

Tight-binding approximation in description of electrostatic position-dependent Qbit, Quantum Swap and Quantum CNOT gate

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Abstract

Analytical solutions describing quantum Swap gate are given by the use of tight-binding approximation.

1 Electrostatic position depedent qubit

In case of 2 well representing coupled quantum dot one can write the Hamiltonian in the tight-binding approximation in the following way

$$H = (t_{1,2}|1\rangle\langle 2| + t_{2,1}|2\rangle\langle 1|) + Ep_1|1\rangle\langle 1| + Ep_2|2\rangle\langle 2|. \quad (1)$$

The quantum state is given as $|\psi\rangle = c_0|1\rangle + c_1|2\rangle$, where $|c_0|^2$ is occupancy probability in q-dot 1 and $|c_1|^2$ is occupancy probability in q-dot 2 so $|c_0|^2 + |c_1|^2 = 1$. We have assumed that quantum dots can be asymmetric but in case of symmetric quantum dots we have $E_p(1) = E_p(2) = E_p$ and $t_{1,2} = t_{2,1} = t$. The Hamiltonian has the matrix representation given as

$$H = \begin{pmatrix} Ep_1 & t_{2,1} \\ t_{1,2} & Ep_2 \end{pmatrix} \quad (2)$$

We have 2 different eigenenergy values (E_1, E_2) given as

$$E_{1(2)} = 1/2(Ep_1 + Ep_2 \pm \sqrt{4t_{1,2}t_{2,1} + Ep_1^2 - 2Ep_1Ep_2 + Ep_2^2}) \quad (3)$$

with eigenvalues

$$|\psi_1\rangle = \begin{pmatrix} -(-Ep_1 + Ep_2 - \sqrt{4t_{1,2}t_{2,1} + Ep_1^2 - 2Ep_1Ep_2 + Ep_2^2})/2t_{1,2} \\ 1 \end{pmatrix} \quad (4)$$

and

$$|\psi_2\rangle = \begin{pmatrix} -((-Ep_1 + Ep_2 + \sqrt{4t_{1,2}t_{2,1} + Ep_1^2 - 2Ep_1Ep_2 + Ep_2^2})/(2t_{1,2})) \\ 1 \end{pmatrix} \quad (5)$$

In case of symmetric wells we have eigenenergies $E_{1(2)} = E_p \pm t$. and eigenstates are $\psi_1 = (-1, 1)$ and $\psi_2 = (1, 1)$. Two eigenstates correspond to simultaneous occupancy of 1 and 2 region so we can write

$$\begin{aligned} |\psi_1(t)\rangle &= \begin{pmatrix} -\frac{-Ep_1+Ep_2-\sqrt{4t_{1,2}t_{2,1}+(Ep_1-Ep_2)^2}}{2t_{1,2}} \\ 1 \end{pmatrix} = \\ &= \frac{-(-Ep_1+Ep_2-\sqrt{4t_{1,2}t_{2,1}+(Ep_1-Ep_2)^2})}{2t_{1,2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \\ &= \frac{-(-Ep_1+Ep_2-\sqrt{4t_{1,2}t_{2,1}+(Ep_1-Ep_2)^2})}{2t_{1,2}} |1,0\rangle + |0,1\rangle \end{aligned} \quad (6)$$

and

$$\begin{aligned} |\psi_2(t)\rangle &= \begin{pmatrix} -\left(\frac{(-Ep_1+Ep_2+\sqrt{4t_{1,2}t_{2,1}+(Ep_1^2-Ep_2)^2})}{(2t_{1,2})}\right) \\ 1 \end{pmatrix} = \\ &= -\left(\frac{(-Ep_1+Ep_2+\sqrt{4t_{1,2}t_{2,1}+(Ep_1^2-Ep_2)^2})}{(2t_{1,2})}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \\ &= -\left(\frac{(-Ep_1+Ep_2+\sqrt{4t_{1,2}t_{2,1}+(Ep_1^2-Ep_2)^2})}{(2t_{1,2})}\right) |1,0\rangle + |0,1\rangle. \end{aligned} \quad (7)$$

1.0.1 Double Q-Dot in external non-uniform time-dependent potential

We can introduce external time-dependent potential acting on points 1 and 2 such as $V(1, t)$ and $V(2, t)$. The Hamiltonian of the system is then given as

$$H = \begin{pmatrix} Ep_1 + V(1, t) & t_{2,1}(t) \\ t_{1,2}(t) & Ep_2 + V(2, t) \end{pmatrix}. \quad (8)$$

If external time-dependent potential is weak than $t_{1,2}(t) \approx t_{1,2}$ and $t_{2,1}(t) \approx t_{2,1}$.

$$H = \begin{pmatrix} Ep_1 + V(1, t) & t_{2,1} \\ t_{1,2} & Ep_2 + V(2, t) \end{pmatrix}. \quad (9)$$

We have 2 different time dependent eigenenergy values ($E_1(t), E_2(t)$) given as

$$E_{1(2)}(t) = 1/2((Ep_1+Ep_2+\frac{1}{2}(V(1, t)+V(2, t)) \pm \sqrt{4t_{1,2}(t)t_{2,1}(t) + ((Ep_1-Ep_2) + \frac{1}{2}(V(1, t) + V(2, t)))^2})). \quad (10)$$

with eigenvalues

$$|\psi_1(t)\rangle = \begin{pmatrix} -\frac{(-Ep_1-V(1, t)+Ep_2+V(2, t)-\sqrt{4t_{1,2}(t)t_{2,1}(t)+(Ep_1-Ep_2+(V(1, t)-V(2, t)))^2})}{2t_{1,2}} \\ 1 \end{pmatrix} \quad (11)$$

and

$$|\psi_2(t)\rangle = \left(-\left(\frac{(-Ep_1 - V(1,t) + Ep_2 + V(2,t) + \sqrt{4t_{1,2}(t)t_{2,1}(t) + (Ep_1 - Ep_2 + (V(1,t) - V(2,t))^2})}{(2t_{1,2})} \right) \right) \quad (12)$$

At any time instant the quantum state is given as

$$|\psi(t)\rangle = c_1(t)|\psi_{1n}(t)\rangle + c_2(t)|\psi_{2n}(t)\rangle, \quad (13)$$

where $|c_1(t)|^2 + |c_2(t)|^2 = 1$ and normalized eigenstates are denoted as $|\psi_{1n}(t)\rangle$ and $|\psi_{2n}(t)\rangle$. Equivalently we obtain

$$\langle \psi_{1n}(t) | \psi(t) \rangle = c_1(t), \langle \psi_{2n}(t) | \psi(t) \rangle = c_2(t). \quad (14)$$

The equation of motion can be written as $|\psi(t+dt)\rangle = |\psi(t)\rangle + \frac{dt}{i\hbar}(H(t)|\psi(t)\rangle)$. Equivalently we obtain 2 coupled recurrent relations for coefficients $c_1(t+dt)$ and $c_2(t+dt)$ depending on coefficients $c_1(t)$ and $c_2(t)$. We have

$$\begin{aligned} c_1(t+dt) &= \langle \psi_{1n}(t+dt) | \psi(t+dt) \rangle = \\ &= \langle \psi_{1n}(t+dt) | \psi(t) \rangle + \frac{dt}{i\hbar} (\langle \psi_{1n}(t+dt) | H(t) | \psi(t) \rangle) = \\ &= \langle \psi_{1n}(t+dt) | (c_1(t)|\psi_{1n}(t)\rangle + c_2(t)|\psi_{2n}(t)\rangle) + \\ &+ \frac{dt}{i\hbar} (\langle \psi_{1n}(t+dt) | \begin{pmatrix} Ep_1 + V(1,t) & t_{2,1}(t) \\ t_{1,2}(t) & Ep_2 + V(2,t) \end{pmatrix} (c_1(t)|\psi_{1n}(t)\rangle + c_2(t)|\psi_{2n}(t)\rangle)). \end{aligned} \quad (15)$$

and

$$\begin{aligned} c_2(t+dt) &= \langle \psi_{2n}(t+dt) | \psi(t+dt) \rangle = \\ &= \langle \psi_{2n}(t+dt) | \psi(t) \rangle + \frac{dt}{i\hbar} (\langle \psi_{2n}(t+dt) | H(t) | \psi(t) \rangle) = \\ &= \langle \psi_{2n}(t+dt) | (c_1(t)|\psi_{1n}(t)\rangle + c_2(t)|\psi_{2n}(t)\rangle) + \\ &+ \frac{dt}{i\hbar} (\langle \psi_{2n}(t+dt) | \begin{pmatrix} Ep_1 + V(1,t) & t_{2,1}(t) \\ t_{1,2}(t) & Ep_2 + V(2,t) \end{pmatrix} (c_1(t)|\psi_{1n}(t)\rangle + c_2(t)|\psi_{2n}(t)\rangle)). \end{aligned} \quad (16)$$

In case of symmetric wells $Ep(1) = Ep(2) = E_p$, $t_{1,2} = |t| = t_{2,1}$ and time-independent Hamiltonian we have

$$\begin{aligned} \frac{d}{dt}c_1(t) &= \frac{1}{i\hbar}(E_p c_1(t) + |t|c_2(t)) \\ \frac{d}{dt}c_2(t) &= \frac{1}{i\hbar}(|t|c_1(t) + E_p c_2(t)). \end{aligned} \quad (17)$$

Adding and subtracting those two equations give us relations $|t|$ -hopping (kinetic) term

$$\begin{aligned} \frac{d}{dt}(c_1(t) + c_2(t)) &= -\frac{i}{\hbar}[(E_p + |t|)(c_1(t) + c_2(t))] \\ \frac{d}{dt}(c_1(t) - c_2(t)) &= -\frac{i}{\hbar}[(E_p - |t|)(c_1(t) - c_2(t))]. \end{aligned} \quad (18)$$

In analogy to the evolution operator in Schroedinger equation we recognize two analytic solutions

$$[c_1(t) + c_2(t)] = e^{-\frac{i}{\hbar}(E_p+|t|)(t-t_0)}[c_1(t_0) + c_2(t_0)] \quad (19)$$

$$[c_1(t) - c_2(t)] = e^{-\frac{i}{\hbar}(E_p-|t|)(t-t_0)}[c_1(t_0) - c_2(t_0)]. \quad (20)$$

By adding or subtracting 2 equations and multiply by 1/2 we obtain $c_1(t)$ or $c_2(t)$ given as

$$c_1(t) = (e^{-\frac{i}{\hbar}(E_p+|t|)(t-t_0)} + e^{-\frac{i}{\hbar}(E_p-|t|)(t-t_0)})\frac{c_1(t_0)}{2} + (e^{-\frac{i}{\hbar}(E_p+|t|)(t-t_0)} - e^{-\frac{i}{\hbar}(E_p-|t|)(t-t_0)})\frac{c_2(t_0)}{2} \quad (21)$$

$$c_2(t) = (e^{-\frac{i}{\hbar}(E_p+|t|)(t-t_0)} - e^{-\frac{i}{\hbar}(E_p-|t|)(t-t_0)})\frac{c_1(t_0)}{2} + (e^{-\frac{i}{\hbar}(E_p+|t|)(t-t_0)} + e^{-\frac{i}{\hbar}(E_p-|t|)(t-t_0)})\frac{c_2(t_0)}{2}. \quad (22)$$

Presence of weak-time dependent potential present in 1 and 2 will change the analytic solutions into

$$c_1(t) = e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt} e^{-\frac{i}{\hbar}E_p(t-t_0)}[(e^{-\frac{i}{\hbar}|t|(t-t_0)} + e^{\frac{i}{\hbar}|t|(t-t_0)})\frac{c_1(t_0)}{2} + (e^{-\frac{i}{\hbar}|t|(t-t_0)} - e^{\frac{i}{\hbar}|t|(t-t_0)})\frac{c_2(t_0)}{2}] \quad (23)$$

$$c_2(t) = e^{-\frac{i}{\hbar}\int_{t_0}^t V(2,t)dt} e^{-\frac{i}{\hbar}E_p(t-t_0)}[(e^{-\frac{i}{\hbar}|t|(t-t_0)} - e^{\frac{i}{\hbar}|t|(t-t_0)})\frac{c_1(t_0)}{2} + (e^{-\frac{i}{\hbar}|t|(t-t_0)} + e^{\frac{i}{\hbar}|t|(t-t_0)})\frac{c_2(t_0)}{2}] \quad (24)$$

The last two equations are equivalent to

$$\begin{aligned} c_1(t) &= e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt} e^{-\frac{i}{\hbar}E_p(t-t_0)}[\cos(\frac{|t|}{\hbar}(t-t_0))c_1(t_0) - \sin(\frac{|t|}{\hbar}(t-t_0))ic_2(t_0)] = \\ &= e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(\cos(\frac{E_p(t-t_0)}{\hbar}) - \sin(\frac{E_p|t-t_0|}{\hbar})i)[\cos(\frac{|t|}{\hbar}(t-t_0))c_1(t_0) - \sin(\frac{|t|}{\hbar}(t-t_0))ic_2(t_0)] = \\ &= e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(c_1(t_0)\cos(\frac{E_p(t-t_0)}{\hbar})^2 - c_2(t_0)\sin(\frac{E_p(t-t_0)}{\hbar})^2) + \\ &-ie^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(c_1(t_0)\sin(\frac{E_p(t-t_0)}{\hbar})\cos(\frac{|t|}{\hbar}(t-t_0)) + c_2(t_0)\cos(\frac{E_p(t-t_0)}{\hbar})\sin(\frac{|t|}{\hbar}(t-t_0))) = \\ &= e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(c_1(t_0) - (c_2(t_0) + c_1(t_0))\sin(\frac{E_p(t-t_0)}{\hbar})^2) + \\ &-ie^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}c_1(t_0)(\sin(\frac{E_p(t-t_0)}{\hbar})\cos(\frac{|t|}{\hbar}(t-t_0)) + \cos(\frac{E_p(t-t_0)}{\hbar})\sin(\frac{|t|}{\hbar}(t-t_0))) + \\ &+ (-i)e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(c_2(t_0) - c_1(t_0))\cos(\frac{E_p(t-t_0)}{\hbar})\sin(\frac{|t|}{\hbar}(t-t_0)) = \\ &= e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(c_1(t_0) - (c_2(t_0) + c_1(t_0))\sin(\frac{E_p(t-t_0)}{\hbar})^2) - ie^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}c_1(t_0)\sin(\frac{(|t|+E_p)}{\hbar}(t-t_0)) + \\ &+ \frac{-i}{2}e^{-\frac{i}{\hbar}\int_{t_0}^t V(1,t)dt}(c_2(t_0) - c_1(t_0))[\sin(\frac{(E_p+|t|)(t-t_0)}{\hbar})t + \sin(\frac{(|t|-E_p)}{\hbar}(t-t_0))]. \end{aligned}$$

In quite analogical way we deal with coefficient $c_2(t)$ whose analytic solution can be written as

$$c_2(t) = e^{-\frac{i}{\hbar}\int_{t_0}^t V(2,t)dt} e^{-\frac{i}{\hbar}E_p(t-t_0)}(\sin(\frac{|t|}{\hbar}(t-t_0))(-ic_1(t_0)) + \cos(\frac{|t|(t-t_0)}{\hbar})c_2(t_0)). \quad (25)$$

1.1 Qbit in tight-binding in density matrix

The most general description for quantum state is by density matrix. In the simplest case it is $\rho = |\psi\rangle\langle\psi|$. Such state has the property $\rho^2 = \rho$ (pure state), where n is positive integer number. If $\rho^2 \neq \rho$ we deal with mixed state. Now we start the considerations from clean state.

1.1.1 Qbit in pure state

If our state has the form

$$|\psi\rangle = c_1(t)|1,0\rangle + c_2(t)|0,1\rangle = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}, \quad (26)$$

(where $|1,0\rangle$ corresponds to occupancy of 1 point in space and $|0,1\rangle$ corresponds to occupancy of 2 point in space) then $\langle\psi| = c_1^*(t)\langle 1,0| + c_2^*(t)\langle 0,1|$ and consequently

$$\rho = |\psi\rangle\langle\psi| = (c_1(t)|1,0\rangle + c_2(t)|0,1\rangle)(c_1^*(t)\langle 1,0| + c_2^*(t)\langle 0,1|) = |c_1(t)|^2|1,0\rangle\langle 1,0| + |c_2(t)|^2|0,1\rangle\langle 0,1| + c_1^*(t)c_2(t)|0,1\rangle\langle 1,0| + c_2^*(t)c_1(t)|1,0\rangle\langle 0,1|. \quad (27)$$

We recognize that ρ is Hermitian matrix. We also recognize that $Tr(\rho) = 1$. The ρ can be written in the matrix form

$$\rho = \begin{pmatrix} |c_1(t)|^2 & c_1^*(t)c_2(t) \\ c_1(t)c_2^*(t) & |c_2(t)|^2 \end{pmatrix}. \quad (28)$$

We have from previous considerations

$$c_1(t) = e^{-\frac{i}{\hbar} \int_{t_0}^t V(1,t)dt} e^{-\frac{i}{\hbar} E_p(t-t_0)} [\cos(\frac{|t|}{\hbar}(t-t_0))c_1(t_0) - \sin(\frac{|t|}{\hbar}(t-t_0))ic_2(t_0)]$$

and

$$c_2(t) = e^{-\frac{i}{\hbar} \int_{t_0}^t V(2,t)dt} e^{-\frac{i}{\hbar} E_p(t-t_0)} (\sin(\frac{|t|}{\hbar}(t-t_0))(-ic_1(t_0)) + \cos(\frac{|t|}{\hbar}(t-t_0))c_2(t_0)).$$

1.1.2 Qbit in mixed state state

In most general case $Tr(\rho) = 1$ and $\rho^2 \neq \rho$ and $\rho^\dagger = \rho$. Thus we can write

$$\rho = |\psi\rangle\langle\psi| = \gamma_1(t)|1,0\rangle\langle 1,0| + (1 - \gamma_1(t))|0,1\rangle\langle 0,1| + \gamma_0(t)|0,1\rangle\langle 1,0| + \gamma_0(t)^*|1,0\rangle\langle 0,1|, \quad (29)$$

where $\gamma_1(t), \gamma_0(t)$ are complex valued numbers. We recognize that external perturbing potential $V(1,t)$ and $V(2,t)$ can bring pure state to mixed state and reversely. One of the examples of mixed matrix can have of the following form

$$\rho = |\psi\rangle\langle\psi| = \gamma_1(t)|1,0\rangle\langle 1,0| + (1 - \gamma_1(t))|0,1\rangle\langle 0,1|. \quad (30)$$

2 Quantum electrostatic Swap gate

We consider the situation as depicted in Fig.1. We have 2 separated in space systems of double quantum dots U (Upper) and L (Lower). One electron is in L

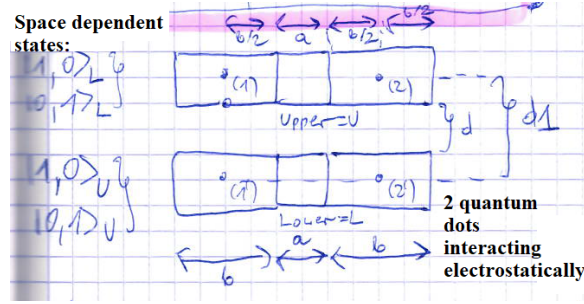


Figure 1: 2 electrons confined in two separated in space double interconnected quantum dots interacting electrostatically.

system and one electron is in U system. If U system is far away from L system than the quantum states of U is independent from L quantum system and in such case we can write $|\psi\rangle_U = c_1|1,0\rangle_U + c_2|0,1\rangle_U$ and $|\psi\rangle_L = c_3|1,0\rangle_L + c_4|0,1\rangle_L$ and normalization conditions $|c_1|^2 + |c_2|^2 = 1$ and $|c_3|^2 + |c_4|^2 = 1$. In case of separated systems we can write the total Hilbert space by factorization so $|\psi\rangle = |\psi\rangle_U |\psi\rangle_L$. However it is not true when we bring L and U systems sufficiently close so Coulomb interaction has no longer perturbative character. In such case we have the most general form of quantum state given as

$$|\psi\rangle = c_a|0,1\rangle_U |0,1\rangle_L + c_b|0,1\rangle_U |1,0\rangle_L + c_c|1,0\rangle_U |0,1\rangle_L + c_d|1,0\rangle_U |1,0\rangle_L. \quad (31)$$

Since we have 2 electrons we can write $|c_a|^2 + |c_b|^2 + |c_c|^2 + |c_d|^2 = 1$. In rare and special case we can write

$$|\psi\rangle = (c_{1U}|0,1\rangle_U + c_{2U}|1,0\rangle_U)(c_{1L}|0,1\rangle_L + c_{2L}|1,0\rangle_L) = c_{1U}c_{1L}|0,1\rangle_U |0,1\rangle_L + c_{1U}c_{2L}|0,1\rangle_U |1,0\rangle_L + c_{2U}c_{1L}|1,0\rangle_U |0,1\rangle_L + c_{2U}c_{2L}|1,0\rangle_U |1,0\rangle_L. \quad (32)$$

If $c_a = c_{1U}c_{1L}$, $c_b = c_{1U}c_{2L}$, $c_c = c_{2U}c_{1L}$ and $c_d = c_{2U}c_{2L}$ and we are dealing with non-entangled state since total quantum state can be factorized as product of 2 quantum subsystems. Such case is rare and in most cases our system depicted in Fig.1 is entangled what especially takes place if U and L are not far away. Now we need to write down the system Hamiltonian from Fig.1. One electron from U can be in points 1 and 2 and second electron can be in points 1' and 2'. We make assumptions that U and L have the same physical structure and are symmetric.

We have total system Hamiltonian as the sum of all potential and kinetic energies given as

$$\begin{aligned} H = & (E_p(1)|1,0\rangle_U \langle 1,0|_U + E_p(2)|0,1\rangle_U \langle 0,1|_U)I_L + I_U(E_p(1')|1,0\rangle_L \langle 1,0|_L + \\ & + E_p(2')|0,1\rangle_L \langle 0,1|_L) + t_U(|1,0\rangle_U \langle 0,1|_U + |0,1\rangle_U \langle 1,0|_U)I_L + I_U t_L(|1,0\rangle_L \langle 0,1|_L + \\ & + |0,1\rangle_L \langle 1,0|_L) + E_c(1,1')(|1,0\rangle_U |1,0\rangle_L \langle 1,0|_U \langle 1,0|_L) + \\ & + E_c(2,2')|0,1\rangle_U |0,1\rangle_L \langle 0,1|_U \langle 0,1|_L + \\ & + E_c(2,1')(|0,1\rangle_U |1,0\rangle_L \langle 0,1|_U \langle 1,0|_L) + E_c(1,2')|1,0\rangle_U |0,1\rangle_L \langle 1,0|_U \langle 0,1|_L. \end{aligned} \quad (33)$$

The last 4 terms are Coulomb interaction terms between one electron confined in L system and one electron confined in U system. The expressions $E_c(1, 1'), E_c(2, 2'), E_c(2, 1'), E_c(1, 2')$ have values Coulomb classical energy between points $(1, 1'), (2, 2'), (2, 1'), (1, 2')$. Two double quantum dots are geometrically parametrized by constants $d1, d, a, b$ and thus we have distances $d_{1,1'} = d1 = d_{2,2'}$ and $d_{1,2'} = d_{1',2} = \sqrt{d1^2 + (b+a)^2}$. Therefore $E_c(1, 1') = \frac{q^2}{d1} = E_c(2, 2')$ and $E_c(1, 2') = \frac{q^2}{\sqrt{(d1)^2 + (b+a)^2}} = E_c(2, 1')$. The electron kinetic energy in U system is parametrized by t_U and in L system by t_L . In simplified case we have $t_U = t_L = t$. We also denoted $I_L = (|0, 1\rangle\langle 0, 1|_L + |1, 0\rangle\langle 1, 0|_L)$ and $I_U = (|0, 1\rangle\langle 0, 1|_U + |1, 0\rangle\langle 1, 0|_U)$. I_L is identity operator and is projection of L state on itself. The same is with I_U operator that is identity operator and is projection of state U on itself. It is convenient to express total system Hamiltonian in matrix representation. We have 4 by 4 matrix given as

$$H = \begin{pmatrix} Ep(2) + Ep(2') + E_c(2, 2') & Ep(2) + Ep(1') + E_c(2, 1') & t_U & 0 \\ t_L & 0 & 0 & t_U \\ t_U & t_U & Ep(1) + Ep(2') + E_c(1, 2') & t_L \\ 0 & t_U & Ep(1) + Ep(1') + E_c(1, 1') & 0 \end{pmatrix} \quad (34)$$

Now we need to find system 4 eigenvalues and eigenstates(4 orthogonal 4-dimensional vectors) so we are dealing with matrix eigenvalue problem) what is the subject of classical algebra. Let us assume that 2 double quantum dot systems are symmetric and biased by the same voltages generating potential bottoms V_s so we have $Ep(1) = Ep(2) = Ep(1') = Ep(2') = V_s$ and that $t_L = t_U = t_s$. Denoting $E_c(1, 1') = E_c(2, 2') = Ec1s$ and $E_c(1, 2') = E_c(2, 1') = Ec2s$ we are obtaining 4 orthogonal eigenvectors

$$V_1 = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, V_2 = \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}, V_{3(4)} = \begin{pmatrix} 1 \\ \mp \frac{4t_s}{\pm(-Ec1s+Ec2s)+\sqrt{(Ec1s-Ec2s)^2+16t_s^2}} \\ \mp \frac{4t_s}{\pm(-Ec1s+Ec2s)+\sqrt{(Ec1s-Ec2s)^2+16t_s^2}} \\ 1 \end{pmatrix} \quad (35)$$

corresponding to 4 eigenenergies

$$\begin{aligned} E_1 &= Ec1s + 2V_s, E_2 = Ec2s + 2V_s, E_1 > E_2 \\ E_3 &= \frac{1}{2}((Ec1s + Ec2s) - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2} + 4V_s) \\ E_4 &= \frac{1}{2}((Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2} + 4V_s), E_4 > E_3. \end{aligned} \quad (36)$$

We observe that setting quantum state to vector V_1 we obtain the state

$$|\psi\rangle = -|0, 1\rangle_U |0, 1\rangle_L + |1, 0\rangle_U |1, 0\rangle_L \quad (37)$$

and such state is indeed entangled. Setting the quantum state to vector V_2 we also obtain the entangled state

$$|\psi\rangle = -|0, 1\rangle_U |1, 0\rangle_L + |1, 0\rangle_U |0, 1\rangle_L. \quad (38)$$

We also notice that the state V_3 and V_4 does not have its classical counterpart since upper electron exists at both positions 1 and 2 and lower electron

exists at both positions at the same time. We observe that when distance between two systems of double quantum dots goes into infinity the energy difference between quantum state corresponding to V_1 and V_2 goes to zero. This makes those two entangled states to be degenerate. We notice that vectors

$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ correspond to states $(|0, 1 \rangle_U |0, 1 \rangle_L), (|0, 1 \rangle_U |1, 0 \rangle_L), (|1, 0 \rangle_U |0, 1 \rangle_L), (|1, 0 \rangle_U |1, 0 \rangle_L)$.

We observe that $|v_1|^2 = 2, |v_2|^2 = 2$ and that

$$|v_3|^2 = \frac{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \quad (39)$$

with

$$|v_4|^2 = \frac{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s}. \quad (40)$$

Thus normalized 4 eigenvectors are of the following form

$$V_{1n} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, V_{2n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} \quad (41)$$

$$, V_{3n} = \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} \frac{1}{4t_s} \\ -\frac{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \\ -\frac{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \\ 1 \end{pmatrix} \quad (42)$$

$$, V_{4n} = \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} \frac{1}{4t_s} \\ \frac{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \\ \frac{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \\ 1 \end{pmatrix} \quad (43)$$

2.0.1 Case of 2 double quantum dots on the line

We consider the situation as depicted in Fig.2.0.1.

We have the following Coulomb interaction terms $E_C(2, 1') = q^2/d, E_C(2, 1') = q^2/(d+2b+2a), E_C(2, 2') = q^2/(d+b+a) = E_C(1, 1')$. We assume $t_L = t_R = |t|$. All energies at the nodes 1, 2, 1' and 2' are controlled with biasing voltage V_s .

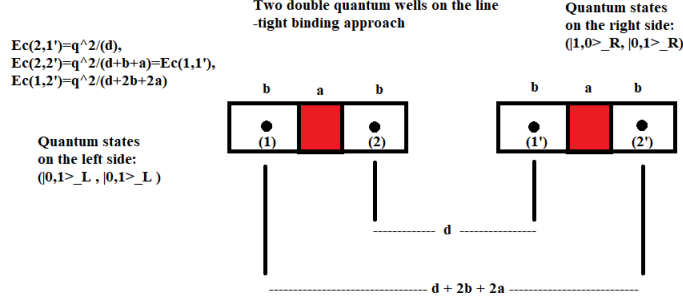


Figure 2: Case of 2 double quantum dots on the line.

We obtain the following Hamiltonian of the system

$$+E_c(1,1')(|1,0>_L |1,0>_R < 1,0|_L < 1,0|_R) + E_c(2,2')(|0,1>_L |0,1>_R < 0,1|_L < 0,1|_R) + E_c(1,2')(|1,0>_L$$

The quantum state of the system can be written as

$$|\psi> = c_a|0,1>_L |0,1>_R + c_b|0,1>_L |1,0>_R + c_c|1,0>_L |0,1>_R + c_d|1,0>_L |1,0>_R. \quad (45)$$

The coefficients $|c_a|^2 + |c_b|^2 + |c_c|^2 + |c_d|^2 = 1$ since $\langle \psi | \psi \rangle = 1$. We assume that

$$|0,1>_L |0,1>_R = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |0,1>_L |1,0>_R = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |1,0>_L |0,1>_R = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |1,0>_L |1,0>_R = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (46)$$

In such case the system Hamiltonian is given as

$$H = \begin{pmatrix} E_p(2) + E_p(2') + E_c(2,2') & t_R(2' \rightarrow 1') & t_L(2 \rightarrow 1) & 0 \\ t_R(1' \rightarrow 2') & E_p(2) + E_p(1') + E_c(2,1') & 0 & t_L(2 \rightarrow 1) \\ t_L(1 \rightarrow 2) & 0 & E_p(1) + E_p(2') + E_c(1,2') & t_R(2' \rightarrow 1') \\ 0 & t_L(1 \rightarrow 2) & t_R(1' \rightarrow 2') & E_p(1) + E_p(1') + E_c(1,1') \end{pmatrix}. \quad (47)$$

We notice that $E_c(2,2') = E_c(1,1')$ since two double symmetric qubits are on the same line. Now we place the dependence of Coulomb energy on geometry. We obtain

$$H = \begin{pmatrix} E_p(2) + E_p(2') + \frac{q^2}{d+b+a} & t_R(2' \rightarrow 1') & t_L(2 \rightarrow 1) & 0 \\ t_R(1' \rightarrow 2') & E_p(2) + E_p(1') + \frac{q^2}{d} & 0 & t_L(2 \rightarrow 1) \\ t_L(1 \rightarrow 2) & 0 & E_p(1) + E_p(2') + \frac{q^2}{d+2(b+a)} & t_R(2' \rightarrow 1') \\ 0 & t_L(1 \rightarrow 2) & t_R(1' \rightarrow 2') & E_p(1) + E_p(1') + \frac{q^2}{d+b+a} \end{pmatrix}. \quad (48)$$

Now we set all hopping coefficients to $-t$ and we set $E_p(1) = E_p(2) = E_p(1') = E_p(2') = V_s$. We obtain

$$H = \begin{pmatrix} 2V_s + \frac{q^2}{d+b+a} & t & t & 0 \\ t & 2V_s + \frac{q^2}{d} & 0 & t \\ t & 0 & 2V_s + \frac{q^2}{d+2(b+a)} & t \\ 0 & t & t & 2V_s + \frac{q^2}{d+b+a} \end{pmatrix}. \quad (49)$$

This matrix has 4 different terms on its diagonal what brings 4 different eigenvalues and 4 orthogonal different eigenstates. In the oversimplified case we can consider the matrix structure to be of the form

$$H_s = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & q1s & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix} \quad (50)$$

. In such case we can recognize the following eigenvalues $E1 = 1$,

$$E2 = (2 + q1s)/3 - \frac{(-13 + 2q1s - q1s^2)}{(3(8 - 6q1s - 3q1s^2 + q1s^3 + 3\sqrt{3}\sqrt{-79 + 34q1s - 25q1s^2 + 8q1s^3 - 2q1s^4})^{1/3}) + 1/3(8 - 6q1s - 3q1s^2 + q1s^3 + 3\sqrt{3}\sqrt{-79 + 34q1s - 25q1s^2 + 8q1s^3 - 2q1s^4})^{1/3}}, \quad (51)$$

$$E3 = (2 + q1s)/3 + \frac{((1 + ISqrt[3])(-13 + 2q1s - q1s^2))}{(6(8 - 6q1s - 3q1s^2 + q1s^3 + 3Sqrt[3]Sqrt[-79 + 34q1s - 25q1s^2 + 8q1s^3 - 2q1s^4])^{1/3}) - 1/6(1 - ISqrt[3])(8 - 6q1s - 3q1s^2 + q1s^3 + 3Sqrt[3]Sqrt[-79 + 34q1s - 25q1s^2 + 8q1s^3 - 2q1s^4])^{1/3}}. \quad (52)$$

$$E4 = (2 + q1s)/3 + \frac{((1 - ISqrt[3])(-13 + 2q1s - q1s^2))}{(6(8 - 6q1s - 3q1s^2 + q1s^3 + 3Sqrt[3]Sqrt[-79 + 34q1s - 25q1s^2 + 8q1s^3 - 2q1s^4])^{1/3}) - 1/6(1 + ISqrt[3])(8 - 6q1s - 3q1s^2 + q1s^3 + 3Sqrt[3]Sqrt[-79 + 34q1s - 25q1s^2 + 8q1s^3 - 2q1s^4])^{1/3}}. \quad (53)$$

The last 2 eigenenergies has imaginary parts and are not corresponding to solution for non-dissipative quantum system.

For the matrix structure of the form

$$H = \begin{pmatrix} q2s & 1 & 1 & 0 \\ 1 & q1s & 1 & 0 \\ 1 & 1 & q3s & 0 \\ 1 & 1 & 1 & q2s \end{pmatrix}. \quad (54)$$

It has following eigenvalues

$$Es1 = q2s = \frac{2V_s}{t_s} + \frac{q^2}{t_s(d+b+a)}, \quad (55)$$

and second eigenvalue is

$$Es2 = (1/3)(q1s + q2s + q3s) +$$

$$\frac{- (2^{\frac{1}{3}} (-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2))}{3(-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 3q_{3s}(6q_{3s} - q_{1s}^2) + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3(q_{1s} + q_{2s})q_{3s}^2 + 2q_{3s}^3 + \frac{1}{\sqrt{4(-12 - q_{1s}^2 + q_{1s}(q_{2s} + q_{3s}) - q_{2s}^2 + q_{2s}q_{3s} - q_{3s}^2)^3 + w}})^{\frac{1}{3}}} +$$

$$+ (1/(32^{1/3}))(-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3 +$$

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$$\sqrt{4(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)^3 + (-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3)^2)^{1/3}}, \quad (56)$$

where

$$w = (-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3)^2. \quad (57)$$

Consequently 3-rd energy eigenvalue $Es3$ with $I = \sqrt{-1}$ is

$$Es3 = 1/3(q1s + q2s + q3s) + [(1 + ISqrt[3])(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)]/[32^{\frac{2}{3}}(-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3) + \sqrt{4(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)^3 + (-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3)^2)^{1/3}] - (1/(62^{\frac{1}{3}}))(1 - ISqrt[3])(-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3 + \sqrt{4(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)^3 + (-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3)^2})^{\frac{1}{3}}.$$

4-th energy eigenvalue is

$$Es4 = 1/3(q1s + q2s + q3s) + [(1 - ISqrt[3])(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)]/[32^{\frac{2}{3}}(-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3) + \sqrt{4(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)^3 + (-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3)^2)^{1/3}] - (1/(62^{1/3}))(1 + ISqrt[3])(-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3 + \sqrt{4(-12 - q_{1s}^2 + q_{1s}q_{2s} - q_{2s}^2 + q_{1s}q_{3s} + q_{2s}q_{3s} - q_{3s}^2)^3 + (-18q_{1s} + 2q_{1s}^3 + 36q_{2s} - 3q_{1s}^2q_{2s} - 3q_{1s}q_{2s}^2 + 2q_{2s}^3 - 18q_{3s} - 3q_{1s}^2q_{3s} + 12q_{1s}q_{2s}q_{3s} - 3q_{2s}^2q_{3s} - 3q_{1s}q_{3s}^2 - 3q_{2s}q_{3s}^2 + 2q_{3s}^3)^2})^{1/3} \quad (58)$$

Numerical testing shows that all eigenenergies has real values. Here $q_{2s} = \frac{2V_s}{t_s} + \frac{q^2}{4\pi\epsilon_0\epsilon t_s(d+b+a)}$, $q_{1s} = \frac{2V_s}{t_s} + \frac{q^2}{t_s d 4\epsilon_0\epsilon}$ and $q_{3s} = \frac{2V_s}{t_s} + \frac{q^2}{4\pi\epsilon_0\epsilon(d+2(a+b))}$, where ϵ is dielectric constant of material where electrons are and ϵ_0 is dielectric constant of vacuum. 4 eigenenergies correspond to 4 eigenstates (eigenvectors). We recognize that energy E_{1s} corresponds to electron oscillations such that they maintain constant distance so they switch between $|1, 0 \rangle_L$ $|1, 0 \rangle_R$ and $|0, 1 \rangle_L$ $|0, 1 \rangle_R$ state what is given below. Such energy is $Es1 = q2s = \frac{2V_s}{t_s} + \frac{q^2}{t_s(d+b+a)}$!!! It will correspond to eigenvector $|v1 \rangle = (-|0, 1 \rangle_L |0, 1 \rangle_R + |1, 0 \rangle_L |1, 0 \rangle_R)$ and this state is entangled and at the same time maximally ordered as it corresponds to energetic minimum of classically charged balls that moves in synchronized way all the time !! . We have the following energy eigenvectors

$$|v1 \rangle = n_1 \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, |v2 \rangle = n_2 \begin{pmatrix} -1 - \frac{((q1s-E_{2s})(q3s-E_{2s})(-q2s+E_{2s}))}{(q1s+q3s-2E_{2s})}, \\ -\frac{((q2s-E_{2s})(-q3s+E_{2s}))}{(-q1s-q3s+2E_{2s})}, \\ \frac{((q1s-E_{2s})(-q2s+E_{2s}))}{(q1s+q3s-2E_{2s})}, \\ 1 \end{pmatrix}, |v3 \rangle = n_3 \begin{pmatrix} -1 - \frac{((q1s-E_{s3})(q3s-E_{s3})(-q2s+E_{s3}))}{(q1s+q3s-2E_{s3})}, \\ -\frac{((q2s-E_{s3})(-q3s+E_{s3}))}{(-q1s-q3s+2E_{s3})}, \\ \frac{((q1s-E_{s3})(-q2s+E_{s3}))}{(q1s+q3s-2E_{s3})}, \\ 1 \end{pmatrix}, \quad (59)$$

$$|v4 \rangle = n_4 \begin{pmatrix} -1 - \frac{((q1s-E_{s4})(q3s-E_{s4})(-q2s+E_{s4}))}{(q1s+q3s-2E_{s4})}, \\ -\frac{((q2s-E_{s4})(-q3s+E_{s4}))}{(-q1s-q3s+2E_{s4})}, \\ \frac{((q1s-E_{s4})(-q2s+E_{s4}))}{(q1s+q3s-2E_{s4})}, \\ 1 \end{pmatrix}. \quad (60)$$

Here n_1, n_2, n_3, n_4 are normalization constants. They have values $n_1 = \frac{1}{\sqrt{2}}$ and

$$n_{k=2,3,4} = \frac{1}{\sqrt{1 + (1 + \frac{((q1s-E_{sk})(q3s-E_{sk})(-q2s+E_{sk}))}{(q1s+q3s-2E_{sk})})^2 + ((\frac{((q2s-E_{sk})(-q3s+E_{sk}))}{(-q1s-q3s+2E_{sk}))})^2 + (\frac{((q1s-E_{sk})(-q2s+E_{sk}))}{(q1s+q3s-2E_{sk})})^2)}. \quad (61)$$

The quantum state at any time instant is given as superposition of its 4 eigenstates with corresponding eigenenergies. Thus we have

$$|\psi(t) \rangle = \alpha_1(t)|v1 \rangle + \alpha_2(t)|v2 \rangle + \alpha_3(t)|v3 \rangle + \alpha_4(t)|v4 \rangle, \quad (62)$$

with condition $\langle \psi | \psi \rangle = 1$ that is $|\alpha_1(t)|^2 + |\alpha_2(t)|^2 + |\alpha_3(t)|^2 + |\alpha_4(t)|^2 = 1$ what is equivalent to 7 different real value numbers parametrizing quantum state. Using orthonormality of eigenstates and the fact that Hamiltonian is time independent we have

$$H|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle = i\hbar \left[\left(\frac{d}{dt}\alpha_1(t) \right) |v1\rangle + \left(\frac{d}{dt}\alpha_2(t) \right) |v2\rangle + \left(\frac{d}{dt}\alpha_3(t) \right) |v3\rangle + \left(\frac{d}{dt}\alpha_4(t) \right) |v4\rangle \right] \quad (63)$$

or equivalently

$$H|\psi(t)\rangle = E_1\alpha_1(t)|v1\rangle + E_2\alpha_2(t)|v2\rangle + E_3\alpha_3(t)|v3\rangle + E_4\alpha_4(t)|v4\rangle. \quad (64)$$

Making projections by applying $\langle v1|, \langle v2|, \langle v3|, \langle v4|$ from the left of $|\psi(t)\rangle$ we obtain

$$E_k\alpha_k(t) = i\hbar \frac{d}{dt}\alpha_k(t) \quad (65)$$

that is equivalent to the equation

$$\alpha_k(t) = \alpha_k(0)e^{\frac{-i}{\hbar}E_k t}, \quad (66)$$

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, where t is time. We observe that probability of occurrence of quantum state in given k -th eigen energy $|c_k|^2 = |c_k(0)|^2$ is constant and time independent. Therefore the final quantum state has the following form of time dependence

$$|\psi(t)\rangle = \alpha_1(0)e^{\frac{-i}{\hbar}E_1 t}|v1\rangle + \alpha_2(0)e^{\frac{-i}{\hbar}E_2 t}|v2\rangle + \alpha_3(0)e^{\frac{-i}{\hbar}E_3 t}|v3\rangle + \alpha_4(0)e^{\frac{-i}{\hbar}E_4 t}|v4\rangle. \quad (67)$$

Now we raise the question of finding of first electron in 1 and 2 points or finding another electron in 1' and 2' geometric points. We need to apply the following projector $\langle 1, 0|_L \langle 0, 1|_R + \langle 1, 0|_R \langle 0, 1|_L$ to the quantum state $|\psi\rangle$ to find the first electron in 1 point. Since we have

$$\langle 1, 0|_L \langle 0, 1|_R = (0, 0, 1, 0), \langle 1, 0|_L \langle 1, 0|_R = (0, 0, 0, 1), \langle 1, 0|_L \langle 0, 1|_R + \langle 1, 0|_R \langle 0, 1|_L = (0, 0, 1, 1). \quad (68)$$

Consequently we obtain

$$\begin{aligned} c_1(t) &= \frac{1}{\sqrt{2}} (\langle 1, 0|_L \langle 0, 1|_R + \langle 1, 0|_R \langle 0, 1|_L) |\psi(t)\rangle = \frac{1}{\sqrt{2}} (0, 0, 1, 1) |\psi(t)\rangle = \frac{1}{\sqrt{2}} \\ &(0, 0, 1, 1) (\alpha_1(0)e^{\frac{-i}{\hbar}E_1 t}|v1\rangle + \alpha_2(0)e^{\frac{-i}{\hbar}E_2 t}|v2\rangle + \alpha_3(0)e^{\frac{-i}{\hbar}E_3 t}|v3\rangle + \alpha_4(0)e^{\frac{-i}{\hbar}E_4 t}|v4\rangle) \end{aligned} \quad (69)$$

. The factor $\frac{1}{\sqrt{2}}$ in projector comes from the fact that $\frac{1}{\sqrt{2}}(<1,0|_L(<0,1|_R+<1,0|_R)(|1,0>_L(|0,1>_R+|1,0>_R)\frac{1}{\sqrt{2}}=1$. Finally we have $c_1(t)$ (where $|c_1(t)|^2$ is the probability of finding electron in 1 node):

$$c_1(t) = \frac{1}{\sqrt{2}}[n_1\alpha_1(0)e^{-\frac{i}{\hbar}E_1t} + n_2\alpha_2(0)e^{-\frac{i}{\hbar}E_2t}(\frac{((q1s-E_{2s})(-q2s+E_{2s}))}{(q1s+q3s-2E_{s2})}+1) + \\ +n_3\alpha_3(0)e^{-\frac{i}{\hbar}E_3t}(\frac{((q1s-E_{s3})(-q2s+E_{s3}))}{(q1s+q3s-2E_{s3})}+1) + n_4\alpha_4(0)e^{-\frac{i}{\hbar}E_4t}(\frac{((q1s-E_{s4})(-q2s+E_{s4}))}{(q1s+q3s-2E_{s4})}+1)] \quad (70)$$

We can look for finding the probability of electron being at maximum distance that is one electron is at node 1 and another electron is at node 2' what we denote $|c_{1,2'}(t)|^2$. Thus we need to apply the projector $<1,0|_L<0,1|_R=(0,0,1,0)$ to the quantum state $|\psi(t)>$. We obtain

$$[<1,0|_L<0,1|_R]|\psi(t)>=(0,0,1,0)|\psi(t)>=c_{1,2'}(t)=[n_2\alpha_2(0)e^{-\frac{i}{\hbar}E_2t}(\frac{((q1s-E_{2s})(-q2s+E_{2s}))}{(q1s+q3s-2E_{s2})}) + \\ +n_3\alpha_3(0)e^{-\frac{i}{\hbar}E_3t}(\frac{((q1s-E_{s3})(-q2s+E_{s3}))}{(q1s+q3s-2E_{s3})}) + n_4\alpha_4(0)e^{-\frac{i}{\hbar}E_4t}(\frac{((q1s-E_{s4})(-q2s+E_{s4}))}{(q1s+q3s-2E_{s4})})] \quad (71)$$

Having particles at maximum distances and making energy projection on one of the energy states brings particles (for example *into* E_{2s} so $\alpha_2=1$) to the situation where we have no longer oscillations of occupancy so

$$c_{1,2'}(t)=[n_2\alpha_2(0)e^{-\frac{i}{\hbar}E_2t}(\frac{((q1s-E_{2s})(-q2s+E_{2s}))}{(q1s+q3s-2E_{s2})})]. \quad (72)$$

In such case the probability of occupancy of first electron in 1 and second electron in 2 is $|c_{1,2'}(t)|^2 = \text{constant}$ so it is time independent. In such case we can achieve system thermodynamical ground state.

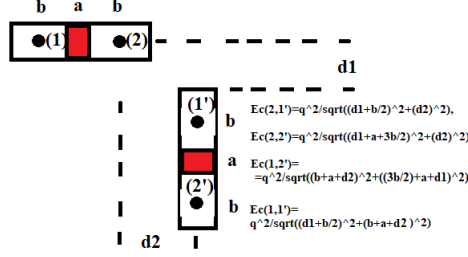


Figure 3: Case of 2 interacting double quantum dots

2.0.2 Case of 2 perpendicular double quantum dots

It is important to consider the situation as depicted in Fig.1A.

In highest simplified case we have

$$H = \begin{pmatrix} 2V_s + \frac{q^2}{\sqrt{(d_1 + a + \frac{3}{2}b)^2 + (d_2)^2}} & t & t & 0 \\ t & 2V_s + \frac{q^2}{\sqrt{(d_1 + \frac{1}{2}b)^2 + (d_2)^2}} & 0 & t \\ t & 0 & 2V_s + \frac{q^2}{\sqrt{(d_1 + \frac{3}{2}b + a)^2 + (d_2 + b + a)^2}} & t \\ 0 & t & t & 2V_s + \frac{q^2}{\sqrt{(d_1 + \frac{1}{2}b)^2 + (d_2 + b + a)^2}} \end{pmatrix} \quad (73)$$

Let us simplify matrix structure by assumption $a = b = d_1 = d_2$. We obtain simplified Hamiltonian as

$$H = \begin{pmatrix} 2V_s + \frac{q_1}{\sqrt{(\frac{7}{2})^2 + (1)^2}} & t & t & 0 \\ t & 2V_s + \frac{q_1}{\sqrt{(\frac{3}{2})^2 + (1)^2}} & 0 & t \\ t & 0 & 2V_s + \frac{q_1}{\sqrt{(\frac{7}{2})^2 + (3)^2}} & t \\ 0 & t & t & 2V_s + \frac{q_1}{\sqrt{(\frac{3}{2})^2 + (3)^2}} \end{pmatrix} \quad (74)$$

where $q_1 = \frac{q^2}{a}$. Now we introduce $V1_s = \frac{V_s}{t}$ and $Q_1 = \frac{q_1}{t}$. We thus have

$$H = t \begin{pmatrix} 2V1_s + \frac{Q_1}{\sqrt{(\frac{7}{2})^2 + (1)^2}} & 1 & 1 & 0 \\ 1 & 2V1_s + \frac{Q_1}{\sqrt{(\frac{3}{2})^2 + (1)^2}} & 0 & t \\ 1 & 0 & 2V1_s + \frac{Q_1}{\sqrt{(\frac{7}{2})^2 + (3)^2}} & t \\ 0 & 1 & 1 & 2V1_s + \frac{Q_1}{\sqrt{(\frac{3}{2})^2 + (3)^2}} \end{pmatrix} = t \begin{pmatrix} 2V1_s + \frac{2Q_1}{\sqrt{50}} & 1 & 1 & 0 \\ 1 & 2V1_s + \frac{2Q_1}{\sqrt{13}} & 0 & 1 \\ 1 & 0 & 2V1_s + \frac{2Q_1}{\sqrt{(7)^2 + (6)^2}} & 1 \\ 0 & 1 & 1 & 2V1_s + \frac{2Q_1}{\sqrt{(3)^2 + (6)^2}} \end{pmatrix} = 2t \begin{pmatrix} V1_s + \frac{Q_1}{\sqrt{50}} & 1 & 1 & 0 \\ 1 & V1_s + \frac{Q_1}{\sqrt{13}} & 0 & 1 \\ 1 & 0 & V1_s + \frac{Q_1}{\sqrt{85}} & 1 \\ 0 & 1 & 1 & V1_s + \frac{Q_1}{\sqrt{45}} \end{pmatrix} = 2H2 \quad (75)$$

Setting $Q_1 = V1_s = 1 = 2t$ we compute the eigenvalues and eigenstates for H2 matrix. We obtain $E1 =$

3.17105, $E2 = 1.19282$, $E3 = 1.14525$, $E4 = -0.832809$ that correspond to normalized eigenvectors

$$V1 = \begin{pmatrix} -0.495619 \\ -0.524431 \\ -0.48149 \\ -0.497494 \end{pmatrix}, V2 = \begin{pmatrix} 0.0274301 \\ -0.705768 \\ 0.707178 \\ 0.0322261 \end{pmatrix}, V3 = \begin{pmatrix} -0.70717 \\ 0.00104358 \\ -0.00374818 \\ 0.707032 \end{pmatrix}, V4 = \begin{pmatrix} 0.503507 \\ -0.476301 \\ -0.517738 \\ 0.501563 \end{pmatrix}, \text{ The quantum}$$

state is thus spanned by $|\psi\rangle = q_1V1 + q_2V2 + q_3V3 + q_4V4$ with condition $|q_1|^2 + |q_2|^2 + |q_3|^2 + |q_4|^2 = 1$. The last matrix has 4 different elements on its diagonal parametrized by geometry of $(-, |)$ system of 2 double quantum dots as well as by polarizing voltages that are set to be the same V_s .

We notice that vectors $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ correspond to states

$(|0, 1\rangle_U |0, 1\rangle_L), (|0, 1\rangle_U |1, 0\rangle_L), (|1, 0\rangle_U |0, 1\rangle_L), (|1, 0\rangle_U |1, 0\rangle_L)$. Here $|0, 1\rangle_L$ denotes L (lower) system with lower position of electron (2' point), while $|1, 0\rangle_L$ denotes L (lower) system with upper position of electron that is 1' so point 2' is placed lower in y coordinates than point 1'. We will be interested in the projection of system state $|\psi\rangle$ to the state $|\psi\rangle_L$ (1-one body L wavefunction) and in particular in occupancy of electron at points 1' and 2'. We have the following projections

$$P(1') = ((\langle 1, 0|_U \langle 1, 0|_L) + (\langle 0, 1|_U \langle 1, 0|_L)) = \begin{pmatrix} 0 & 0 & 0 & 1 \end{pmatrix}, + \begin{pmatrix} 0 & 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 1 \end{pmatrix}, \quad (76)$$

and

$$\begin{aligned} P(2') &= ((\langle 1, 0|_U \langle 0, 1|_L) + (\langle 0, 1|_U \langle 0, 1|_L)) = \\ &= \begin{pmatrix} 0 & 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix}, = \begin{pmatrix} 1 & 0 & 1 & 0 \end{pmatrix}, \end{aligned} \quad (77)$$

Therefore finally the occupancy of 1' point is given as

$$c(1', t) = P(1')|\psi(t)\rangle = ((\langle 1, 0|_U \langle 0, 1|_L) + (\langle 0, 1|_U \langle 1, 0|_L))|\psi(t)\rangle = \begin{pmatrix} 1 & 1 & 0 & 0 \end{pmatrix} |\psi(t)\rangle$$

and occupancy of 2' point is given as

$$c(2', t) = P(2')|\psi(t)\rangle = ((\langle 1, 0|_U \langle 1, 0|_L) + (\langle 0, 1|_U \langle 0, 1|_L))|\psi(t)\rangle = \begin{pmatrix} 1 & 0 & 1 & 0 \end{pmatrix} |\psi(t)\rangle.$$

The occupancy at 1 and 2 points can be expressed as

$$\begin{aligned} c(1, t) &= P(1)|\psi(t)\rangle = ((\langle 1, 0|_U (\langle 0, 1|_L + \langle 1, 0|_L))|\psi(t)\rangle = \\ &= (\langle 1, 0|_U \langle 0, 1|_L + \langle 1, 0|_U \langle 1, 0|_L)|\psi(t)\rangle = \\ &= (\begin{pmatrix} 0 & 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 1 \end{pmatrix})|\psi(t)\rangle = \begin{pmatrix} 0 & 0 & 1 & 1 \end{pmatrix} |\psi(t)\rangle \end{aligned} \quad (78)$$

and

$$\begin{aligned} c(2, t) &= P(2)|\psi(t)\rangle = (\langle 0, 1|_U (\langle 0, 1|_L + \langle 1, 0|_L))|\psi(t)\rangle = \\ &= (\langle 0, 1|_U \langle 0, 1|_L + \langle 0, 1|_U \langle 1, 0|_L)|\psi(t)\rangle = \\ &= (\begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \end{pmatrix})|\psi(t)\rangle = \begin{pmatrix} 1 & 1 & 0 & 0 \end{pmatrix} |\psi(t)\rangle. \end{aligned} \quad (79)$$

2.1 Quantum dynamics with time for Q-SWAP gate

We refer to the case depicted in Fig.1. Obviously the quantum system is subjected to the equation of motion as

$$H|\psi\rangle = i\hbar \frac{d}{dt}|\psi\rangle. \quad (80)$$

We assume that $|\psi\rangle = c_{1n}(t)|V_{1n}\rangle + c_{2n}(t)|V_{2n}\rangle + c_{3n}(t)|V_{3n}\rangle + c_{4n}(t)|V_{4n}\rangle$, where $|c_{1n}(t)|^2 + \dots + |c_{4n}(t)|^2 = 1$. The quantum state have the form as

$$\begin{aligned} |\psi(t)\rangle = & \frac{c_{1n}(t)}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \frac{c_{2n}(t)}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} + \\ & + c_{3n}(t) \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} 1 \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ 1 \end{pmatrix} + \\ & + c_{4n}(t) \begin{pmatrix} \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \end{pmatrix} \end{aligned} \quad (81)$$

Now we can trace the system dynamics with time-independent or with time independent Hamiltonian. We have $|\psi(t+dt)\rangle = |\psi(t)\rangle + \frac{1}{i\hbar} H dt |\psi(t)\rangle$. At first we consider time independent Hamiltonian. We have 2 symmetric double quantum dots with the same effective confiment potentials $V_s = Ep(2) = Ep(2') = Ep(1) = Ep(1')$ and the same t hopping terms so $t_U = t_L = t_s$ so we obtain for Fig.1 the Hamiltonian

$$H = \begin{pmatrix} 2V_s + \frac{q^2}{d1} & t_s & t_s & 0 \\ t_s & 2V_s + \frac{q^2}{(d1)^2 + (b+a)^2} & 0 & t_s \\ t_s & 0 & 2V_s + \frac{q^2}{(d1)^2 + (b+a)^2} & t_s \\ 0 & t_s & t_s & 2V_s + \frac{q^2}{d1} \end{pmatrix} \quad (82)$$

and system dynamics is as follows

$$\begin{aligned}
|\psi(t+dt) \rangle &= |\psi(t) \rangle + \frac{dt}{i\hbar} \begin{pmatrix} 2V_s + \frac{q^2}{d1} & t_s & t_s & 0 \\ t_s & 2V_s + \frac{q^2}{(d1)^2+(b+a)^2} & 0 & t_s \\ t_s & 0 & 2V_s + \frac{q^2}{(d1)^2+(b+a)^2} & t_s \\ 0 & t_s & t_s & 2V_s + \frac{q^2}{d1} \end{pmatrix} \left[\frac{c_{1n}(t)}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \right. \\
&\quad \left. \frac{c_{2n}(t)}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} + \right. \\
&\quad \left. + c_{3n}(t) \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} 1 \\ \frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ 1 \end{pmatrix} + \right. \\
&\quad \left. + c_{4n}(t) \begin{pmatrix} \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \end{pmatrix} \right]
\end{aligned}$$

Since

$$c_{1n}(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 & 0 & 1 \end{pmatrix} |\psi(t) \rangle = \langle \psi_1 | \psi(t) \rangle \quad (84)$$

and

$$c_{2n}(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 1 & 0 \end{pmatrix} |\psi(t) \rangle = \langle \psi_2 | \psi(t) \rangle \quad (85)$$

and

$$\begin{aligned}
c_{3n}(t) &= \sqrt{\frac{4t_s}{\left(-\frac{1}{d1} + \frac{1}{\sqrt{(d1)^2+(b+a)^2}}\right)q^2 + 8t_s - \sqrt{\left(\left(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}}\right)q^2\right)^2 + 16t_s^2}}} \\
&\quad \left(1, -\frac{\frac{4t_s}{\left(-\frac{q^2}{d1} + \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right) + \sqrt{\left(\frac{q^2}{d1} - \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right)^2 + 16t_s^2}}}{\left(-\frac{q^2}{d1} + \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right) + \sqrt{\left(-\frac{q^2}{d1} + \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right)^2 + 16t_s^2}}, 1\right) |\psi(t) \rangle = \\
&\quad = \langle \psi_3 | \psi(t) \rangle
\end{aligned}$$

and

$$\begin{aligned}
c_{4n}(t) &= \sqrt{\frac{4t_s}{\left(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}}\right)q^2 + 8t_s - \sqrt{\left(\left(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}}\right)q^2\right)^2 + 16t_s^2}}} \\
&\quad \left(1, \frac{\frac{4t_s}{\left(+\frac{q^2}{d1} - \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right) + \sqrt{\left(\frac{q^2}{d1} - \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right)^2 + 16t_s^2}}}{\left(+\frac{q^2}{d1} - \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right) + \sqrt{\left(+\frac{q^2}{d1} - \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}\right)^2 + 16t_s^2}}, 1\right) |\psi(t) \rangle = \\
&\quad = \langle \psi_4 | \psi(t) \rangle \quad (87)
\end{aligned}$$

Denoting T as transpose of vector we notice that

$$[V_{1n}]^T(|\psi(t+dt) \rangle - |\psi(t) \rangle) = (c_{1n}(t+dt) - c_{1n}(t)) = \frac{dt}{i\hbar} [V_{1n}]^T H |\psi(t) \rangle \quad (88)$$

and consequently

$$[V_{2n}]^T(|\psi(t+dt) \rangle - |\psi(t) \rangle) = (c_{2n}(t+dt) - c_{2n}(t)) = \frac{dt}{i\hbar} [V_{2n}]^T H |\psi(t) \rangle \quad (89)$$

and

$$[V_{3n}]^T(|\psi(t+dt) \rangle - |\psi(t) \rangle) = (c_{3n}(t+dt) - c_{3n}(t)) = \frac{dt}{i\hbar} [V_{3n}]^T H |\psi(t) \rangle \quad (90)$$

and

$$[V_{4n}]^T(|\psi(t+dt) \rangle - |\psi(t) \rangle) = (c_{4n}(t+dt) - c_{4n}(t)) = \frac{dt}{i\hbar} [V_{4n}]^T H |\psi(t) \rangle. \quad (91)$$

Therefore we obtain 4 recurrent equations where r-th coefficient $c_{rn}(t+dt)$ depends on linear combination of coefficients from previous time step $c_{kn}(t+dt)$, where k is from 1 to 4 and i-th is any among 1-4. We have

$$c_{rn}(t+dt) = c_{rn}(t) + \frac{dt}{i\hbar} [V_{rn}]^T H |\psi(t) \rangle. \quad (92)$$

Let us use last relation for r=1. We have

$$\begin{aligned} c_{1n}(t+dt) = c_{1n}(t) + \frac{dt}{i\hbar} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 & 0 & 1 \end{pmatrix} \left(\begin{pmatrix} 2V_s + \frac{q^2}{d1} & t_s & t_s & 0 \\ t_s & 2V_s + \frac{q^2}{(d1)^2 + (b+a)^2} & 0 & t_s \\ t_s & 0 & 2V_s + \frac{q^2}{(d1)^2 + (b+a)^2} & t_s \\ 0 & t_s & t_s & 2V_s + \frac{q^2}{d1} \end{pmatrix} \left[\frac{c_{1n}(t)}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \frac{c_{2n}(t)}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} + \right. \right. \\ \left. + c_{3n}(t) \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} 1 \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ 1 \end{pmatrix} + \right. \\ \left. + c_{4n}(t) \begin{pmatrix} \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \end{pmatrix} \right) \Bigg). \quad (93) \end{aligned}$$

and consequently we have

$$\begin{aligned}
c_{2n}(t+dt) &= c_{2n}(t) + \frac{dt}{i\hbar} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 1 & 0 \end{pmatrix} \left(\begin{pmatrix} 2V_s + \frac{q^2}{d1} & t_s & t_s & 0 \\ t_s & 2V_s + \frac{q^2}{(d1)^2 + (b+a)^2} & 0 & t_s \\ t_s & 0 & 2V_s + \frac{q^2}{(d1)^2 + (b+a)^2} & t_s \\ 0 & t_s & t_s & 2V_s + \frac{q^2}{d1} \end{pmatrix} \left[\frac{c_{1n}(t)}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \frac{c_{2n}(t)}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} \right] + \right. \\
&+ c_{3n}(t) \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} \frac{1}{4t_s} \\ -\frac{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \\ -\frac{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}{4t_s} \\ 1 \end{pmatrix} + \\
&\left. + c_{4n}(t) \begin{pmatrix} \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \end{pmatrix} \right]. \tag{94}
\end{aligned}$$

and

$$\begin{aligned}
& c_{3n}(t+dt) = c_{3n}(t) + \\
& + \frac{dt}{i\hbar} \sqrt{\frac{4t_s}{(-\frac{1}{d1} + \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2 + 8t_s - \sqrt{((\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2)^2 + 16t_s^2}}} \\
& \left(1, -\frac{q^2}{(-\frac{q^2}{d1} + \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}) + \sqrt{(\frac{q^2}{d1} - \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}})^2 + 16t_s^2}}, -\frac{q^2}{(-\frac{q^2}{d1} + \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}}) + \sqrt{(-\frac{q^2}{d1} + \frac{q^2}{\sqrt{(d1)^2+(b+a)^2}})^2 + 16t_s^2}}, 1 \right) \left(\begin{array}{cccc} 2V_s + \frac{q^2}{d1} & t_s & t_s & 0 \\ t_s & 2V_s + \frac{q^2}{(d1)^2+(b+a)^2} & 0 & t_s \\ t_s & 0 & 2V_s + \frac{q^2}{(d1)^2+(b+a)^2} & t_s \\ 0 & t_s & t_s & 2V_s + \frac{q^2}{d1} \end{array} \right) \left[\frac{c_{1n}(t)}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \frac{c_{2n}(t)}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} + \right. \\
& + c_{3n}(t) \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} 1 \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ -\frac{4t_s}{(-Ec1s + Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ 1 \end{pmatrix} + \\
& \left. + c_{4n}(t) \left(\begin{array}{c} \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \frac{4t_s}{(Ec1s - Ec2s) + \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s - Ec2s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \end{array} \right) \right].
\end{aligned}$$

and consequently

$$\begin{aligned}
& c_{4n}(t+dt) = c_{4n}(t) + \\
& + \frac{dt}{i\hbar} \sqrt{\frac{4t_s}{(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2 + 8t_s - \sqrt{((\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2)^2 + 16t_s^2}}} \\
& \left(1, \frac{\frac{4t_s}{(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2 + 8t_s - \sqrt{((\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2)^2 + 16t_s^2}}}{(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2 + 8t_s - \sqrt{((\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2)^2 + 16t_s^2}}, \frac{4t_s}{(\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2 + 8t_s - \sqrt{((\frac{1}{d1} - \frac{1}{\sqrt{(d1)^2+(b+a)^2}})q^2)^2 + 16t_s^2}}, 1 \right) \left(\begin{array}{cccc} 2V_s + \frac{q^2}{d1} & t_s & t_s & 0 \\ t_s & 2V_s + \frac{q^2}{(d1)^2+(b+a)^2} & 0 & t_s \\ t_s & 0 & 2V_s + \frac{q^2}{(d1)^2+(b+a)^2} & t_s \\ 0 & t_s & t_s & 2V_s + \frac{q^2}{d1} \end{array} \right) \left[\frac{c_{1n}(t)}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \frac{c_{2n}(t)}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} + \right. \\
& + c_{3n}(t) \sqrt{\frac{4t_s}{(Ec2s - Ec1s) + 8t_s - \sqrt{(Ec1s - Ec2s)^2 + 16t_s^2}}} \begin{pmatrix} 1 \\ -\frac{4t_s}{(-Ec1s+Ec2s)+\sqrt{(Ec1s-Ec2s)^2+16t_s^2}} \\ -\frac{4t_s}{(-Ec1s+Ec2s)+\sqrt{(Ec1s-Ec2s)^2+16t_s^2}} \\ 1 \end{pmatrix} + \\
& \left. + c_{4n}(t) \begin{pmatrix} \sqrt{\frac{4t_s}{(Ec1s-Ec2s)+8t_s-\sqrt{(Ec1s-Ec2s)^2+16t_s^2}}} \\ \sqrt{\frac{4t_s}{(Ec1s-Ec2s)+8t_s-\sqrt{(Ec1s-Ec2s)^2+16t_s^2}}} \frac{4t_s}{(Ec1s-Ec2s)+\sqrt{(Ec1s-Ec2s)^2+16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s-Ec2s)+8t_s-\sqrt{(Ec1s-Ec2s)^2+16t_s^2}}} \frac{4t_s}{(Ec1s-Ec2s)+\sqrt{(Ec1s-Ec2s)^2+16t_s^2}} \\ \sqrt{\frac{4t_s}{(Ec1s-Ec2s)+8t_s-\sqrt{(Ec1s-Ec2s)^2+16t_s^2}}} \end{pmatrix} \right]. \tag{96}
\end{aligned}$$

2.2 Extraction of 1-body quantum state from 2-body quantum state

Now we need to be able to extract one body wavefunction from 2-body wavefunction. Let us extract the wavefunction for U system. Thus we need to apply the following projection operators $P1_U$ and $P2_U$ on general quantum state (U, L) to obtain only U wavefunction subcomponents:

$$P1_U = \frac{1}{\sqrt{2}} |1, 0\rangle_U ((\langle 1, 0|_U \langle 1, 0|_L) + (\langle 1, 0|_U \langle 0, 1|_L)) \tag{97}$$

and

$$P2_U = \frac{1}{\sqrt{2}} |0, 1\rangle_U ((\langle 0, 1|_U \langle 1, 0|_L) + (\langle 0, 1|_U \langle 0, 1|_L)). \tag{98}$$

Consequently the whole U 1-body wavefunction is given as follows

$$\begin{aligned}
|\psi\rangle_U = (P1_U + P2_U)|\psi\rangle = & \left(\frac{1}{\sqrt{2}} |1, 0\rangle_U ((\langle 1, 0|_U \langle 1, 0|_L) + (\langle 1, 0|_U \langle 0, 1|_L)) + \right. \\
& \left. \frac{1}{\sqrt{2}} |0, 1\rangle_U ((\langle 0, 1|_U \langle 1, 0|_L) + (\langle 0, 1|_U \langle 0, 1|_L))) \right) |\psi\rangle. \tag{99}
\end{aligned}$$

In quite analogical way we can introduce the following projection operators $P1_L$ and $P2_L$ on general quantum state (U, L) to obtain only L wavefunction subcomponents:

$$P1_L = \frac{1}{\sqrt{2}}|1, 0\rangle_L ((\langle 1, 0|_U \langle 1, 0|_L) + (\langle 0, 1|_U \langle 1, 0|_L)) \quad (100)$$

and

$$P2_L = \frac{1}{\sqrt{2}}|0, 1\rangle_L ((\langle 1, 0|_U \langle 0, 1|_L) + (\langle 0, 1|_U \langle 0, 1|_L)). \quad (101)$$

Consequently the whole L: 1-body wavefunction is given as follows

$$|\psi\rangle_L = (P1_L + P2_L)|\psi\rangle = \left(\frac{1}{\sqrt{2}}|1, 0\rangle_L ((\langle 1, 0|_U \langle 1, 0|_L) + (\langle 0, 1|_U \langle 1, 0|_L)) + \frac{1}{\sqrt{2}}|0, 1\rangle_L ((\langle 1, 0|_U \langle 0, 1|_L) + (\langle 0, 1|_U \langle 0, 1|_L))\right)|\psi\rangle \quad (102)$$

2.3 The action of strong measurement on one of the sub-systems L and U

Making the measurement determining the position of particle from U system on the left side is represented by the projection

$$PL_U = \frac{1}{\sqrt{2}}(|1, 0\rangle_U (|1, 0\rangle_L + |0, 1\rangle_L))(\langle 1, 0|_U (\langle 1, 0|_L + \langle 0, 1|_L)). \quad (103)$$

Thus after the determination of the state of electron in U to be on the left side we have the total quantum state after measurement $|\psi'\rangle$ expressed by the state before measurement $|\psi\rangle$ to be of the form

$$\begin{aligned} |\psi'\rangle &= PL_U|\psi\rangle = \\ &= \frac{1}{\sqrt{2}}(|1, 0\rangle_U (|1, 0\rangle_L + |0, 1\rangle_L))(\langle 1, 0|_U (\langle 1, 0|_L + \langle 0, 1|_L))|\psi\rangle. \end{aligned} \quad (104)$$

Making the measurement determining the position of particle from U system on the right side is represented by the projection

$$PR_U = \frac{1}{\sqrt{2}}(|0, 1\rangle_U (|1, 0\rangle_L + |0, 1\rangle_L))(\langle 0, 1|_U (\langle 1, 0|_L + \langle 0, 1|_L)). \quad (105)$$

Thus after the determination of the state of electron in U to be on the left side we have the total quantum state after measurement $|\psi'\rangle$ expressed by the state before measurement $|\psi\rangle$ to be of the form

$$\begin{aligned} |\psi'\rangle &= PR_U|\psi\rangle = \\ &= \frac{1}{\sqrt{2}}(|0, 1\rangle_U (|1, 0\rangle_L + |0, 1\rangle_L))(\langle 0, 1|_U (\langle 1, 0|_L + \langle 0, 1|_L))|\psi\rangle. \end{aligned} \quad (106)$$

Quite obviously instead of measurement of position of electron from U system we can make the determination of electron state from the L system to be on the left what we obtain with the projection operator PL_U that is represented as following

$$PL_L = \frac{1}{\sqrt{2}}(|1,0\rangle_U + |0,1\rangle_U)|1,0\rangle_L (|1,0\rangle_U + |0,1\rangle_U) \langle 1,0|_L. \quad (107)$$

In similar way we can introduce the projection measurement determining the position of electron to be on the right side of system L in the way as

$$PR_L = \frac{1}{\sqrt{2}}(|1,0\rangle_U + |0,1\rangle_U)|0,1\rangle_L (|1,0\rangle_U + |0,1\rangle_U) \langle 0,1|_L. \quad (108)$$

In similar way as before the state of the quantum system after determination of particle position in L subsystem to be on the left side is $PL_L|\psi\rangle$ while the state of the total quantum system after measurement determination of particle position in L subsystem to be on the right side is $PR_L|\psi\rangle$.

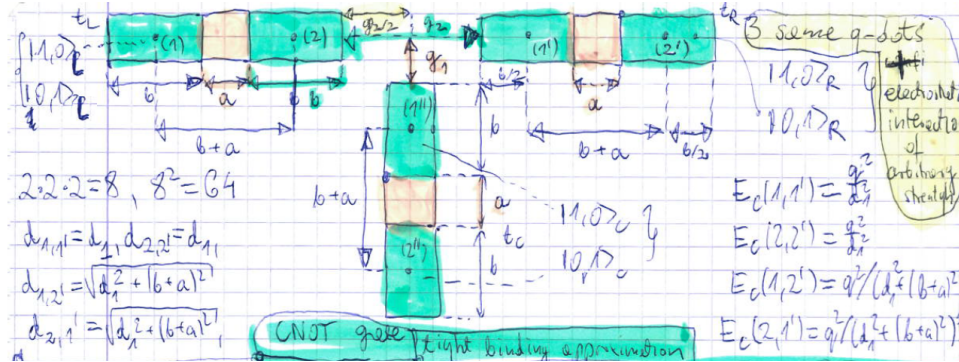


Figure 4: 3 electrons confined in 3 separated in space double interconnected quantum dots interacting electrostatically.

3 Quantum electrostatic CNOT gate

In the same methodology as we have studied q-SWAP gate we are studying the CNOT quantum gate but with considerations of 3 body system (3 separated in space electrons) of 3 double separated in space quantum dots as depicted in Fig.2. The system is parametrized by a, b, g and g_2 geometric parameters. If 3 double quantum dot systems (L-Left, R-Right, C-Center) are very far one from each other we can consider 3 different separate Hilbert spaces. If L (R,C) system is far away from R (L,C) and C system than the quantum states of L is independent from R(C) quantum system and in such case we can write $|\psi\rangle_L = c_1|1,0\rangle_L + c_2|0,1\rangle_L$, $|\psi\rangle_R = c_3|1,0\rangle_R + c_4|0,1\rangle_R$ and $|\psi\rangle_C = c_5|1,0\rangle_C + c_6|0,1\rangle_C$ and normalization conditions $|c_1|^2 + |c_2|^2 = 1$, $|c_3|^2 + |c_4|^2 = 1$ and $|c_5|^2 + |c_6|^2 = 1$. In case of separated systems we can write the total Hilbert space by factorization so $|\psi\rangle = |\psi\rangle_L |\psi\rangle_R |\psi\rangle_C$. However it is not true when we bring L and R and C systems sufficiently close so Coulomb interaction has no longer perturbative character. In such case we have the most general form of quantum state given as

$$|\psi\rangle = c_a|0,1\rangle_L|0,1\rangle_R|0,1\rangle_C + c_b|0,1\rangle_L|0,1\rangle_R|1,0\rangle_C + c_c|0,1\rangle_L|1,0\rangle_R|0,1\rangle_C + c_d|0,1\rangle_L|1,0\rangle_R|1,0\rangle_C + c_e|1,0\rangle_L|0,1\rangle_R|0,1\rangle_C + c_f|1,0\rangle_L|0,1\rangle_R|1,0\rangle_C + c_g|1,0\rangle_L|1,0\rangle_R|0,1\rangle_C + c_h|1,0\rangle_L|1,0\rangle_R|1,0\rangle_C \quad (109)$$

We have parametrization of kinetic energy in 3 double-quantum dot systems given by coefficients t_L, t_R, t_C . We also denoted $I_L = (|0,1\rangle_L\langle 0,1| + |1,0\rangle_L\langle 1,0|_L)$ and $I_R = (|0,1\rangle_R\langle 0,1|_R + |1,0\rangle_R\langle 1,0|_R)$ and $I_C = (|0,1\rangle_C\langle 0,1|_C + |1,0\rangle_C\langle 1,0|_C)$. I_L is identity operator and is projection of L state on itself. The same is with I_R operator that is identity operator and is projection of state R on itself. Also the operator I_C is the projection of state C on state C. We preassume that electron in L can be either in 1 or in 2, electron in R can be in 1' or 2' and that electron in C can be either in 1'' and in 2''. Now we construct the tight-binding Hamiltonian for 3 electrostatically interacting electrons confined by some local potential in 3 different regions of space. We have total system

Hamiltonian as the sum of all potential and kinetic energies given as

$$\begin{aligned}
H = & (E_p(1)|1,0\rangle_L\langle 1,0|_L + E_p(2)|0,1\rangle_L\langle 0,1|_U)_L I_R I_C + I_L(E_p(1')|1,0\rangle_R\langle 1,0|_R)I_C + \\
& + I_L E_p(2')|0,1\rangle_R\langle 0,1|_R)I_C + I_L I_R(E_p(1'')|1,0\rangle_C\langle 1,0|_C + E_p(2'')|0,1\rangle_C\langle 0,1|_C) + \\
& + t_L(|1,0\rangle_L\langle 0,1|_L + |0,1\rangle_L\langle 1,0|_L)I_R I_C + I_L t_R(|1,0\rangle_R\langle 1,0|_R I_C + \\
& + I_L t_R(|0,1\rangle_R\langle 1,0|_R)I_C + I_L I_R t_C(|1,0\rangle_C\langle 0,1|_C + |0,1\rangle_C\langle 1,0|_C) + \\
& + E_c(1,1')(|1,0\rangle_L |1,0\rangle_R I_C \langle 1,0|_L \langle 1,0|_R) + \\
& + E_c(1,2')(|1,0\rangle_L |0,1\rangle_R I_C \langle 1,0|_L \langle 0,1|_R) + E_c(1,1'')(|1,0\rangle_L |1,0\rangle_C I_R \langle 1,0|_L \langle 1,0|_C) + \\
& + E_c(1,2'')(|1,0\rangle_L |0,1\rangle_C I_R \langle 1,0|_L \langle 0,1|_C) + \\
& + (E_c(2,1')|0,1\rangle_L |1,0\rangle_R\langle 0,1|_L \langle 1,0|_R)I_C + E_c(2,2')(|0,1\rangle_L |0,1\rangle_R\langle 0,1|_L \langle 0,1|_R)I_C + \\
& + E_c(2,1'')(|0,1\rangle_L |1,0\rangle_C I_R \langle 0,1|_L \langle 1,0|_C) + I_L E_c(1',1'')(|1,0\rangle_R |1,0\rangle_C\langle 1,0|_R \langle 1,0|_C) + \\
& + I_L E_c(1',2'')(|1,0\rangle_R |0,1\rangle_C\langle 1,0|_R \langle 0,1|_C) + I_L E_c(2',1'')(|0,1\rangle_R |1,0\rangle_C\langle 0,1|_R \langle 1,0|_C).
\end{aligned}$$

We have the following expressions to be evaluated $E_c(1,1') = q^2/(2b + a + g_2) = E_c(2,2'), E_c(1,2') = \frac{q^2}{3b+2a+g_2}, E_c(1,1'') = \frac{q^2}{\sqrt{(\frac{3}{2}b+a+\frac{g_2}{2})^2+(g_1+\frac{b}{2})^2}} = E_c(2',1''), E_c(1,2'') = \frac{q^2}{\sqrt{(\frac{3}{2}b+a+\frac{g_2}{2})^2+(g_1+\frac{3b}{2})^2}} = E_c(2',2''), E_c(2,1') = q^2/(b + g_2), E_c(2,2'), E_c(2,1''), E_c(2,2''), E_c(1',1''), E_c(1',2'')$. It is convenient to express total system Hamiltonian in matrix representation. We have 8 by 8 matrix H given as $H = [A1, A2, A3, A4]$ so A1, A2, A3 and A4 matrices are given as

$$\begin{aligned}
A_1 = & \begin{pmatrix} E_p(2) + E_p(2') + E_p(2'') + \textcolor{red}{E_c(2,2')} + \textcolor{yellow}{E_c(2,2'')} + \textcolor{green}{E_c(2',2'')} = a_0 & \begin{matrix} t_C, \\ E_p(2) + E_p(2') + E_p(1'') + \textcolor{red}{E_c(2,2')} + \textcolor{blue}{E_c(2,1'')} + E_c(2',1'') = a_1, \\ 0, \\ t_R, \\ 0, \\ t_L, \\ 0, \\ 0, \end{matrix} \end{pmatrix}, \\
A_2 = & \begin{pmatrix} \begin{matrix} t_R \\ 0 \\ t_C \\ 0 \\ 0 \\ t_L \\ 0 \end{matrix} & \begin{matrix} 0, \\ t_R, \\ t_C, \\ 0, \\ 0, \\ 0, \\ t_L, \end{matrix} \end{pmatrix}, \\
A_3 = & \begin{pmatrix} \begin{matrix} t_L \\ 0 \\ 0 \\ 0 \\ t_C \\ t_R \\ 0 \end{matrix} & \begin{matrix} 0 \\ t_L \\ 0 \\ 0 \\ t_C \\ 0 \\ t_R \end{matrix} \end{pmatrix}, \\
A_4 = & \begin{pmatrix} \begin{matrix} 0 \\ 0 \\ t_L \\ 0 \\ t_R \\ 0 \\ t_C \end{matrix} & \begin{matrix} 0 \\ 0 \\ 0 \\ t_L \\ 0 \\ t_R \\ t_C \end{matrix} \end{pmatrix} \quad (110)
\end{aligned}$$

We limit ourselves to the situation depicted in Fig.2. In such case $d(1,1') = d(2,2')$ (points (1,1') and (2,2'') are on the same line but in general case they does not

need to be), $d(2, 2'') = d(1', 2'')$ (system has symmetry around OY axis but in general case it does not need to have it). For the sake of simplicity we can set $t_L = t_R = t_C = t$ and we can set all potential energies to be V_s . In such case the Hamiltonian matrix has 6 independent terms on its diagonal since we have identified terms set to a_0 and a_1 .

In most general case we have 8 different eigenenergies and 8 different eigen-solutions. The determination of eigenenergies is the problem of determination of roots of polynomial of 8th order. Therefore it is the numerical problem. The polynomials of 4th order have analytic solutions. The polynomial of higher order than 4th have only numerical solutions. We consider the Hamiltonian from Fig.2 in case of all potential energies set to V_s and $t_L = t_R = t_C = t$. We have

$$H = [H1, H2],$$

$$H1 = \begin{pmatrix} 3V_s + E_c(2, 2') + E_c(2, 2'') + E_c(2', 2'') & t & 0 & 0 \\ t & 3V_s + E_c(2, 2') + E_c(2, 1'') + E_c(2', 1'') & 0 & 0 \\ t_R & 0 & 3V_s + E_c(2, 1') + E_c(2, 2') + E_c(1', 2'') & 0 \\ 0 & t & 0 & 3V_s + E_c(2, 1') + E_c(2, 1'') + E_c(1', 1'') \\ 0 & 0 & 0 & 0 \\ 0 & 0 & t & 0 \\ 0 & 0 & 0 & t \end{pmatrix},$$

$$H2 = \begin{pmatrix} t & 0 & 0 & 0 \\ 0 & t & 0 & 0 \\ 0 & 0 & t & 0 \\ 0 & 0 & 0 & t \\ 3V_s + E_c(1, 2') + E_c(1, 2'') + E_c(2', 2'') & 3V_s + E_c(1, 2') + E_c(1, 1'') + E_c(2', 1'') & 3V_s + E_c(1, 1') + E_c(1, 2'') + E_c(2', 2'') & 3V_s + E_c(1, 1') + E_c(1, 1'') + E_c(1', 1'') \\ t & 0 & 0 & t \\ t & 0 & 0 & 0 \\ 0 & t & 0 & 0 \end{pmatrix},$$

If all 3 double quantum dots are very far away than we can simplify Coulomb interaction $E_c = E_c(1, 1') = E_c(1, 2') = E_c(1, 1'') = E_c(1, 2'') = E_c(2, 1') = E_c(2, 2') = E_c(2, 1'') = E_c(2, 2'') = E_c(1', 1'') = E_c(1', 2'') = E_c(2', 1'') = E_c(2', 2'')$. In such case we obtain the simplified Hamiltonian of the form

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$$H = \begin{pmatrix} 3V_s + 3E_c & t & t & 0 & t & 0 & 0 & 0 \\ t & 3V_s + 3E_c & 0 & t & 0 & t & 0 & 0 \\ t & 0 & 3E_c & t & 0 & 0 & t & 0 \\ 0 & t & t & 3V_s + 3E_c & 0 & 0 & 0 & t \\ t & 0 & 0 & 0 & 3V_s + 3E_c & t & t & 0 \\ 0 & t & 0 & 0 & t & 3V_s + 3E_c & 0 & t \\ 0 & 0 & t & 0 & t & 0 & 3V_s + 3E_c & t \\ 0 & 0 & 0 & t & 0 & t & t & 3V_s + 3E_c \end{pmatrix}. \quad (111)$$

This Hamiltonian has all diagonal terms set to the same value. This simplifies its solutions. Setting the diagonal terms to be

$a_1 = 3V_s + 3E_c$ we obtain the following eigenenergies

$$E1s = a1 - 3ts$$

$$E2s = a1 - ts$$

$$E3s = a1 - ts,$$

$$E4s = a1 - ts,$$

$$E5s = a1 + ts,$$

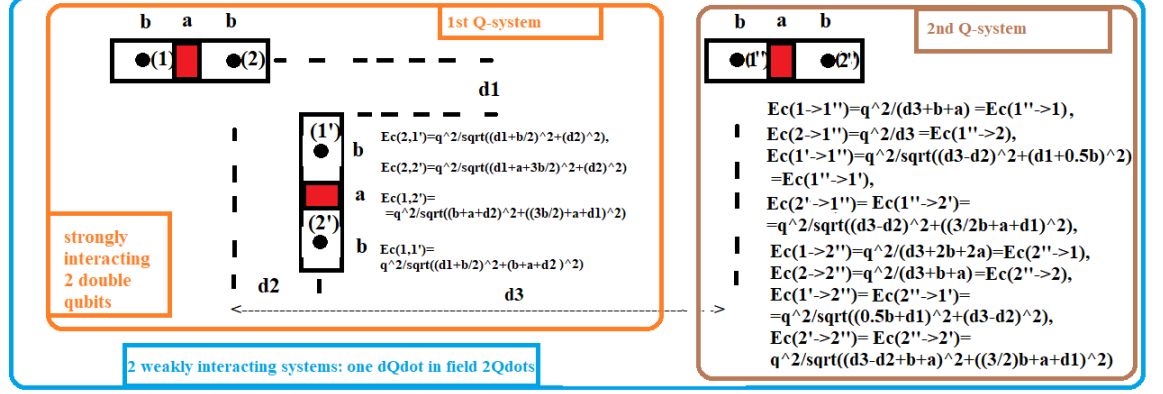
$$E6s = a1 + ts,$$

$$E7s = a1 + ts,$$

$$E8s = a1 + 3ts$$

Thus we have 3 different eigenenergies. Values $a1 - ts$ are occurring 3 times and thus are degenerated eigenenergies. Also values $a1 + ts$ are occurring 3 times and thus are degenerated eigenenergies. The eigenvectors are as following

$$|\psi1\rangle = \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \\ 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}, |\psi2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \\ -1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, |\psi3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \\ -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |\psi4\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \\ -1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |\psi5\rangle = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \\ -1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, |\psi6\rangle = \begin{pmatrix} 0 \\ -1 \\ 0 \\ -1 \\ 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |\psi7\rangle = \begin{pmatrix} 0 \\ 0 \\ -1 \\ -1 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |\psi8\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad (112)$$



ELECTROSTATIC CNOT,
-semianalytical approach [tight-binding + integro-differential eqn.]

1st Q-Systems has strong effect on 2nd Q-System,
while 2-nd Q-System has weak effect on dynamics of 1-st Q-System
[effect of 2-nd Q-System on 1-st Quantum system can be neglected (in 1st step)]

Figure 5: CNOT gate treated by combined approach:tight-binding+integro-differential equations, where SWAP Q-Gate (1st q-system) is weakly affected by 2nd q-system.

4 Symmetries and analytic vs numerical solutions for Q-SWAP and Q-CNOT gate

CNOT gate in shape of Mercedes has the highest level of symmetries. Than T CNOT gate has lower number of symmetries. In case of qubits in configuration $(-|)$, $-$ where elements $(-,|)$ are close and when $-$ is far away from $(-|)$ we can use 2 double quantum dots rigorous solutions and perturbative approach for the electric field coming to qubit element $-$ that is far away. The situation is depicted in Fig.4.

4.1 Combined approach of tight-binding + integro-differential equations for Q-CNOT gate

The effect of 1-st quantum system from Fig.4 on the second quantum system (1-qubit:double Q-Dot system) can be accounted by the following Hamiltonian. We assume that $d_3 > d_2$. The Hamiltonian of 2-nd quantum system that is CNOT output in its functional dependence from Hamiltonian of 1-st quantum system [Q-SWAP gate]. 2-nd quantum system Hamiltonian has the matrix

$$\begin{aligned}
&= H_{2,non-interaction} + H_{1 \rightarrow 2}[1] + H_{1 \rightarrow 2}[2] = \begin{pmatrix} V_{s2} & t_2 \\ t_2 & V_{s2} \end{pmatrix} + \begin{pmatrix} \frac{q^2 |c_1(t)|^2}{d_3+b+a} + \frac{q^2 |c_2(t)|^2}{d_3} & 0 \\ 0 & \frac{q^2 |c_1(t)|^2}{d_3+2(b+a)} + \frac{q^2 |c_2(t)|^2}{d_3+b+a} \end{pmatrix} + \\
&+ \begin{pmatrix} \frac{q^2 |c_{1'}(t)|^2}{\sqrt{(d_{32})^2 + (\frac{2d_1+b}{2})^2}} + \frac{q^2 |c_{2'}(t)|^2}{\sqrt{(d_{32})^2 + (d_1 + \frac{2a+3b}{2})^2}} & 0 \\ 0 & \frac{q^2 |c_{1'}(t)|^2}{\sqrt{|d_{32}|^2 + |\frac{b+2d_1}{2}|^2}} + \frac{q^2 |c_{2'}(t)|^2}{\sqrt{|d_{32}+a+b|^2 + (\frac{3b+2a}{2} + d_1)^2}} \end{pmatrix} = \\
&\begin{pmatrix} Ep_{1''} + Ec(1 \rightarrow 1'') + Ec(2 \rightarrow 1'') & t_2 \\ t_2 & Ep_{2''} + Ec(1 \rightarrow 2'') + Ec(2 \rightarrow 2'') + Ec(1' \rightarrow 2'') + Ec(2' \rightarrow 2'') \end{pmatrix}
\end{aligned}$$

representation, where $d_{32} = d_3 - d_2$) and $|c_1|^2, |c_2|^2, |c_{1'}|^2, |c_{2'}|^2$ are the probabilities of occupancies of nodes 1,1',2,2' by electrons. Thus we need to know dynamics of system 1 to determine dynamics of system 2. We need to use formulas 78 and 78. The terms $H_{1 \rightarrow 2}[1], H_{1 \rightarrow 2}[2]$ can be treated as the perturbation to $H_{2, non-interaction}$. Analyzing more precisely we can introduce perturbation to the system 1 coming from system 2. This perturbation of system 1 from system 2 is later affecting the dynamics of system 2 as well. However in the first level of approximation we can recognize that only system 1 is affecting system 2 and that system 2 is no-having impact on the system 1.