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Simulation of the Entanglement Creation for Identical Particles Scattering in a 2D System

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We study, by means of a time-dependent numerical analysis, the entanglement between an electron freely propagating in a 2D system and another electron bound to a specific site by a harmonic potential. This physical system can be used as guideline to analyze the entanglement formation in the case of a carrier-impurity scattering event in bulk semiconductors. The dynamics of the bound particle in the harmonic potential is coupled to the incoming particle through a screneed Coulumb potential.

The above model has been already studied for a system of two distinguishable particles[2]. The aim of this work is to overcome this restriction taking into account the issues arising fro the indistinguishability of the particles. Some theoretical questions about the notion and the evaluation of the entanglement between indistinguishable particles are adressed. In the present work we use a criterion, given by Schliemann, based on the Schmidt decomposition theorem for the state $|\Psi_F\rangle$ of two fermionic particles [3], [4]. Through an unitary transformation the antisymmetric wavefunction is expressed into a basis of N Slater determinants with a minimum number of non vanishing 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^f as:

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

with

$$\rho^f_{\mu\nu} = \frac{\mathrm{Tr}[\rho_F f^\dagger_\nu f_\mu]}{\mathrm{Tr}[\rho_F \sum_\mu f^\dagger_\mu f_\mu]} \quad (2)$$

where ρ_F is two particles density matrix $\rho_F = |\Psi_F\rangle\langle\Psi_F|$ and $2N$ is the dimension of the single particle Hilbert space and corresponds, in the present case, to 2 times the number of discretization points in the space degree of freedom.

In our approach we solve numerically the time-dependent Schroedinger equation for the wavefunction of the system by means of a Crank-Nicholson finite difference scheme. From such wavefunction we calculate the one-particle reduced density matrix, related to each initial state, at different time steps. In order to calculate at any time, the entanglement by means of the von Neumann entropy from (1), we need to diagonalize the one-particle reduced density matrix ρ^f. This procedure turns out to be extremely demanding from the point of view of the numerical calculation. In fact these matrices are dense and tipically of the order of 10^{10} complex elements. Such a numerical problem has been faced by resorting to a parallel algorithms for matrices diagonalization. As a reference, a typical a simulation runs for 8 hours on 128 CPUs on a IBM-SP5 machine. As an example in Fig. 1 we show the evolution of the entanglement for the state with two electrons having same spin at three different values of the incoming electron initial energy, namely 10, 20, 30 meV, when the harmonic trap energy is $\hbar\omega = 2meV$. As the particles get closer their quantum correlation builds up and entanglement reaches a stationary value once scattering event is completed. From the square modulus of the two-particle space wavefunction before and after the scattering event (Fig. 2), we can evaluate the role played in entanglement creation by the correlations between the spatial degrees of freedom.

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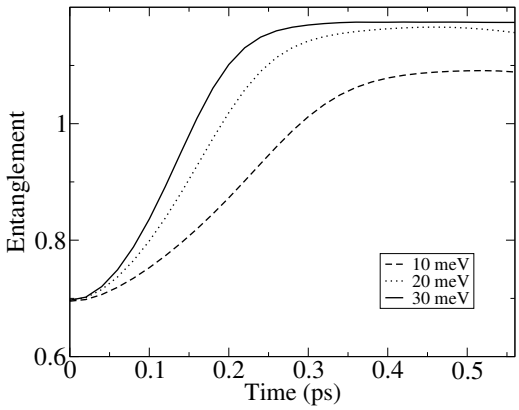

Fig. 1. The time evolution of entanglement for the state $|\Psi_F\rangle$ at three different values of the incoming electron initial energy when the harmonic oscillator energy is $\hbar\omega = 2meV$

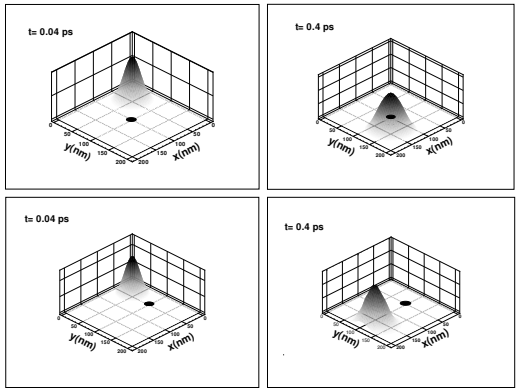

Fig. 2. Square modulus of the two-particle antisymmetrized wavefunction $\psi(\mathbf{r})\,\phi(\mathbf{R}) - \phi(\mathbf{R})\,\psi(\mathbf{r})$ for $|\Psi\rangle$ at two different times before($t = 0.04$ ps) and after ($t = 0.4$ ps) scattering, calculated keeping fixed at a specific value **R** (black spot) the position of one of the two particles. In the two upper graphs **R**=(100 nm,100 nm), while in the two lower graphs **R**=(50 nm,150 nm)

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