Simulation of entanglement dynamics for a scattering between a free and a bound carrier in a quantum wire

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We present a numerical analysis of the creation of entanglement between an electron freely propagating along a quantum wire and a charged particle bound to a specific site by a harmonic potential. The latter can be considered as a simplified model of an ionized impurity with an internal sctructure or of a localized phonon mode. Its dynamics is coupled to that of the free electron through a screened Coulomb potential.

The time-dependent Schrödinger equation is solved numerically for the two-particle wave function [1] thus describing the coherent evolution of the bipartite system (see Fig. 1). The two particle are considered distinguishible. As initial condition the product of a minimum uncertainty wave packet and the ground state of the harmonic oscillator is considered:

$$\Psi(x_A,x_B)=\frac{1}{\left(\sqrt{2\pi}\sigma_A\right)^{1/2}}\exp\left(-\frac{\left(x_A-\langle x_A\rangle\right)^2}{4\sigma_A^{\,2}}+i\langle k_A\rangle x_A\right)\cdot\left(\frac{m\omega}{\pi}\right)^{1/4}\exp\left(-\frac{m\omega x_B^{\,2}}{2}\right)$$

with σ_A, $\langle x_A\rangle$ and $\langle k_A\rangle$ mean dispersion, position and wave vector of the free electron, ω and m energy and mass of the harmonic oscillator. The above initial condition represents a pure separable state. The coupling effect of the Coulomb interaction during the evolution can be seen from a two-particle or from a single-particle perspective. In the first case the two particles get entangled and the pure state described by $\Psi(x_A,x_B)$ becomes not separable in the two particle subspaces. In the second case, i.e. tracing over the degrees of freedom of one particle (thus considered as the environment), the state of the other has to be described in terms of a density matrix representing a mixed state, since the interaction induces decoherence. As a consequence, the amount of entanglement between the two subsystems quantifies the amount of decoherence of one of the subsystems, when the other is considered as the environment [2].

The entanglement between the particles is evaluated numerically at several time steps of the quantum evolution as the von Neumann entropy of the reduced density matrix [3]. As an example in Fig. 2 the time evolution of the entanglement for different values of the free-electron initial energy E_A is presented. After the scattering, the entanglement reachs a stationary value that exibits a dependence from the initial kinetic energy of the free electron and its initial dispersion σ_A. This computational scheme allows a quantitative evaluation of the decoherence undergone by a carrier in a single unelastic scattering.

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A full journal publication of this work will be published in the Journal of Computational Electronics.

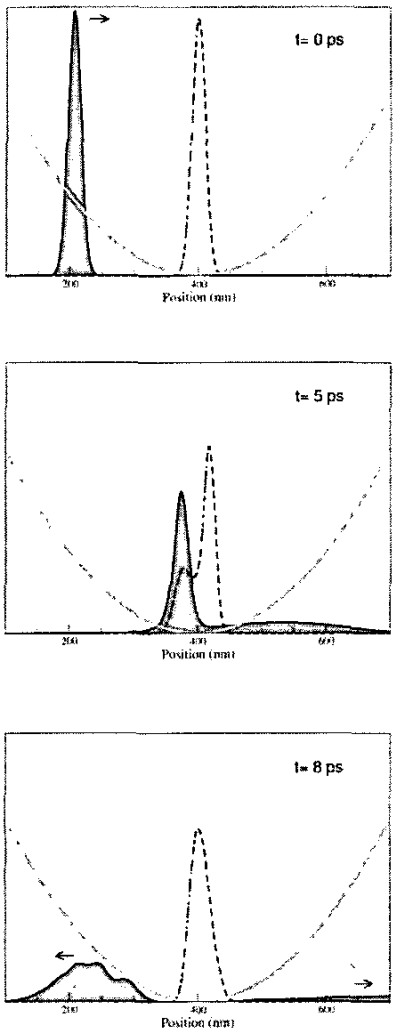

FIG. 1. Particle density at three different time steps. The solid line, and the shaded area below, represents the expression: $\int\left|\Psi\left(x_A,x_B\right)\right|^2 dx_B$, while the dashed curve represents the expression: $\int\left|\Psi\left(x_A,x_B\right)\right|^2 dx_A$. The grey solid line sketches (in qualitative way) the harmonic potential. In the initial condition the mean dispersion σ_A and the kinetic energy of the freely propagating electron are 20 nm and 5 meV respectively, the mass of the harmonic oscillator is m=0.32 m_0 (where m_0 is the electron rest mass), and $\hbar\omega$ is 1 meV.

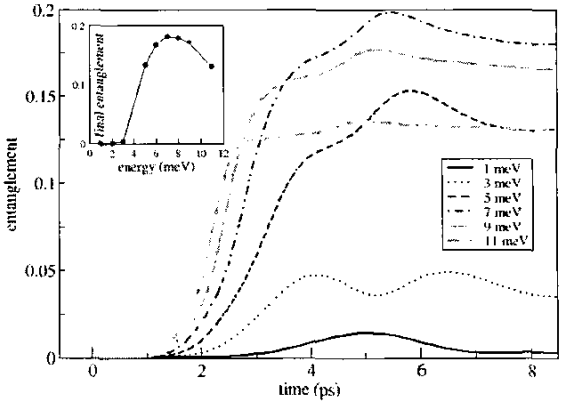

Fig. 2. Entanglement as a function of time at different values of the initial kinetic energy (ε_A) of the freely propagating electron, for an initial mean dispersion σ_A=20 nm. The inset shows the stationary values of the entanglement at different values of ε_A for σ_A=20 nm.

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