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Validity of the single-particle approach for electron transport in quantum wires assisted by surface acoustic waves

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Abstract
We study by means of time-dependent numerical simulations the quantum entanglement stemming from the Coulomb interaction between two electrons trapped in the minima of the piezoelectric potential generated by surface acoustic waves. We find that for particles captured in low-energy bound states the quantum correlations turn out to be negligible, thus validating a single-particle approach to the dynamics of such systems. At long times, for high-energy electrons, a substantial entanglement appears, which is an indicator of a mostly correlated dynamics.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In piezoelectric semiconductors, surface acoustic waves (SAWs) are experimentally produced by high frequency AC transducers generating lattice vibrations that propagate through the structure as longitudinal waves. These in turn couple to charge carriers and can be modeled as a sinusoidal traveling electric potential which traps the carriers into its moving minima [1–4]. A number of devices exploiting SAW–electron interactions have been designed, realized and also proposed as basic building blocks for quantum computing applications. Here the use of the acoustically driven electron transport has been shown to constitute a highly controllable means to inject and drive electrons along quasi-one-dimensional channels [5–7]. Indeed, although the SAW technology was originally introduced in the context of metrological application for defining a new standard of electric current [1–4], the use of SAWs has been shown to improve significantly the performances of some systems proposed as solid-state devices for quantum computation [5, 8, 9]. In fact, a better performance of such devices can be obtained with respect to the free electron propagation case, being SAW efficient to prevent the spreading of the electron wavefunction and to reduce undesired reflection effects and uncontrolled entanglement [6, 10].

In the analysis of charge transport assisted by SAW, the dynamics of the system is usually investigated in terms of single-particle non-interacting wavepackets [1–5], and the quantum correlations between electrons due to their Coulomb interaction are neglected. Such a description not only allows us to solve in a simple way the dynamics of the transport phenomena but is also crucial to guarantee the correct functionality of the quantum computation devices mentioned above. In fact, the possible appearance of quantum correlations between the charged carriers along a single wire can be interpreted as a manifestation of an undesired spatial entanglement which could represent a threat to perform the basic quantum computing operations [6, 7].

The focus of the present paper is on the analysis of the validity of the single-particle approach in electron transport through low-dimensional semiconductor structures assisted by SAWs, as commonly assumed in the experimental works [1–4]. To this purpose, we assess the correlation between two electrons by computing their mutual quantum entanglement. In particular we study numerically (by using the physical parameters corresponding to the experimental setups) a specific model which mimics SAW charge transport in a GaAs quantum wire. Indeed, in the last few years the entanglement created as a consequence of the Coulomb

interaction between two free propagating and/or bound charged particles has been studied in low-dimensional semiconductor structures [13–15]. Now we intend to move a step forward by investigating the time development of quantum correlations in a specific model of physical interest which describes the quantum transport of both low- and high-energy electrons trapped in the minima of a sinusoidal potential.

2. The physical model

We consider two electrons, interacting via the Coulomb potential, in a one-dimensional (1D) channel and localized into two next minima of a periodic potential modeling the 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 the two next potential minima and high-energy particles taken in bound excited states or in their linear superpositions. 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 [11, 12].

The two-particle Hamiltonian for two charged carriers in a GaAs quantum wire reads

$$H(x_a, x_b) = H_0(x_a) + H_0(x_b) + \frac{e^2}{\epsilon\sqrt{(x_a - x_b)^2 + d^2}}, \quad (1)$$

where ϵ is the GaAs dielectric constant, d the width of the quantum wire and

$$H_0(x) = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + \alpha\left(\sin\left(\frac{2\pi}{\lambda}x\right) + 1\right) \quad (2)$$

is the single-particle Hamiltonian, with m^* indicating the GaAs electron mass, α the amplitude of the SAW oscillation and λ its wavelength. We assume that the Hamiltonian given in equation (1) describes a couple of electrons interacting with the traveling piezoelectric potential of the SAW, in the reference frame moving with the SAW itself. In our numerical calculation we have taken the amplitude of the oscillation α equal to 50 meV, corresponding to the value used in the experiments [4].

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

$$\Phi_0(x_a, x_b) = \frac{1}{\sqrt{2}}(\varphi_0(x_a)\varphi_0(x_b - \lambda) - \varphi_0(x_b)\varphi_0(x_a - \lambda)) \quad (3)$$

where $\varphi_0(x)$ is the ground state of $H_0(x)$ in the closed domain $x \in [\frac{\pi}{2\lambda}, \frac{5\pi}{2\lambda}]$. To be specific, $\varphi_0(x)$ and $\varphi_0(x - \lambda)$ describe two electrons trapped in two next minima of a SAW with wavelength λ, as shown in the inset of figure 1. To evaluate the system dynamics, we solve numerically the time-dependent Schrödinger equation for the two-particle spatial wavefunction by means of a Crank–Nicholson finite difference scheme. At each time step we compute the state of the system and from this

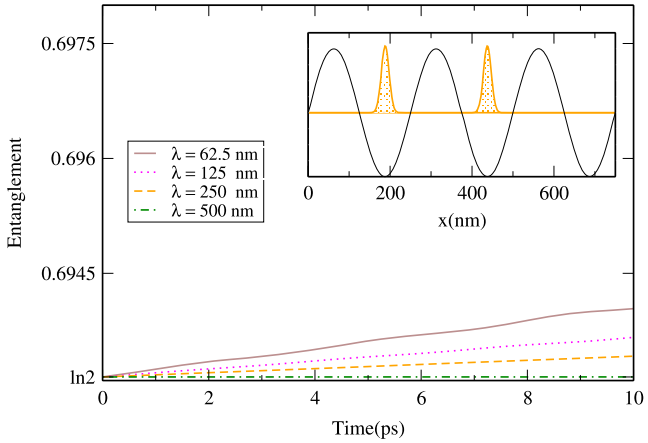

Figure 1. Entanglement dynamics of two electrons described at the initial time by Φ_0. Different values of the SAW potential wavelength λ are considered: 62.5 nm (solid line), 125 nm (dotted line), 250 nm (dashed line), and 500 nm (dash-dotted line). The inset shows the square modulus of the initial two-particle wavefunction describing the two electrons in two ground states of two next minima of the sinusoidal potential (thin black line). Note the scale on the vertical axis: the entanglement is almost constant in all the cases considered.

we obtain the two-particle density matrix $\rho(x_a, x_b, x'_a, x'_b) = \Phi_0^*(x_a, x_b)\Phi_0(x'_a, x'_b)$.[4] The latter is used to compute the one-particle reduced density matrix ρ_r, 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 ε_{vN}:

$$\varepsilon_{vN} = -\operatorname{Tr}[\rho_r \ln \rho_r] = -\sum_{i=1} |z_i|^2 \ln |z_i|^2, \quad (4)$$

where $|z_i|^2$ are the eigenvalues of the matrix ρ_r. As recently shown in the literature [11, 12], ε_{vN} provides a quantitative estimation of the entanglement in a pure-state system of two fermions and therefore it is an indicator of its non-separability into an antisymmetrized product of single-particle states. In this sense, the more entangled the quantum state is, the more unreliable the system dynamics computed in terms of single-particle states is. Thus the estimation of the possible appearance of quantum correlations created as a consequence of the Coulomb interaction between the charged carriers in our system turns out to be of great importance.

In order to illustrate with an example the relation between the errors incurred in the use of the single-particle approach and the appearance of quantum correlations, here we shall evaluate the von Neumann entropy of a simple two-fermion system in a state $|\Xi\rangle$ given by

$$\Xi(x_a, x_b) = \frac{1}{\sqrt{2}}\Bigg[\sqrt{1-\gamma^2}(\chi_1(x_a)\chi_2(x_b) - \chi_1(x_b)\chi_2(x_a)) + \sum_{k=2}^{M} a_k(\chi_{2k-1}(x_a)\chi_{2k}(x_b) - \chi_{2k-1}(x_b)\chi_{2k}(x_a))\Bigg], \quad (5)$$

[4] In our computational approach the spatial coordinate x of the electrons is discretized with a M-point grid, thus the dimension of the single-particle Hilbert space is M. This makes possible to define and evaluate numerically the density matrices in the x-space representation.

where the χ_ks are the states of an arbitrary orthonormal basis spanning the single-particle Hilbert space of dimension M and the real parameter γ is related to the coefficients a_k by $\gamma^2 = \sum_{k=2}^{M} |a_k|^2$. If the coefficients a_k are small so that $\gamma^2 \ll 1$, the second term in the right-hand side (rhs) of equation (5) can be considered as a perturbation that brings some correlation in the otherwise uncorrelated $|\Xi\rangle$ state. In fact, we observe that for $\gamma^2 = 0$ the state of equation (5) can be set in terms of a single Slater determinant

$$\tilde{\Xi}(x_a, x_b) = \frac{1}{\sqrt{2}}(\chi_1(x_a)\chi_2(x_b) - \chi_1(x_b)\chi_2(x_a)), \quad (6)$$

with no quantum correlations between the particles apart from the one due to the exchange symmetry. This means that $|\tilde{\Xi}\rangle$ can be written in terms of the two single-particle wavefunctions χ_1 and χ_2 suitably antisymmetrized. The amount of quantum correlation evaluated according to equation (4) is $\ln 2$. This value is related to the lack of knowledge only due to indistinguishability of the particles and therefore does not represent a manifestation of a 'genuine' entanglement [11, 12, 16]. On the other hand for $\gamma^2 \neq 0$, $|\Xi\rangle$ is given by a linear superposition of Slater determinants and after some calculations its von Neumann entropy can be written as

$$\varepsilon_{\mathrm{vN}} = \ln 2 - (1-\gamma^2)\ln(1-\gamma^2) - \sum_{k=2}^{M} |a_k|^2 \ln |a_k|^2. \quad (7)$$

Here $\varepsilon_{\mathrm{vN}}$ is larger than the minimum value $\ln 2$, thus indicating a 'genuine' entanglement.

Now we can relate $\varepsilon_{\mathrm{vN}}$, namely the number of quantum correlations in $|\Xi\rangle$, to the quantitative estimation of the errors incurred in the description of the system in terms of single-particle wavefunctions. In fact, the projection of the state $|\tilde{\Xi}\rangle$ on the state $|\Xi\rangle$ is

$$\int\int \mathrm{d}x_a\, \mathrm{d}x_b\, \tilde{\Xi}^*(x_a, x_b)\, \Xi(x_a, x_b) = \sqrt{1-\gamma^2}, \quad (8)$$

which, remarkably, is the same coefficient of the Slater determinant coming from the antisymmetrization of χ_1 and χ_2 in the rhs of equation (5). The expression (8) gives an estimation of how accurately $|\tilde{\Xi}\rangle$ can describe the state of a system where quantum correlations are present not only because of the exchange statistics. Since the factor $1-\gamma^2$ also appears in equation (7), a relation between the von Neumann entropy and the estimation of the effectiveness of a single-particle approach can be established. In particular we note that the less a description of the system by means of single-particle wavefunctions is accurate, the more $|\langle\tilde{\Xi}|\Xi\rangle|^2$ is far from 1 and the larger is $\varepsilon_{\mathrm{vN}}$.

3. Results

In figure 1, we report for different values of the wavelength λ of the sinusoidal potential, the time evolution of the entanglement evaluated by means of equation (4) for the system composed of two electrons initially in Φ_0 and mimicking SAW charge transport in GaAs quantum wires. At the initial time, no correlation is present, apart from that due to the exchange symmetry. As the time increases, the entanglement does not vary significantly (only a few per cent of the initial value), though it becomes higher for smaller wavelengths, as expected. We stress that the ordinate scale of figure 1 is very contracted. Since the entanglement between the electrons taken in the ground state of the potential minima remains essentially constant, one can immediately conclude that during the time evolution of the two-particle wavefunction the Coulomb interaction does not become sufficiently strong to build up significant quantum correlations between the two electrons. This implies that the time evolution of the system can be studied in terms of the dynamics of two non-interacting single-particle wavepackets, at least up to times of the order of tens of picoseconds.

Now we want to investigate the behavior of the entanglement when the electrons are, at the initial time, in excited eigenstates of the single-particle Hamiltonian of equation (2). This can help us to gain a better insight into the transport assisted by SAWs when the electrons are in higher-energy levels. To this aim we consider two different quantum states:

$$\Phi_n(x_a, x_b) = \frac{1}{\sqrt{2}}(\varphi_n(x_a)\varphi_n(x_b-\lambda) - \varphi_n(x_b)\varphi_n(x_a-\lambda)), \quad (9)$$

where $\varphi_n(x)$ is the nth excited eigenstate of the single-particle Hamiltonian of equation (2) with eigenvalue E_n, and

$$\tilde{\Phi}_n(x_a, x_b) = \frac{1}{\sqrt{2}}(\tilde{\varphi_n}(x_a)\tilde{\varphi_n}(x_b-\lambda) - \tilde{\varphi_n}(x_b)\tilde{\varphi_n}(x_a-\lambda)), \quad (10)$$

where $\tilde{\varphi_n}(x)$ is given by

$$\tilde{\varphi_n}(x) = \frac{1}{\sqrt{n+1}}(\varphi_0(x) + \cdots + \varphi_i(x) + \cdots \varphi_n(x)), \quad (11)$$

i.e. it is a linear combination of the lowest $n+1$ single-particle H_0 eigenstates with mean energy $\tilde{E}_n = (E_0 + \cdots + E_i + \cdots E_n)/(n+1)$. Again, Φ_n and $\tilde{\Phi}_n$ describe two electrons trapped into two next minima, but now they are in a single or a combination of excited states, respectively.

The results for these cases are reported in figures 2 and 3, where we show the evolution of the entanglement of two electrons initially in Φ_n and $\tilde{\Phi}_n$ respectively, for different values of n. We observe that when higher-energy states (corresponding to higher values of n) are involved, the quantum correlation is larger. Unlike the previous case, here the entanglement is not negligible and reaches values significantly different from the initial one, $\ln 2$, at times of the order of ten picoseconds. The reasons for this behavior can be related to the real-space two-particle wavefunction. As shown in the top panels of figures 2 and 3, 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. Note that a similar effect is present in the simulations of figure 1 as the λ is decreased. However in that case the SAW confinement is also reduced and the energy distance between bound states

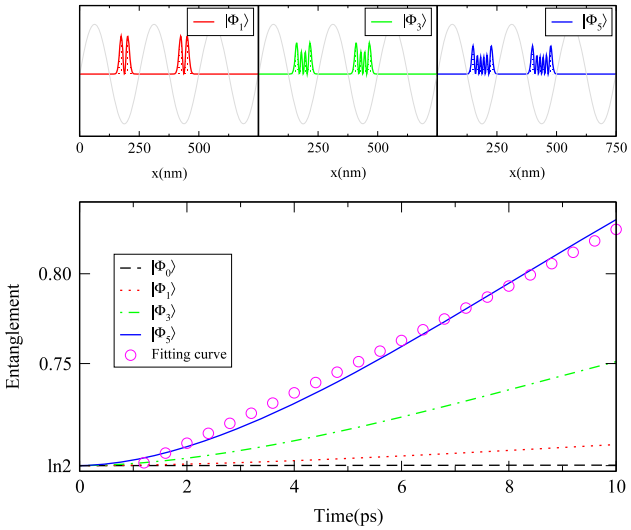

Figure 2. Top panel: single-electron probability density $\int |\Phi_n(x_a, x_b)|^2 \, \mathrm{d}x_a$ evaluated for $n = 1$ (left graph), $n = 3$ (middle graph), and $n = 5$ (right graph). The thin solid line sketches the sinusoidal potential. The amplitude of the oscillation is $\alpha = 50$ meV and the wavelength is $\lambda = 250$ nm, in order to mimic a SAW potential. Bottom panel: 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. The circles show the values of the function $A_0 \exp\{A_1 t\}$ fitting the time evolution of the entanglement of Φ_5. Here $A_0 = 0.68$ and $A_1 = 0.019 \times 10^{12}$ s^{-1}.

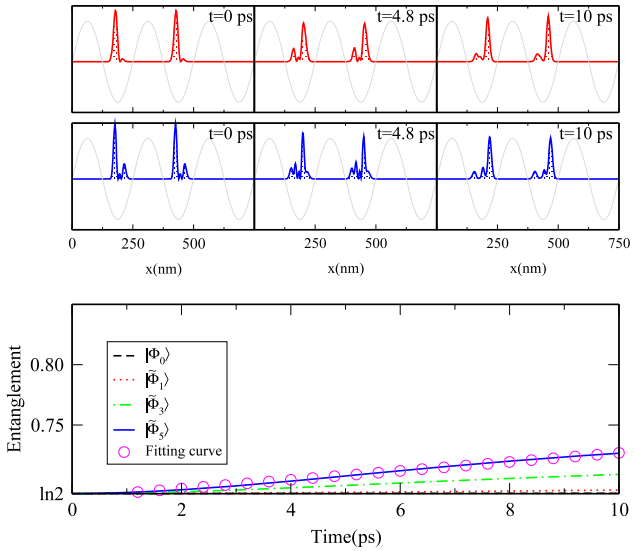

Figure 3. Top panel: single-electron probability density $\int |\tilde{\Phi}_n(x_a, x_b)|^2 \, \mathrm{d}x_a$ evaluated at different time steps for $n = 1$ (in the upper row of graphs) and $n = 3$ (in the lower row of graphs). The thin solid line sketches the sinusoidal potential. Bottom panel: entanglement dynamics of Φ_0 (dashed line) with $E_0 = -47.17$ meV, $\tilde{\Phi}_1$ (dotted line) with $\tilde{E}_1 = -44.35$ meV, $\tilde{\Phi}_3$ (dash-dotted line) with $\tilde{E}_3 = -38.83$ meV, and $\tilde{\Phi}_5$ (solid line) with $\tilde{E}_5 = -33.43$ meV. The circles show the values of the function $A_0 \exp\{A_1 t\}$ fitting the time evolution of the entanglement of $\tilde{\Phi}_5$. Here $A_0 = 0.69$ and $A_1 = 0.005 \times 10^{12}$ s^{-1}.

increases. This makes the wavefunction less sensitive to their mutual repulsion.

For electrons initially in the nth excited state of the SAW, the entanglement increase turns out to be larger than the one found for particles with energy $\tilde{E}_n < E_n$, described at the initial time by the linear superposition $\tilde{\varphi}_n(x)$. This behavior implies that moving from low-energy states to higher-energy states yields an entanglement enhancement. Since the function $A_0 \exp\{A_1 t\}$ fits well the entanglement dynamics of Φ_n and $\tilde{\Phi}_n$ evaluated numerically (see figures 2 and 3), we can reasonably assume that, as a first approximation, the entanglement rise in time is described by an exponential law and that such behavior also holds for longer times.

The above results suggest that for electrons captured in high-energy bound states of the SAW a description in terms of single-particle states is less and less accurate as time goes by. In particular, for times of the order of a few tens of picoseconds, as required for a single quantum operation in SAW-based quantum logic gates [17], only the low-energy bound carriers can safely be assumed to keep coherence, the effects of their mutual quantum correlations being negligible.

4. Conclusions

Acoustically driven single-electron transport constitutes a fundamental resource to produce a standard of electric current [1–4] and in the last few years it has also been recognized as a viable means to implement quantum gate networks in semiconductor nanodevices [5, 6, 8, 9]. Here, the assumption that the quantum transport assisted by SAW does not produce entanglement between two carriers in two different minima of the same wire plays a key role to ensure the functionality of logic quantum gates.

In this paper, we assessed the validity of the single-particle approximation in a peculiar model describing the SAW-driven propagation of electrons through a GaAs quantum wire. As we have shown in a theoretical toy-model of a pure two-fermion state, the validity of such an approximation is strictly related to the entanglement between the two particles. In particular, a description of the dynamics of the SAW charge transport in terms of single-particle wavepackets requires that the quantum correlations due to Coulomb interaction between the two carriers can be neglected during the evolution of the system. In this spirit we have evaluated by means of the von Neumann entropy the entanglement dynamics of two electrons with the same spin localized into two next minima of a standing SAW. In our investigation we have considered two different initial conditions: low-energy electrons occupying the ground state of the two next minima and high-energy electrons in bound excited states or in a linear combination of excited states.

The outcomes of our simulations suggest that the low-energy particles remain essentially uncorrelated during the time evolution of the systems. Therefore, in this case the description of the electron transport assisted by SAWs in terms of single-particle wavefunctions represents an acceptable approximation. On the other hand, for high-energy electrons, SAWs are less efficient at preventing the spread of the spatial

wavepackets, and the entanglement due to the Coulomb interaction between carriers turns out to be significant even after a few picoseconds. This time represents the timescale required experimentally for quantum computing operations [17]. In this context the observation of quantum effects related to the coherent single-electron regime, such as the single-particle interference, will be limited by the appearance of quantum correlations destroying the coherence of single carriers.

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