangle \) of system-A, \( P_{|0\rangle} (t) = P_{|0A\rangle} (t) + P_{|0B\rangle} (t) \), and the evolution of the probability with time of the localized state \( |0\rangle \) of system-B, \( P_{|0\rangle} (t) = P_{|0A\rangle} (t) + P_{|0B\rangle} (t) \). In this case, the anti-correlation is not trivial, and the result will depend on initial conditions. This is expected since we assumed that there is no electrostatic interaction between the two particles, i.e., the Coulomb force is negligible. Considering
this, the position of each particle is not expected to be “strongly” affected by the position of the other, only its energy states. Here we should note that if one considers a non-negligible Coulomb force, the positional anti-correlation will be also observed. This was also demonstrated in [26] where the quantum states entanglement was due to a Coulomb interaction.

To conclude this section, we investigate the entanglement in the system under study. Figure 8 plots the Von Neumann entanglement entropy $S_N$ defined between system-A and system-B. As shown in Section 4.4, the maximum value of $S_N$ for this system is $2 \ln 2$. At such an instance of time, when $S_N = \text{max}$, the quantum states are maximally entangled (inseparable). Thus, the wave-function cannot be represented as a product of the wave-functions of each particle. From the plot, one can observe that $S_N$ is a time-dependent quantity and for this system, it reaches the maximum value of $2 \ln 2$. We conclude that the states of the two coupled qubits via the waveguide are entangled. Therefore, when a photon communication is allowed between two qubits, as constructed via the methodology discussed in this study, one is expected to achieve quantum operations between the qubits over longer distances.

**Figure 8.** Von Neumann entanglement entropy $S_N$ defined between system-A and system-B. The maximum value of $S_N$ for this system is $2 \ln 2$. When this is the case, the quantum states are maximally entangled (inseparable). Thus, the wave-function cannot be represented as a product of the wave-functions of each particle. One can observe from the plot that $S_N$ is a time-dependent quantity. For this system it reaches a maximum value $2 \ln 2$. The states of the two coupled qubits via the waveguide are entangled.

5. Conclusions

In this study, we investigated semiconductor position-based qubits (a.k.a. charge qubits) in the context of photon communication. Electrostatic simulations under the assumption of freezeout operation show that with appropriate voltages applied to the gates of CMOS devices (based on FDSOI technology) it would be possible to achieve the desired potential energy profile meeting the requirements of a specific quantum operation. This can allow one to control the energy levels of the bound states of the system and the tunneling probabilities of particles between the barriers separating quantum wells. We discussed that the system can be approximated as quantum dots (QD), and each double QD (DQD) implements a position-based qubit.

We defined position-based qubits and their coupling with a cavity. We showed that in the presence of an external perturbative driving field, in the rotating wave approximation, the Rabi flopping frequency predicts analytically the evolution of the quantum states. The various states of the system of the simple qubit are found to be anti-correlated, both in energy-basis and position-basis representation.

We further expanded the model to include the description of the photon emission and entanglement of coupled position-based qubits based on the Jaynes–Cummings–Hubbard formalism.
We demonstrated that for a given geometry and potential energy profile it is possible to construct entangled states and trace their time evolution. We quantified the magnitude of entanglement due to the photon communication by calculating the entanglement entropy. The modelling provided in this work can offer the tools towards the optimization of relevant semiconductor photon-assisted applications and can easily be expanded in a straightforward manner to describe multi-particle systems.

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