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Dynamics of electron entanglement in semiconductor nanostructures

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Abstract. Quantum entanglement, the most remarkable feature of quantum physics, is recognized as a resource for quantum information processing. The quest for quantum-computing devices has also produced great interest in entanglement formation in solid-state systems involving quantum effects. Indeed, the functionality of an increasing number of nanodevices is influenced by quantum correlations. In this work a theoretical approach developed in recent years to study the entanglement of fermions interacting via a Coulomb potential is presented, together with a number of applications to specific situations of physical interest in the field of charge transport in semiconductor nanostructures.

1. Introduction

Quantum entanglement undoubtedly represents one of the most peculiar aspects of quantum mechanics as it can be viewed as the furthest departure of the quantum world from the classical one [1, 2]. Quantum entanglement between two charge carriers can be created when they interact through the Coulomb potential. Indeed, after a scattering the two-particle system is in general described by a two-particle state that is not separable in two single-particle states. This entanglement building up is an intrinsically dynamical process and its analysis is not only useful to understand the nature of the scattering process itself, but it can also contribute significantly to design quantum information processing devices. In fact, on one hand, controlled entanglement has been recognized as the fundamental resource for quantum computation and communication [2], on the other hand entanglement with the environment (i.e., decoherence) represents the main threat to the proper functioning of a feasible quantum computer [1].

For these reasons, the study of the entanglement dynamics in scattering events in solid-state systems has became more and more relevant in recent years [3, 4, 5, 6] and different proposals to produce entangled states between charge carriers, have been presented [7, 8, 9].

In this context, the entanglement dynamics has been evaluated in 1D- and 2D-scattering events between two carriers explicitely considered as indistinguishable. To this aim, numerical approaches have been developed which allow one to evaluate the mechanisms governing entanglement creation and their connection with the characteristic physical parameters and initial condition of the systems. Estimations of the entanglement time-evolution show a deep relation between spin and space degrees of freedom of the states, even for interactions not involving spin-orbit terms [10, 11].

Entanglement and its effects have been investigated in semiconductors devices realized with semiconductor quantum dots (QD) by solving the multi-particle open-boundary Schrödinger equation. In particular numerical simulations show that the production of entanglement in QD structures may be controlled through external fields [12].

Dynamics of entanglement has also been analyzed for carrier-carrier collisions in low-dimensional semiconductor structures in presence of an external periodic potential. In particular the latter has been shown to provide a way to control electron decoherence due to carrier-carrier scattering, this model being of interest to study the building up of quantum correlations in electron transport assisted by surface acoustic waves (SAW).

2. Entanglement creation for identical particles

A quantitative evaluation of the entanglement dynamics for electron-electron collisions in 1D and 2D systems has been performed applying a method, suitable for indistinguishable particles, based on the Slater rank and the von Neumann entropy of the reduced density matrix [10]. The quantum entanglement of both spatial and spin degrees of freedom can be computed for various initial conditions of the system. Here, for the sake of brevity, we analyze only a 2D case. We consider an electron freely propagating in a 2D system interacting through a Coulomb potential with a second carrier confined in a harmonic potential. The latter can be viewed as a simple model of shallow impurity. Spin orbit effects are not taken into account. At the initial time one of the two particles (incoming electron) is represented by a minimum uncertainty wavepacket, while the bound electron is in the ground state of a 2D harmonic oscillator. Considering the spin degrees of freedom, we take four initial spin configurations, as given in the following quantum states: $|\Psi\rangle$ same spin, $|\Upsilon\rangle$ different spin, $|\Phi\rangle_-$ singlet, $|\Phi\rangle_+$ triplet;

$$\begin{aligned} |\Psi\rangle &= \frac{1}{\sqrt{2}}\Big(|\psi\,\phi\rangle - |\phi\,\psi\rangle\Big)|\uparrow\uparrow\rangle, \\ |\Upsilon\rangle &= \frac{1}{\sqrt{2}}\Big(|\psi\,\phi\rangle|\uparrow\downarrow\rangle - |\phi\,\psi\rangle|\downarrow\uparrow\rangle\Big), \\ |\Phi\rangle_\mp &= \frac{1}{2}\Big(|\psi\,\phi\rangle \pm |\phi\,\psi\rangle\Big)\Big(|\uparrow\downarrow\rangle \mp |\downarrow\uparrow\rangle\Big), \end{aligned}$$

where the ket $|\uparrow\rangle$ ($|\downarrow\rangle$) indicates a spin up (down) state.

In our approach we solve numerically the time-dependent Schröndinger equation for the 2D two-particle wavefunction in the center of the mass coordinate system. In order to quantify numerically the entanglement we have implemented the theoretical criterion, given by Schliemann, based on the Schmidt decomposition theorem for two-fermion state [13, 14]. Through a unitary transformation the antisymmetric wavefunction is expressed into a combination of Slater determinants with a minimum number of non vanishing terms with coefficients z_i. This number, the Slater rank, gives the measure of the entanglement that can still be equivalently expressed as the von Neumann entropy of the one particle reduced density operator ρ as:

$$\varepsilon = -\mathrm{Tr}[\rho \ln \rho] = \ln 2 - 2\sum_{i=1}^{N} |z_i|^2 \ln 2|z_i|^2 \qquad (1)$$

$2N$ is the dimension of the single particle Hilbert space and corresponds, in the present case, to twice the number of discretization points in the real space. For identical particles the von Neumann entropy reaches its minimum value $\varepsilon = \ln 2$ in case of non entangled states, whose Slater rank is equal to 1. This value indicates the uncertainty coming from indistinguishability of the particles, but the correlations due to exchange symmetry cannot represent a resource for quantum information [14].

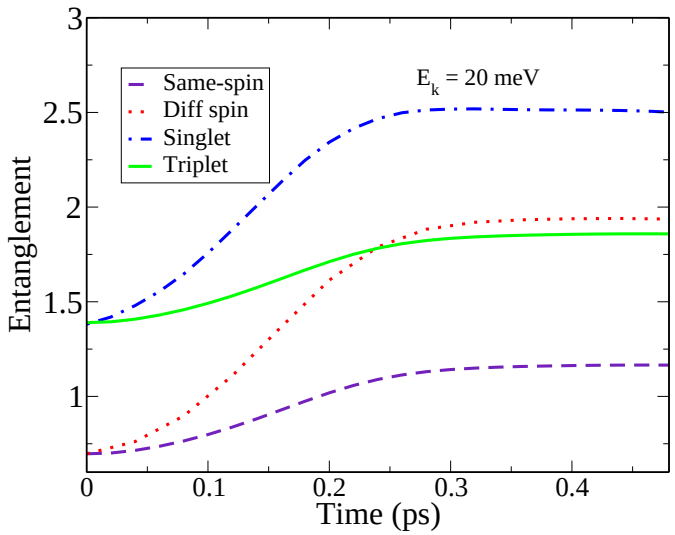

Figure 1. Entanglement as a function of time: two electrons with same spin $|\Psi\rangle$(dashed line), with different spin $|\Upsilon\rangle$(dotted line), singlet $|\Phi\rangle_-$ (dash-dotted line) and triplet $|\Phi\rangle_+$ (solid line).

Numerical result have been obtained adopting GaAs material parameters but can be considered representative of a more general behavior. At initial time, when the centers of the wavepackets are distant enough so that the Coulomb energy is negligible, the von Neumann entropy for the states $|\Psi\rangle$ and $|\Upsilon\rangle$ is $\ln 2$ as expected. In fact no correlation is present a part from the one due to the exchange symmetry and therefore $|\Psi\rangle$ and $|\Upsilon\rangle$ must be considered as non entangled. As the particles get closer their quantum correlation builds up and entanglement reaches a stationary value once particles get closer. In Fig.1 we report the time evolution of the entanglement for an initial kinetic energy of the incoming electron $E_k = 20$ meV, and for all the considered spin configurations. Note that at the initial time the von Neumann entropy of the singlet $|\Phi\rangle_-$ and the triplet state $|\Phi\rangle_+$ is $2\ln 2$. In fact such states have to be considered as initially entangled, being their Slater rank greater than 1: note that $|\Phi\rangle_-$ and $|\Phi\rangle_+$ cannot be factorized in terms of a single Slater determinant.

From our simulations we found a dependence of the entanglement dynamics upon the spin components of the state vector describing the system at initial time, even if we have neglected spin-orbit effects.

3. Effects of scattering resonance on carrier-carrier entanglement in quantum dots

Here we address numerically the problem of entanglement generation for a two-electron scattering in a 1D double-barrier resonant tunnelling device. Specifically, we consider an electron incoming from a source lead and described by a scattering state, while the other is localized in a bound state between the two small potential barriers, that separate the internal region from the two contacts. The system is depicted in the left panel of Fig. 2. The N bound energies of the so-formed QD will be indicated as E_n (with $n = 0, 1, \ldots, N$ in order of increasing energy), respectively.

Let us consider the envelope function of two spinless electrons in 1D $\psi(x_1, x_2)$, describing the state with a particle in a QD bound state χ_0 and a second electron incoming from the left lead with energy E_{IN}, and scattered by the structure potential V_s, sketched in the left panel of Fig. 2, and by the Coulomb interaction with the bound particle. The two-particle scattering state is obtained by solving by means of QTBM [16] the time-independent open-boundary Schrödinger equation $\mathbf{H}\psi = E\psi$ in the square domain $x_1, x_2 \,\epsilon\, [0, L]$ with $\mathbf{H}$ the two-particle Hamiltonian of the system. As a consequence of the scattering, quantum correlations appear between the energy levels E_n of the electron bound in the potential well and the energies T_n of the scattered electron. The calculation of the entanglement formation is performed, also in this case, by means

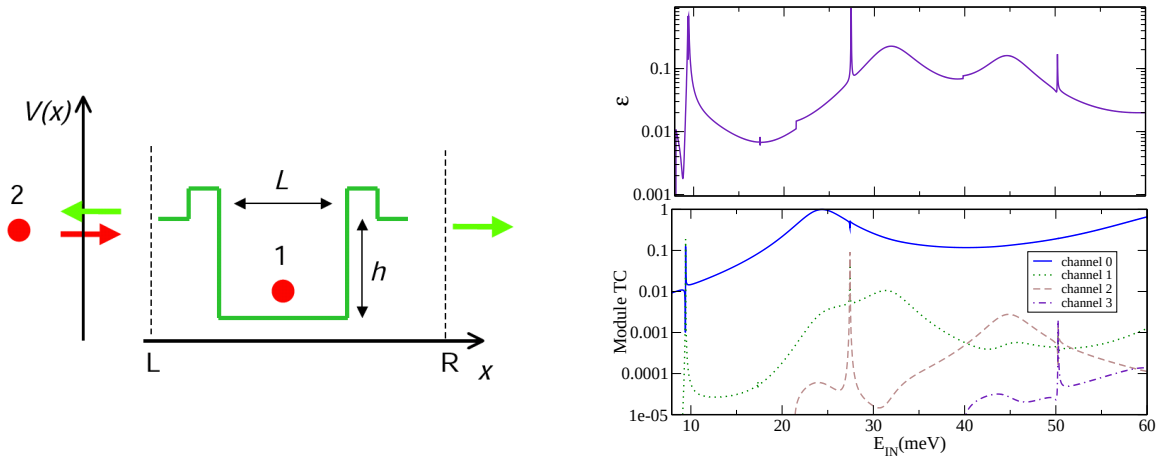

Figure 2. Left panel: Potential profile $V(x)$ of the simulated system: $V(x)$ is zero in both left and right contacts.The bound electron (1) is initialized in the QD ground state while the scattered electron (2) arrives from the left lead. Right top panel: the entanglement ε as a function of the initial kinetic energy of the incoming electron E_{IN}. Right bottom panel: modulus of the TC of the four channels as a function of E_{IN}: channel 0 (solid line), 1 (dotted line), 2 (dashed line) and 3 (dash-dotted line).

of the von Neumann entropy [10] that can here be expressed as:

$$\varepsilon = -\sum_{n=0}^{M} |c_n|^2 \ln |c_n|^2. \tag{2}$$

where c_n are the transmission probability amplitudes of two-particle state.

In the top right panel of Fig. 2 we report the entanglement as a function of the kinetic energy of the incoming particle E_{IN}. In our calculations we consider a potential well 150 meV deep and 40 nm wide. For E_{IN} around 10 meV, with only two possible scattering channels, a Fano resonance [17] of the transmission coefficient (TC) is observed for channel 0. In this case entanglement shows a peculiar behavior. It presents a minimum between two close maxima (where von Neumann entropy is equal to $\ln 2$), indicating the maximum amount of quantum correlations between the transmitted and QD electron in a two-channel scattering. It is worth noting that the TC of channel 1 presents, in correspondence of the Fano resonance of channel 0, a Breit-Wigner resonance. On the other hand, the broad Breit-Wigner resonance for $E_{IN} \simeq 25$ meV of channel 0, does not influence the TCs of other channels (1 and 2), which does not show, at the specific energy, resonances of any kind and moreover the entanglement curve does not display maxima. Such a behavior is ascribed to the different mechanisms characterizing the two types of resonances. When the initial energy of the incoming electron increases new channels become effective in the scattering process thus influencing the entanglement curve. Our results suggest that the production and detection of entanglement in quantum dot structures may be controlled by the manipulation of Fano resonances through external fields [4].

4. Carrier-carrier entanglement in presence of a periodic potential

Let us now consider two electrons, interacting via the Coulomb potential, in a 1D channel and localized into two next minima of a periodic potential. To be more specific, we use a sinusoidal potential suitable for modeling SAW. The two particles are explicitly considered as indistinguishable and have the same spin. Two different physical conditions will be examined:

low-energy particles occupying the ground state of two next potential minima and high-energy particles taken in bound excited states. In our approach we solve numerically the time-dependent two-particle Schrödinger equation and then compute, at each time step, the bipartite entanglement which gives a measure of the correlation between the two electrons due to their mutual Coulomb interaction [10, 13]. We assume that the Hamiltonian describes a couple of electrons interacting with the traveling piezoelectric potential of the SAW, in the reference frame moving with the SAW itself [12].

We consider two electrons with the same spin so that the quantum state describing the system at the initial time $t_0 = 0$ is

$$\Phi_n(x_a, x_b) = \frac{1}{\sqrt{2}}\Big(\varphi_n(x_a)\varphi_n(x_b - \lambda) - \varphi_n(x_b)\varphi_n(x_a - \lambda)\Big) \tag{3}$$

where $n \geq 0$, with $\varphi_0(x)$ the ground state, and $\varphi_n(x)$ the n-th excited state, of the single-particle Hamiltonian in a closed domain with eigenvalues indicated by E_n. To be more specific, $\varphi_n(x)$ and $\varphi_n(x - \lambda)$ describe two electrons trapped in two next minima of a SAW with wavelength λ. To evaluate the system dynamics, we solve numerically the time-dependent Schrödinger equation for the two-particle spatial wavefunction. At each time step we compute the state of the system and from this we obtain the two-particle density matrix. The latter is used to compute the one-particle reduced density matrix by tracing over the degrees of freedom of one of the two electrons. Finally the entanglement is calculated in terms of the von Neumann entropy. We want to compare the behavior of the entanglement when the electrons are, at the initial

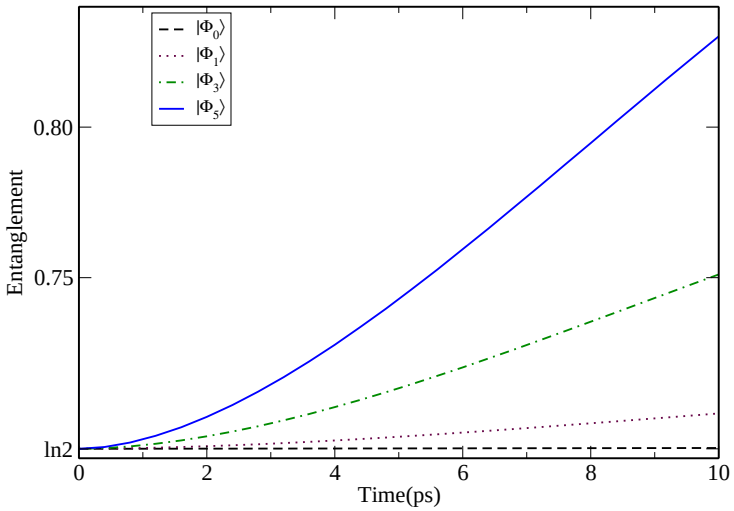

Figure 3. Entanglement dynamics of Φ_0 (dashed line) with E_0=-47.17 meV, Φ_1 (dotted line) with E_1=-41.54 meV, Φ_3 (dash-dotted line) with E_3=-30.59 meV, and Φ_5 (solid line)with E_5=-20.03 meV.

time, in the ground state of the single-particle Hamiltonian, or in one of its excited eigenstates. The results are reported in Fig. 3. When the ground state is considered, at initial time no correlation is present, apart from that due to the exchange symmetry, and the entanglement does not vary significantly with time. One can therefore conclude that during the time evolution of the two-particle wavefunction the Coulomb interaction does not become sufficiently strong to build up significative quantum correlations between the two electrons. On the other hand, when higher-energy states are involved, the quantum correlation is larger. Now, unlike the previous case, the entanglement is not negligible and reaches values significantly different from

the initial one, ln2, at times of the order of ten ps. The reasons for this behavior can be related to the real-space two-particle wavefunction. Its spatial spreading is larger for high-energy states and the single-electron probability densities localized in the two next minima get closer. This leads to an increase of the Coulomb interaction between the particles that is responsible for the quantum correlation. The results suggest that for electrons captured in high-energy bound states of the SAW a description in terms of single-particle states is less accurate as time goes by. In particular, for times of the order of a few tens of ps, as required for a single quantum operation in SAW-based quantum logic gates[18], only the low-energy bound carriers can safely be assumed to keep coherence, the effect of their mutual quantum correlations being negligible.

5. Conclusions

The attempt to shed more light on the phenomenon of entanglement between electrons, with special attention to semiconductors systems, is the motivation of this work. To this purpose, numerical approaches have been developed allowing to investigate the processes ruling entanglement creation and their connection with the physical parameters and initial conditions of the systems. The entanglement dynamics has been evaluated in 2D-scattering events between two indistinguishable carriers, showing a deep relation between spin and space degrees of freedom of the states, even for interaction not involving spin-orbit terms. Entanglement generation for a two-electron scattering in a 1D double-barrier resonant tunneling device has been investigated. Results suggest that the production and detection of entanglement in such structures may be controlled by suitably tuning the resonances of the system through external fields. Finally carrier-carrier quantum correlations in a 1D semiconductor in presence of a periodic potential modeling SAW have been studied. In this context, the validity of the single-particle approximation to describe the acoustically driven charge transport in semiconductors quantum wires has been discussed.

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