# Lund University

## Master Thesis

# Correlation and Entanglement

### Scattering Through two Coupled Quantum Dots

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# Contents

# 1    Abstract

In this thesis we theoretically investigate quantum correlations and entanglement of electron scatterers through two coupled quantum dots (QDs). The interaction is described in terms of two-particle collisions modeled by two-particle scattering matrix. The correlation between the two dots is expressed in terms of density-of-states matrices. Wave packets are introduced into each system and for the entanglement measure we use concurrence.

# 2    Introduction

Entanglement, the term coined by Schrödinger in 1935 [1], has fascinated scientists for more than 70 years. It is a quantum correlation between systems that lacks analogy in classical physics. A measurement done on one of two entangled parties will instantly determine the outcome of the measurement done on the other one. Historically, the interest concerned the interpretation of quantum mechanics and the question of non-locality and physical realism. In 1935 Einstein, Rosen and Podolsky produced a paper (called the EPR-paper [2] after their names) where they argued that, since entanglement was not compatible with local realism quantum mechanics was incomplete. Einstein argued that such correlation between entangled particles had to be due to some hidden variables that are inaccessible. In1964 John Bell showed that quantum correlations were stronger than classical ones and that predictions of quantum mechanics are incompatible with the hidden variables theory [3]. Experiments conducted from 1970's and onward demonstrated entanglement of spatially separate particles unambiguously and the hidden variables model was discarded.

During the last decades, entanglement has been shown to be a great resource for quantum information (QI) and quantum computation (QC) [4], where it is a key component in QI-processes such as teleportation and super dense coding. In superdense coding one is able to send two bits of information using only one classical bit. When it comes to QC, entanglement between qubits allows for computational operations that cannot be realized

on a classical computer. Parallel to the development of a more complete and consistent theory of quantum information, modern technology advanced towards miniaturization of electronic devises such as nanowires, nanotubes and quantum dots and the ability to do controlled measurements on them. In the nano regime classical physics breaks down and quantum effects take place, effects such as quantum tunneling, superposition of states and entanglement. The ability to control semiconductor materials at such small scales makes it possible to create quantum wells and QDs. It is thus natural to look at prospects of QI and QC with single electrons in nano structures. For the last 15 years a number of papers has emerged on QI and QC where schemes for entanglement generation and detection have been proposed. One key proposal was given by Loss and Divincenzo on spin entanglement [5]. Several works have investigated theoretically entanglement detection in QDs [6]. However, no experiment so far has verified the existence of entanglement between coupled QDs, which calls for further investigation. In this thesis we study theoretically quantum correlation between two capacitively coupled QDs. Following the work of Büttiker and Goorden, where they have derived a two particle scattering approach for the interaction between electrons in two mesoscopic conductors [7], we examine if entanglement can be created. We have used the scattering matrix approach combined with a density matrix formalism. We find clear signatures of interaction induced correlations between the two electrons. However no entanglement was found for the system properties and parameter ranges investigated.

This thesis is structured as follows. In chapter 3 we give a basic introduction to quantum bits, density matrices and the entanglement measure concurrence. We proceed by giving a brief description of QDs in chapter 4 . In chapter 5 we give a more thorough derivation of scattering theory where we start by introducing a single-particle scattering matrix and discuss the Breit-Wigner formula for transmission. Then from single-particle scattering theory we derive a two-particle scattering matrix where the correlation term between the two systems is introduced. Further in chapter 6 we present our results and in chapter 7 we give our conclusion and outlook.

# 3 Quantum Bits and Entanglement

In this chapter we take a look at quantum bits and describe how they differ from classical bits. We clarify and mathematically define the concept of superposition and describe briefly the outcome of measurements in quantum information. We even introduce the density matrix operator and finally explain the entanglement measure met in form of concurrence.

## 3.1 Qubits

One can argue that information is physical in the sense that it can only be realized using some physical quantity. For classical computers, zeros and ones are realized by applied different voltages in a circuit. Quantum mechanically information can be realized using the spin of a charged particle or the polarity of a photon. Yet by treating bits as mathematical abstracts, one is not cumbered by the limitations of state of the art technological realizations of computational systems and thus it is possible to create a more general and complete theory of QI and QC. This also allows for different technological approaches for realizing a computational device. In classical information theory (i e not based on principles of quantum mechanics) a bit is an abstract concept that contains one piece of information about the state of a system, often denoted by 0 or 1, and constitutes a computational basis. Any measurement done in this basis will yield the result of either 0 or 1. Just as classical information theory has the bit as its fundamental building block, QI theory has a quantum bit, or qubit, as its fundamental building block. In analogy with a classical bit a qubit can be in either state of $|0\rangle$ or $|1\rangle$, which now constitute the computational basis in the quantum system. Here we have introduced Dirac's notation to denote the two quantum states $|0\rangle$ or $|1\rangle$. Most general a qubit can be found in superposition of these two states, namely

$$\alpha|0\rangle + \beta|1\rangle. \tag{1}$$

Upon measurement in the computational basis the state above will collapse into either state $|0\rangle$ or $|1\rangle$ with probabilities $|\alpha|^2$ or $|\beta|^2 = 1 - |\alpha|^2$ respectively. Similarly a two qubit system has four dimensional computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Most generally a state vector can be written as a superposition of those four states, namely

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle, \qquad (2)$$

with probabilities $|\alpha_x|^2$ where $x = 00, 01, 10$ or $11$ and the total probability adds up to unity.

## 3.2 Density Matrix

A state vector or wave function contains all the information about the physical state of a system. For a pure state the density matrix is obtained by taking the outer product of the state vector with its dual vector and contains the same information as the state vector. For a mixed state where each quantum system is in one of the states $|\psi_i\rangle$ with respective probability $p_i$, the density matrix is defined by

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|. \qquad (3)$$

Thus a quantum state is pure it can be written as $\rho = |\psi\rangle\langle\psi|$, otherwise it is mixed. An observable can be represented by a density operator, formalized by a density matrix, acting on the state vector. A matrix that is Hermitian satisfies the condition $M^\dagger = M$, where the $M^\dagger = (M^*)^T$ and $M^T$ is the transpose of $M$. Thus a Hermitian matrix must have real eigenvalues, which correspond to physically observable quantities. Further an $n \times n$ matrix is said to be positive semi-definite if for some complex valued vector $z$, $z^* M z$ is non-negative. It follows naturally that a positive semi-definite matrix also is Hermitian. Whenever the outcome of the density matrix acting on the vector space is a constant times the vector, the vector is said to be an eigenstate and the constant is an eigenvalue corresponding to that eigenstate. Any measurement of the observable will then yield the eigenvalue as a result. A

density matrix in the bipartite Hilbert space $H_A \otimes H_B$ is separable it can be written as a tensor product of the respective density matrix

$$\rho = \sum_i p_i \rho_i^A \rho_i^B. \tag{4}$$

While the diagonal elements of the two-state density matrix give us information about the population of the basis states, coherence between the two states is found in the off diagonal elements [4].

## 3.3  Entanglement and Concurrence

Non separable states are quantum states that cannot be written in the form of equation (4), and are said to be entangled. Different measures for entanglement have been proposed over the years, such as fidelity (a measure of how distinguishable two states are) , entanglement cost and concurrence. [8] A convenient measure used throughout this thesis is concurrence. For a bipartite system constituted of two qubits, the concurrence can be expressed directly in terms of $\rho$ as [9]

$$C = max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}, \tag{5}$$

where $\lambda_i$ are the eigenvalues of

$$\rho \cdot (\sigma_y \otimes \sigma_y) \cdot \rho^* \cdot (\sigma_y \otimes \sigma_y). \tag{6}$$

Here $\sigma_y$ is the Pauli matrix given by

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{7}$$

and $\otimes$ denotes the direct or tensor product.

# 4 Quantum Dots

Analysis in this thesis is based on electron tunneling in QDs. Those are $0D$ structures with quantized energy levels, hence sometimes referred to as artificial atoms. During the last decades it has become possible to experimentally control and design materials in order to create low-dimensional, $2D$, $1D$ and also $0D$, electronic structures by means of quantum confinement, see figure (1).
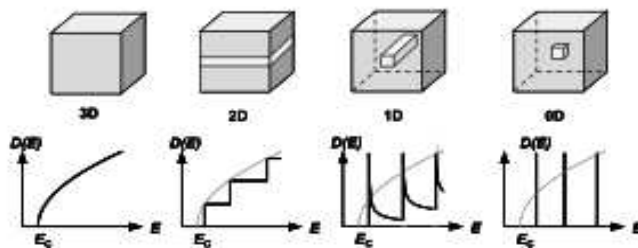


Figure 1: Top: Schematic representation of three, two, one and zero-dimensional nanostructures made using semiconductor heterostructures. Bottom: The corresponding densities of electronic states, image taken from [10]

$QDs$ are typically fabricated in nanostructures such as nanowires, nanotubes, gated semiconductors and $2D$ gas. For our purpose, electrons in QDs are the smallest possible carriers of QI. Here we utilize position/orbital degrees of freedom, i e left/right lead, for investigating quantum correlations. Electron spin degrees of freedom can also be used as qubits.

# 5 Scattering Theory

In this chapter we introduce the scattering matrix for single-particle scattering and then present the Breit-Wigner formula for the transmission and reflection amplitudes. Relating this to the results derived for single-particle scattering, we thereafter present two-particle scattering approach for two coupled conductors, where the interaction between the two systems is treated as a first order perturbation. Constructing the two-particle wave function

and tracing over the energy degree of freedom we then arrive at the reduced density matrix description of the outgoing orbital states.

## 5.1 Single-particle Scattering



Figure 2: Single particle scattering. Scattering properties are determined by the shape of the scattering potential

Consider a single-particle scatterer. For the general theory one permits for the particles to be incident from either direction left ($L$) or right ($R$) and to be scattered in either direction. Finding the quantum transport properties for such a composition is reduced to solving a quantum mechanical scattering problem across a potential defined by the mesoscopic system. For an individual particle all interactions with the system are described by a single-particle scattering potential. This approximation gives a simple model to work with where all the information concerning the transport properties is encoded in the scattering matrix. The wave function for the incoming and outgoing particles with energy $E$ is given by $|\alpha E\rangle_\sigma$, where $\alpha$ stands for ($L/R$) and the subscript $\sigma = in, out$ is to distinguish the incident and scattered wave functions. For a mesoscopic system connected to two leads the single-particle scattering matrix $S(E)$ relates the incoming states to the outgoing as

$$\begin{bmatrix} |LE\rangle_{out} \\ |RE\rangle_{out} \end{bmatrix} = S^* \begin{bmatrix} |LE\rangle_{in} \\ |RE\rangle_{in,} \end{bmatrix} \tag{8}$$

where

$$S = \begin{bmatrix} S_{LL} & S_{LR} \\ S_{RL} & S_{RR} \end{bmatrix}. \tag{9}$$

The matrix elements are reflection and transmission amplitudes and are energy dependent, so the matrix in equation 9 can equivalently be written as

$$S = \begin{bmatrix} r(E) & t'(E) \\ t(E) & r'(E) \end{bmatrix}. \tag{10}$$

To ensure conservation of particle number during scattering the scattering matrix must be unitary $S^\dagger S = 1$. If the particles coming from left with probability amplitude equal to unity, we define the incoming wave function as

$$|\psi_{in}\rangle = |L\ E\rangle_{in}. \tag{11}$$

The outgoing scattering state is then, by definition, the incoming state rewritten via equation (8) as

$$|\psi_{out}\rangle = \sum_{\alpha\ L} S_{\alpha L}|\alpha\ E\rangle_{out} \tag{12}$$

Having determined the relation between the incoming and outgoing states and defined the scattering matrix it is now time to determine the shape of the matrix elements.

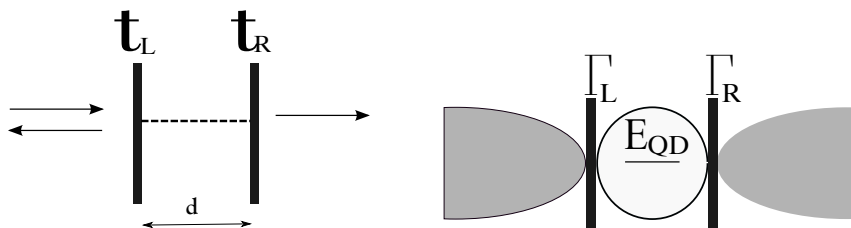## 5.2  Breit-Wigner Transmission Probability Amplitude



Figure 3: Left: Two barriers denoted $L$ and $R$ separated a distance $d$. Right: Two leads connected to a QD giving rise to a localised energy level $E_{QD}$.

Let two barriers be separated a distance $d$. The barriers will give rise to a localized quantum state with energy $E_{QD}$. A free propagating electron

with kinetic energy $h^2k^2/2m$ traveling a round trip between the barriers will gain a phase $\theta(E) = 2kd$ before exiting the entire system. The transmission through the entire system is given by the transmission amplitude

$$t_{tot} = \frac{t_L t_R e^{i\theta/2}}{1 - r_L r_R e^{i\theta}},$$

(13)

where $t_L, r_L$ $(t_R, r_R)$ are the transmission and reflection amplitudes of the the left (right) barrier. This gives the total transmission probability

$$T_{tot} = \frac{T_L T_R}{1 + R_L R_R - 2\sqrt{R_L R_R}\cos(\phi(E))},$$

(14)

where $\phi = 2kd + \arg(r_1 r_2)$ and $T_L = 1 - R_L$ $(T_R = 1 - R_R)$ is the transmission probability of the left (right) barrier. In the limit where $T_L, T_R \ll 1$, the electron will reflect back and forth multiple times between the barriers, each time gaining more phase, before exiting. In this limit the transmission amplitude is of the Breit-Wigner form given by, for a resonance energy $E_{QD}$

$$t(E) = \frac{\sqrt{\Gamma_L \Gamma_R}}{(E - E_{QD}) + i(\Gamma_L + \Gamma_R)/2},$$

(15)

while for reflection amplitude one obtains the following expression

$$r(E) = \frac{i(E - E_{QD}) - i(\Gamma_L - \Gamma_R)/2}{(E - E_{QD}) + i(\Gamma_L + \Gamma_R)/2}.$$

(16)

Here $\Gamma_{L,R} = \frac{\Delta}{2\pi}T_{L,R}$ is the escape rate for the electron across each barrier, with $\Delta$ the distance between two adjacent energy levels. The transmission and reflection probabilities are thus

$$T(E) = |t(E)|^2 = \frac{\Gamma_L \Gamma_R}{(E - E_{QD})^2 + (\Gamma_L + \Gamma_R)^2/4},$$

(17)

and $R(E) = 1 - T(E)$, giving

$$R(E) = |r(E)|^2 = \frac{(E - E_{QD})^2 + (\Gamma_L - \Gamma_R)^2/4}{(E - E_{QD})^2 + (\Gamma_L + \Gamma_R)^2/4}.$$
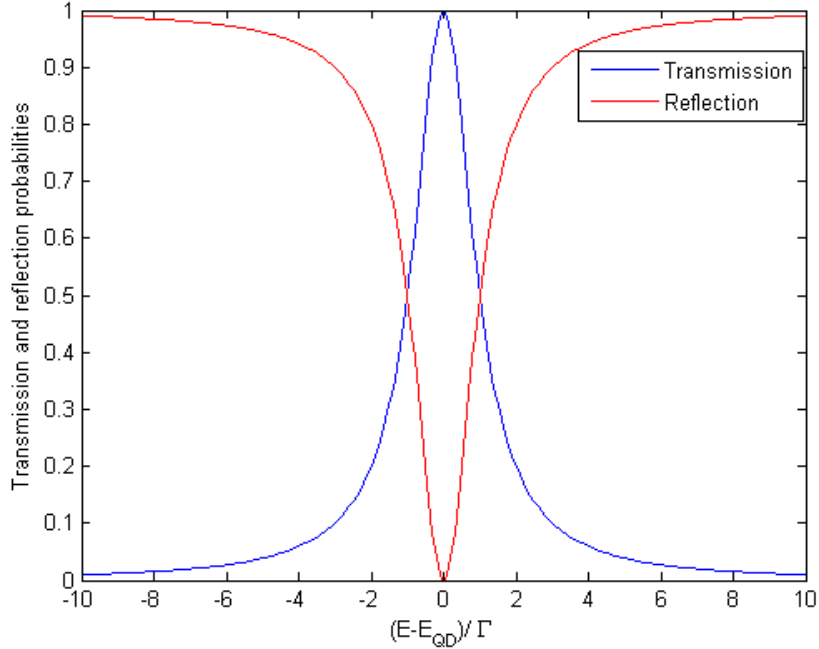
(18)

Figure 4: Transmission and reflection amplitudes of the Breit-Wigner form. On the $x$-axes we have the energy difference between incident particles and the energy of the QD, with $\Gamma = \Gamma_L = \Gamma_R$

We see from figure (4) that the transmission amplitude is maximal when the incident particle is at resonance with the dot level $E = E_{QD}$. Resonant tunneling through a QD is modeled in a good way using Breit-Wigner and therefore we use it throughout the thesis.

## 5.3 Two-particle Scattering

As mentioned before we are interested in the quantum correlation between two coupled systems, here denoted $A$ and $B$, and thus consider two weakly coupled QDs with respective energy $E_A$ and $E_B$, see figure (5). The dots are connected to two separate electron reservoirs via noninteracting leads $L, R$. Due to the coupling, electrons in the two dots can exchange an energy $\hbar\omega$ upon scattering.
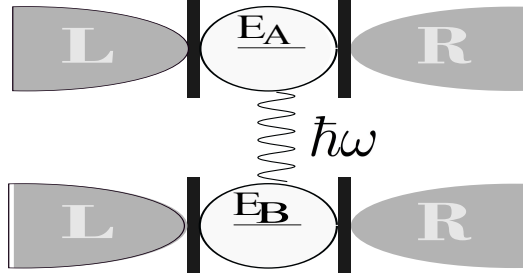
Figure 5: Two coupled quantum dots. Two electrons occupying each quantum dot exchange an energy of $\hbar\omega$ before being scattered

Considering first the case without interaction between the dots we can write the two-particle scattering relation, extending on equation (8)

$$
\begin{bmatrix}
|LE,\ LE'\rangle_{out} \\
|LE,\ RE'\rangle_{out} \\
|RE,\ LE'\rangle_{out} \\
|RE,\ RE'\rangle_{out}
\end{bmatrix}
= S^*
\begin{bmatrix}
|LE,\ LE'\rangle_{in} \\
|LE,\ RE'\rangle_{in} \\
|RE,\ LE'\rangle_{in} \\
|RE,\ RE'\rangle_{in}
\end{bmatrix},
\tag{19}
$$

where we use the convention that for a ket $|\alpha E,\ \beta E'\rangle_{in}$, $\alpha E$ ($\beta E'$) describes the lead and energy of a particle at dot $A$ ($B$). The two-particle scattering matrix is

$$
S = S^A(E) \otimes S^B(E'),
\tag{20}
$$

where $S^A(E)$ and $S^B(E')$ are the single particle scattering matrices of dot $A$ and $B$ respectively.

In the presence of interactions there is also a possible exchange of energy between the particles in the two dots. The two particle scattering matrix then in general describes the amplitudes for two particles incident from leads $\alpha$ in $A$ and $\beta$ in $B$, with energies $E_1$ and $E_2$, to scatter out at leads $\alpha'$ in $A$ and $\beta'$ in $B$ at energies $E_3$ and $E_4$. The corresponding element of the scattering matrix is denoted

$$
S^{A,B}_{\alpha\alpha',\beta\beta'}(E_1, E_2, E_3, E_4).
\tag{21}
$$

We note that in this configuration where we have single-electron injections in respective lead and each electron exists in its own Hilbert space we don't have

to worry about problems with identical particles and fermionic commutation properties and hence use the standard Dirac notation for the two-particle state. Since we consider detection of the electrons on either side of the reservoir the orbital degrees of freedom $L$ and $R$ will now constitute the quantum numbers for our system.

To proceed we consider the case with two particles injected from the left side, with energies $E_1$ and $E_2$, in leads $A$ and $B$ respectively. The wave function for the incoming particles is then given by

$$|\psi_{in}\rangle = |LE_1, LE_2\rangle. \tag{22}$$

In analogy to equation (12) the outgoing states relate to the incoming states via the general expression

$$|\psi_{out}\rangle = \sum_{\alpha,\beta} \int dE_3 dE_4 S^{AB}_{\alpha L,\beta L}(E_1, E_2, E_3, E_4)|\alpha E_3, \beta E_4\rangle. \tag{23}$$

To determine the two-particle scattering matrix for arbitrary strong interactions is a formidable task. Here we focus on weak, capacitive coupling, treated by Goorden and Büttiker [7]. To leading order in the coupling strength $\lambda$ they find that the scattering matrix element in equation (21) can be written

$$
\begin{aligned}
S^{A,B}_{\alpha\alpha',\beta\beta'}(E_1, E_2, E_3, E_4) &= S^{A}_{\alpha\alpha'}(E_1)S^{B}_{\beta\beta'}(E_2)\delta(E_1 - E_3)\delta(E_2 - E_4) \\
&+ \delta S^{A,B}_{\alpha\alpha',\beta\beta'}(E_1, E_2, E_3, E_4)\delta(E_1 + E_2 - (E_3 + E_4)),
\end{aligned}
\tag{24}
$$

where the first term on the right hand side is just the product of the single particle scattering amplitudes (energy conserving) and the second term contains the coupling and is given by

$$\delta S^{AB}_{\alpha\alpha',\beta\beta'}(E_1, E_2, E_3, E_4) = -2\pi i\lambda \frac{S^{A}_{\alpha\alpha'}(E_1) - S^{A}_{\alpha\alpha'}(E_3)}{2\pi i(E_1 - E_3)} \frac{S^{B}_{\beta\beta'}(E_2) - S^{B}_{\beta\beta'}(E_4)}{2\pi i(E_2 - E_4)}. \tag{25}$$

We thus have our wavefunction in (23) as

$$
\begin{aligned}
|\psi_{out}\rangle = & \sum_{\alpha,\beta} \int dE_3 dE_4 \big[ S^A_{\alpha L}(E_3) S^B_{\beta L}(E_4) \delta(E_1 - E_3)\delta(E_2 - E_4) \quad (26) \\
& + \; \delta S^{A,B}_{\alpha L,\beta L}(E_1, E_2, E_3, E_4)\big] |\alpha\, E_3, \beta\, E_4\rangle
\end{aligned}
$$

Having elaborated on the scattering theory we now turn to the generation of wave packets in our system.

## 5.4   Wave Packet Injections

In recent series of experiments [11, 12] a controlled creation of electron wave packets in nanoscale systems has been demonstrated. Motivated by these experiments we here focus on the case when the incident particles are described by synchronized wave packets. Here the wave packets are modeled with a lorentzian spectral amplitude

$$
g^\kappa(E) = \frac{\sqrt{\Delta_\kappa}}{\pi(E - \overline{E}_i - i\Delta_\kappa)}, \tag{27}
$$

where $\overline{E}_i, i = 1, 2$ is the mean value of respective wave packet, $\Delta_\kappa$ its width the subscript $\kappa$ is to distinguish between the two systems $A$ and $B$. The wave packet is normalized such that $\int dE |g(E)|^2 = 1$. For simplicity we let the injected packets in both system have the same width $\Delta_A = \Delta_B = \Delta$. The incoming two-particle state can then be written

$$
|\psi_{in}\rangle = \int dE_1 dE_2\, g^A(E_1) g^B(E_2) |E_1 L, E_2 L\rangle. \tag{28}
$$

To obtain the outgoing state we can make use of the wave function in equation (23) for mono-energetic incoming states, giving

$$
\begin{aligned}
|\psi_{out}\rangle = & \sum_{\alpha,\beta} \int dE_3 dE_4 \big[ g^A(E_3) g^B(E_4) S^A_{\alpha L}(E_3) S^B_{\beta L}(E_4) \quad (29) \\
& + \int d\omega\, g^A(E_3 - \omega) g^B(E_4 + \omega) \delta S^{A,B}_{\alpha L,\beta L}(E_3 + \omega, E_4 - \omega, E_3, E_4)\big] |\alpha E_3, \beta E_4\rangle.
\end{aligned}
$$

Here $\omega$ is the energy exchanged in the scattering, i e $E_1 = E_3 + \omega$ and $E_2 = E_4 - \omega$. Below we omit the subscript *out* in the total wave function. To obtain a simplified notation we introduce

$$P_{\alpha,\beta}^{AB}(E_3, E_4) = g^A(E_3)g^B(E_4)S_\alpha^A(E_3)S_\beta^B(E_4) \tag{30}$$

and

$$\delta P_{\alpha,\beta}^{AB}(\omega, E_3, E_4) = g^A(E_3 - \omega)g^B(E_4 + \omega)\delta S_{\alpha,\beta}^{A,B}(E_3 - \omega, E_4 + \omega, E_3, E_4). \tag{31}$$

We thus have the outgoing wavefunction

$$|\psi\rangle = \sum_{\alpha,\beta} \int dE_3 dE_4 \left[ P_{\alpha,\beta}^{AB}(E_3, E_4) + \int d\omega \delta P_{\alpha,\beta}^{AB}(\omega, E_3, E_4) \right] |\alpha E_3, \beta E_4\rangle. \tag{32}$$

As a next step we then construct the full two-particle density matrix of the outgoing state $\rho = |\psi\rangle\langle\psi|$ which can be written

$$
\begin{aligned}
\rho &= \sum_{\alpha,\beta,\alpha',\beta'} \int dE_3 dE_3' dE_4 dE_4' \left[ P_{\alpha,\beta}^{AB}(E_3, E_4) + \int d\omega \delta P_{\alpha,\beta}^{AB}(\omega, E_3, E_4) \right] \\
&\times \left[ [P_{\alpha',\beta'}^{AB}(E_3', E_4')]^* + \int d\omega [\delta P_{\alpha',\beta'}^{AB}(\omega, E_3', E_4')]^* \right] \\
&\times |E_3\alpha, E_4\beta\rangle\langle E_3'\alpha', E_4'\beta'|
\end{aligned} \tag{33}
$$

Now that we have given the necessary background theory we are ready to address our main question, which also will be our contribution to this paper, what do the orbital quantum states of the system look like? In other words we want to examine correlations and entanglement in the $L, R-$space of the composite system. We consider a measurement situation where only the spatial degrees of freedom can be accessed, as is typically the case for standard electrical current measurements. As a consequence, the energy degree of freedom can not be investigated and we thus trace it out from the outgoing quantum state. The result is a state characterized by a reduced

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density matrix

$$\tilde{\rho} = tr_E[\rho] \equiv \int dEdE' \langle EE' | \rho | E'E \rangle \tag{34}$$

Performing the trace and keeping only terms to first order in coupling $\lambda$, it is then practical to divide the resulting $\tilde{\rho}$ into three matrices, which will be denoted $M_1$, $M_2$ and $M_3$, given by

$$M_1 = \sum_{\alpha,\beta,\alpha',\beta'} \int dEdE' P_{\alpha,\beta}^{AB}(E,E') [P_{\alpha',\beta'}^{AB}(E,E')]^* |\alpha,\beta\rangle\langle\alpha',\beta'|, \tag{35}$$

$$M_2 = \sum_{\alpha,\beta,\alpha'\beta'} \int dEdE'd\omega P_{\alpha,\beta}^{AB}(E,E') [\delta P_{\alpha',\beta'}^{AB}(E-\omega, E'+\omega, E, E')]^* \tag{36}$$

$$\times \ |\alpha,\beta\rangle\langle\alpha',\beta'| \tag{37}$$

and

$$M_3 = M_2^*. \tag{38}$$

The matrix $M_1$ describes the properties of the uncoupled systems while the matrices $M_2$ and $M_3$ describe, to largest order in $\lambda$, the effect of the coupling.

# 6    Results

To provide a clear physical picture, we look at each term separately. Calculations are done using residue integration. For simplicity we set the transmission rate over both barriers to the same value namely $\Gamma_L = \Gamma_R = \Gamma$. Further we denote the difference in energy between the mean value of the incoming wave packet and the energy of the dot $Z_\kappa = \overline{E}_i - E_\kappa$.
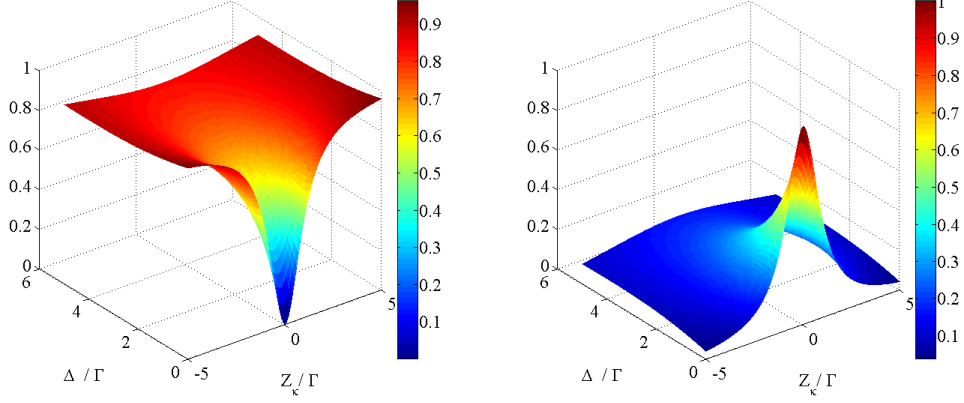
Figure 6: Left: The diagonal matrix element $M_{1\kappa}(1,1)$. Right: The diagonal matrix element $M_{1\kappa}(2,2)$

## 6.1   Uncoupled system $M_1$

The matrix $M_1$ can be written as the tensor product of two by two matrices $M_{1A} \otimes M_{1B}$, giving for $\kappa = A, B$

$$M_{1\kappa} = \sum_{\alpha,\alpha'=L,R} \int dE |g^{\kappa}(E)|^2 S^{\kappa}_{\alpha L}(E)[S^{\kappa}_{\alpha' L}(E)]^* |\alpha\rangle\langle\alpha'|. \tag{39}$$

After integration and simplification we obtain the following result in matrix form

$$M_{1\kappa} = \frac{1}{\pi(\Delta + \Gamma)^2 + Z_{\kappa}^2} \begin{bmatrix} (\Delta(\Delta + \Gamma) + Z_{\kappa}^2) & i\Gamma Z_{\kappa} \\ -i\Gamma Z_{\kappa} & \Gamma(\Delta + \Gamma) \end{bmatrix}, \tag{40}$$

where we note that $tr(M_{1\kappa}) = 1$. The diagonal matrix elements are plotted in figure 6 and the off-diagonal ones in figure 7.
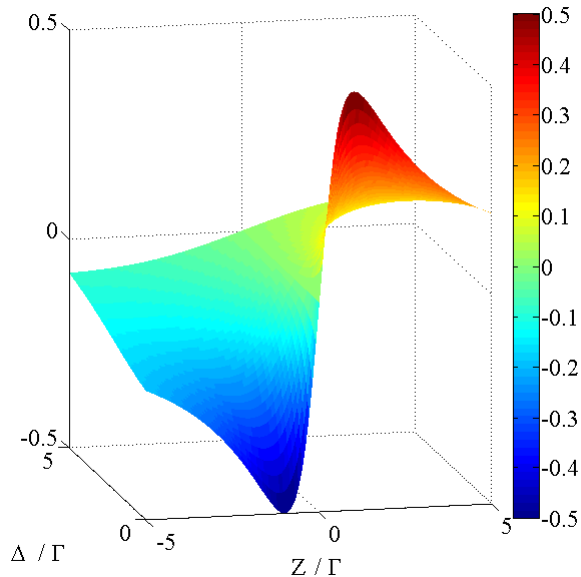
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Figure 7: Imaginary part of the off-diagonal matrix element $M_{1\kappa}(1,2)$.

Discussing the diagonal elements we first note that we can write

$$M_{1\kappa}(1,1) = \int dE |g^\kappa(E)|^2 T^\kappa(E)$$

$$M_{1\kappa}(2,2) = \int dE |g^\kappa(E)|^2 R(E) = 1 - M_{1\kappa}(1,1), \qquad (41)$$

where $T^\kappa = |S_{L,R}^\kappa|^2$ is the transmission probability and $R^\kappa = 1 - T^\kappa$ is the reflection probability. In the limit where the width of the wave packet of the incoming particle is much smaller than the width of the resonance in the dot, $\Delta \ll \Gamma$, we get back the shape of Breit-Wigner for transmission $T(z_\kappa)$ and reflection $R(z_\kappa)$ probabilities, see figure 4. In the opposite limit, $\Delta \gg \Gamma$, the matrix element $M_{1\kappa}(1,1)$ goes towards $\frac{\Gamma}{\pi}|g^\kappa(z_\kappa)|^2$, i. e. proportional to the wave packet spectral probability. For the intermediate values of $\Delta$ vs $\Gamma$ we note that the matrix elements have maxima and minima respectively when the mean value of the wave packet $\overline{E}$ is at resonance with the dot, at $Z_\kappa = 0$. Turning to the off-diagonal elements we note that they have the same shape and can be understood as a mixture of the diagonal elements. While the diagonal elements represents pure outgoing states correlations between the

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states is to be found in the off-diagonal elements, see figure 7. With a clear picture established for the uncoupled system we turn to the coupled elements.

## 6.2   Correlations $M_2$ and $M_3$

When analyzing equation 37 we realize that the interaction correction to the uncoupled scattering matrix can be written as

$$
\begin{aligned}
\delta S^{AB}(E - \omega, E' + \omega, E, E') & = & -\frac{\lambda \Gamma^2}{2\pi i} \xi(E, E_A) \xi(E - \omega, E_A) \\
& \times & \xi(E', E_B) \xi(E' + \omega, E_B),
\end{aligned}
\tag{42}
$$

where

$$
\xi(E, E_\kappa) = \frac{1}{E - E_\kappa - i\Gamma}.
\tag{43}
$$

Thus $\delta S^{AB}$ is independent of the indexes $\alpha'$ and $\beta'$. We can then write the amplitudes for the matrix elements of $M_2$ and $M_3$ in terms of functions $F_{\alpha\beta}$ defined as

$$
F_{\alpha\beta} = \int d\omega f_{L\alpha}^A(\omega) f_{L\beta}^B(-\omega),
\tag{44}
$$

where

$$
f_{L\alpha}^\kappa(\omega) = \int dE g(E) g^*(E - \omega) \xi(E, E_\kappa) \xi(E - \omega, E_\kappa) S_{L\alpha}^\kappa(E),
\tag{45}
$$

and evaluate the integral in equation 45 to get

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$$
\begin{aligned}
f_{LL}^{\kappa}(\omega) &= \frac{1}{D_{\kappa}}\Big[ -\Delta(\Delta + \Gamma)(2\Delta E + 3i\omega) \\
&+ \Delta(-2\Delta - 4\Gamma + i\omega)Z \Big] \tag{46} \\
f_{LR}^{\kappa}(\omega) &= \frac{1}{D_{\kappa}}\Big[ -\Delta(\Delta + \Gamma)(2\Delta E + 4\Gamma + i\omega) \\
&+ i\Delta(-2i\Delta + \omega)Z_{\kappa} \Big] \tag{47}
\end{aligned}
$$

$$
\tag{48}
$$

where we have introduced the following identity

$$
D_{\kappa} = \pi(2\Delta + i\omega)(2i\Gamma + \omega)\big[(\Delta + \Gamma)^2 + Z_{\kappa}^2\big]\big[(\Delta + \Gamma + i(\omega + Z_{\kappa}))\big] \tag{49}
$$

Performing the integrals in equation 44 and assembling everything we get the result for $M_2$, namely

$$
M_2 = \frac{\lambda}{2\pi i\Gamma}
\begin{bmatrix}
F_{LL} & F_{LL} & F_{LL} & F_{LL} \\
F_{LR} & F_{LR} & F_{LR} & F_{LR} \\
F_{RL} & F_{RL} & F_{RL} & F_{RL} \\
F_{RR} & F_{RR} & F_{RR} & F_{RR}
\end{bmatrix}
\tag{50}
$$

Again for clarity we define a denominator $Den$ as, assuming $Z_A = -Z_B = Z$

$$
Den = 2\pi(\Delta + \Gamma)\big[(\Delta + \Gamma)^2 + Z^2\big]^2\big[(3\Delta + \Gamma)^2 + Z^2\big], \tag{51}
$$

in the expressions for density matrix elements, given by

$$
\begin{aligned}
F_{LL} &= \frac{\Delta\Gamma}{Den}\big[-3\Delta(\Delta+\Gamma)^2(3\Delta+\Gamma) \\
&\quad - (\Delta^2+7\Delta\Gamma+4\Gamma^2)Z^2\big] \tag{52} \\
F_{RR} &= \frac{\Delta\Gamma}{Den}\big[-(\Delta+\Gamma)^2(3\Delta+\Gamma)(3\Delta E+4\Gamma) \\
&\quad - \Delta(\Delta+3\Gamma)Z^2\big] \tag{53} \\
F_{LR} &= \frac{\Delta\Gamma}{Den}\big[-3\Delta(\Delta+\Gamma)^2(3\Delta+\Gamma) \\
&\quad - 4i\Gamma(\Delta+\Gamma)(2\Delta+\Gamma)Z_A + \Delta(-\Delta+\Gamma)Z^2\big] \tag{54} \\
F_{RL} &= F_{LR}^*. \tag{55}
\end{aligned}
$$

We notice that the matrix $M_2$ has identical column vectors. This follows from $\alpha', \beta'$ independence of $\delta S^{AB}$. We also notice that the matrix elements $F_{LR}$ and $F_{RL}$ are each others complex conjugates. Further we know that $M_3 = M_2^\dagger$. A good picture of the leading order effect of the correlation can thus be found by investigating in detail $F_{LL}$, $F_{RR}$ as well as the real and imaginary parts of $F_{LR}$.
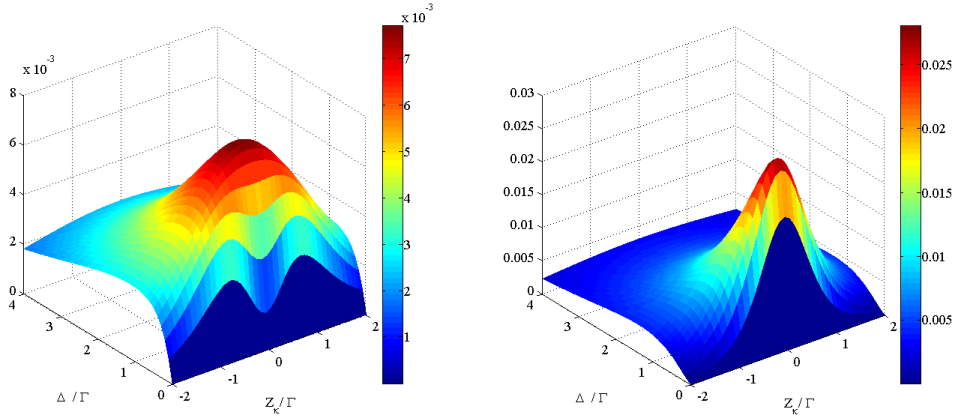


Figure 8: Left: The function $F_{LL}$. Right: The fucntion $F_{RR}$.

Studying the plots for $F_{LL}$ and $F_{RR}$ in figure 8 we notice that the functions decreases to zero for $\frac{\Delta}{\Gamma} \to 0$ and levels off $\frac{\Delta}{\Gamma} \gg 1$. Maximum is reached somewhere in the interval $0 < \frac{\Delta}{\Gamma} < 1$ and when $Z = 0$. This could be

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understood in the following manner. For an interaction to occur the wave packets need to be well localized in the dots. For $\Delta/\Gamma \approx 0$ we get back the picture where there are only planar waves existing in all space and no interaction is possible. On the other hand if $\Delta \gg \Gamma$ the particles with larger probability will be reflected and no interaction is possible. The optimal situation where the interaction is maximal seems to occur when both the incoming wave packets are at resonance with the dots, i e $Z = 0$, and when the wave packets just have the right width to enter the dots and interact with each other.
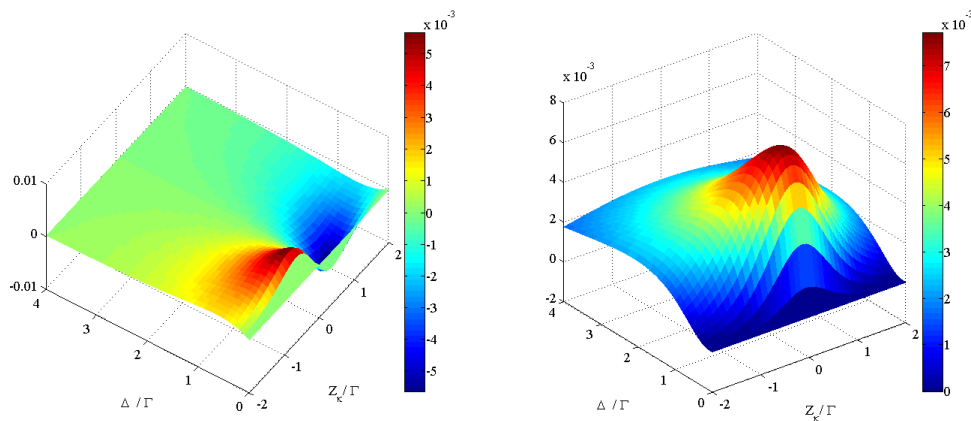


Figure 9: Left: The real part of the matrix element $F_{LR}$. Right:The imaginary part of the matrix element $F_{LR}$.

For $F_{LR}$ plotted in figure 9 we find a qualitatively similar behavior, with the largest effect close to $Z = 0$ and $\Delta/\Gamma \approx 1$.

## 6.3   Concurrence

Having investigated the different parts of $M_1$, $M_2$ and $M_3$ of the matrix in equation 34, we now turn to the question of entanglement quantified via concurrence. Since different entanglement measures should adhere to the same basic properties our results should not depend on a specific choice of entanglement measure, so we choose concurrence out of convenience. As

pointed out in section 3.3, the concurrence can be written as

$$C = max[\tilde{C}, 0] \tag{56}$$

where $\tilde{C}$ is a function of the reduced density matrix $\tilde{\rho}$.
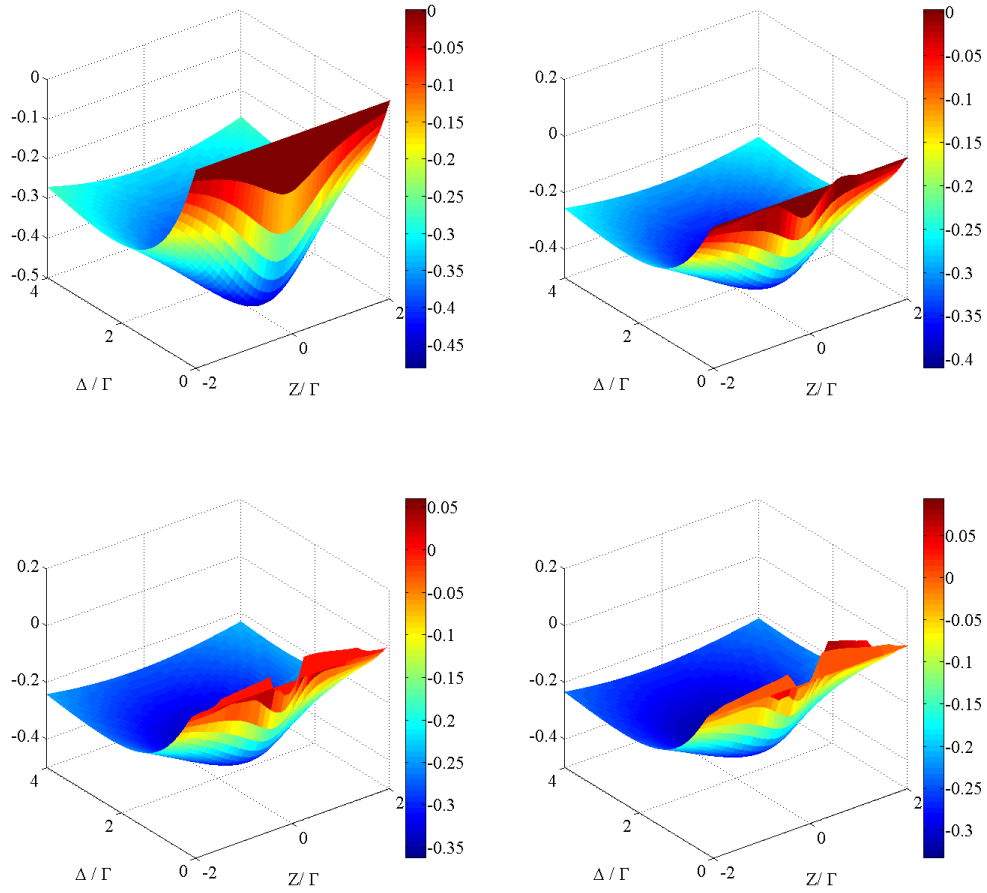


Figure 10: Concurrence function $\tilde{C}$ for $\lambda = 0.1$ (upper left), $\lambda = 0.5$ (upper right), $\lambda = 0.8$ (lower left) and $\lambda = 1.0$ (lower right).

To investigate the possibility of finding entanglement we plot the concurrence function $\tilde{C}$ as a function of $\Delta/\Gamma$ and $Z/\Gamma$, for the same range as in figures 8 and 9. The plots shown in figure 10 are presented for different $\lambda/\Gamma$, with the only constraint that the resulting density matrix remains positive

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definite and hence represent a physical system. From the plots we find that for no single case is $\tilde{C}$ larger than zero, i.e. we do not find entanglement. It is however clear that for large $\lambda/\Gamma$ (not to be considered due to the fact that we are dealing with perturbation theory) and parameters $Z/\Gamma \approx 0$ and $\Delta/\Gamma \approx 1$ there are clear effects on $\tilde{C}$, as one would expect from the results for $M_2$ and $M_3$ above. We can thus conclude that we have investigated a situation where there are strong and clear correlations induced between the orbital properties of the electrons in the two dots. However those correlations are not of a true quantum nature, i.e. there is no entanglement.

# 7   Conclusion and Outlook

As noted before no concurrence could be found but we find clear evidence of correlation close to resonance. The absence of concurrence could be due to the simplifications made where we for instance set $\Gamma_L = \Gamma_R$. However there is an indication that the greatest cause for not detecting any concurrence could be contributed to the tracing over all energies. Still, taking into account the energies off all scattered particles is a tedious work. So for further investigation we suggest studying a small window of energies instead of tracing them out. This could be done by setting an energy filter with a certain width for the outgoing particles. It also seems natural given our findings that one should confine the studies to systems close to resonance and with a well defined wave packet widths.

# 8   Self Reflection

I remember during the first days when Peter presented me with some materials to read. All the terminologies were very abstract and I didn't know what to do with everything. Professor Peter Samuelsson put me to work and during the months to pass I had to do a lot of derivations. This gave me some intuitive insight to how such terminologies work. Terminologies such as the density matrix, scattering matrix approach and concurrence became more

concrete. I guess physics studies are like learning a new language. When ones learns a new word, one knows how to use that word within the context it been learned. One can use it in that same context but still does not understand the full meaning of that word. Later when encountering that word in other contexts a deeper and more intuitive understanding of the world starts to develop. At this stage, I feel like I have learned a few new words, concepts, in physics. I know how they work within the context of my thesis and I can derive them and do some calculations and with time a deeper and more intuitive understanding will hopefully develop within me.

On the practical level, I had a lot of troubles with softwares such as Latex, Mathematica and Matlab. Every such difficulty had to be resolved and every resolution led to better mastering of those tools. Something that is necessary if one is to take on any technological job these days. Further on the personal level, even if I didn't actually had to learn a lot of concepts from different disciplines in physics, I have this assuring feeling that I can take on any new subject and be able to learn it. Compared to how I felt previous to finishing my thesis where I always was in doubt of my ability to really learn physics. Last I would like to say that overall I have matured in many ways and I am very thankful for the help and guidance I got from Peter Samuelsson.

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