Entanglement dynamics of a two-particle scattering in pulsed sinusoidal potentials

F Buscemi$^{1,2}$, P Bordone$^{3,2}$ and A Bertoni$^2$

$^1$ ARCES, Alma Mater Studiorum, University of Bologna, Via Toffano 2/2, 40125 Bologna, Italy
$^2$ S3 Research Center, CNR-INFM, Via Campi 213/A, I-Modena 41100, Italy
$^3$ Dipartimento di Fisica, Università di Modena e Reggio Emilia, I-41100 Modena, Italy

E-mail: fabrizio.buscemi@unimore.it

Abstract. We study by means of time-dependent numerical simulations the behavior of the entanglement stemming from the Coulomb scattering between two charged particles subject to a pulse of sinusoidal potential. We show that the splitting of the spatial wavefunction brought about by the interaction with the potential pulse plays a key role in the appearance of quantum correlation, thus leading under specific conditions to a peculiar behavior. The dependence of the final entanglement upon the physical parameters describing the pulse is discussed. Our results can be applied to a number of physical systems, such as electron-electron scattering in semiconductors or cold-ions dynamics in external fields.

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1. Introduction

Quantum entanglement between two spatially separated particles can be created as a consequence of their non local mutual interactions [1] [2]. In particular, entangled states are produced from the collision between two charged particles interacting via 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 pure 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 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 [3], on the other hand entanglement with the environment (i.e. decoherence) represents the main threat to the proper functioning of a feasible quantum computer [4]. For those reasons, the study of the entanglement dynamics in scattering
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Events have become more and more relevant in recent years\cite{5, 6, 7, 8} and different proposals to produce entangled states between charged carriers in solid-state systems have been presented\cite{9, 10, 11}.

In this work, we analyze the time evolution of the entanglement during the scattering of two particles in presence of an external periodic potential. Our model and results are representative of a broad variety of situations in which two interacting carriers are constrained in a quasi-1D domain and a sinusoidal-like potential is present. Such kind of systems are of interest in different areas of physics, such as condensed matter\cite{12}, quantum optics\cite{13} and astrophysics\cite{14}. In particular, great attention has been devoted to the scattering of an electron beam by a standing wave of light (the so-called Kaptiza-Dirac effect)\cite{15}, stemming from the possibility of using such a system to investigate the wave nature of electrons. The latter model of matter-field interaction also raises conceptual and theoretical issues about the momentum exchange between electrons and electromagnetic radiation\cite{16, 17, 18, 19}, which can be generalized to fields other than quantum optics.

The focus of the present work is on the creation of quantum entanglement between two interacting electrons, in the presence of a further external periodic potential. The two particles are explicitly considered as indistinguishable and have the same spin. Specifically, we simulate numerically a two-particle scattering in a 1D structure and determine how the tailoring of a standing pulse of sinusoidal potential is able to affect electron-electron correlation. Here we intend to move a step forward in the investigation of the entanglement formation in electron-electron scattering processes, recently addressed by many works\cite{5, 6, 7, 20}. We analyze how the momentum exchange between the particles affects the entanglement arising in the binary collision, and how the inclusion of a potential oscillating in space modifies the entanglement dynamics. To this aim we tackle the problem by solving numerically the time-dependent two-particle Schrödinger equation and by computing, at each time step, the bipartite entanglement. Such an approach allows us to investigate also the case of a non-adiabatic switching on/off of the potential, that would make analytical techniques not applicable.

The paper is organized as follows. In Sec. 2, to better introduce our model system, we study the dynamics of a free electron that is subject to a sinusoidal potential only for a small time interval. In Sec. 3 we evaluate the entanglement generated in a collision between two electrons subject to a pulsed potential. We comment on the results and draw final remarks in Sec. 4.

2. Single-particle system

In this section we study the dynamics of a free electron propagating in a quasi-1D system and subject to a single pulsed sinusoidal potential. Our aim is to investigate the role played by the sine-like time-dependent potential in the time evolution of a simple single-particle wave function. The results will be of help in understanding the two-particle dynamics of the following section.
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The single particle is described at the initial time $t_0 = 0$ by a minimum uncertainty wave-packet, with the following wave function

$$\psi(x, t_0) = \frac{1}{(\sqrt{2\pi}\sigma)^{1/2}} \exp\left(-\frac{(x - x_0)^2}{4\sigma^2} + \frac{i}{\hbar}p_{in} \cdot x\right)$$

(1)

where $\sigma$ is the mean dispersion in position and $p_{in}$ the initial momentum.

The particle feels a pulsed sine-like potential, and the Hamiltonian of the system takes the form

$$H_{on-off}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + A \sin(k_0 x) \Theta(t - t_{on}) \Theta(t_{off} - t)$$

(2)

where $m$ is the particle mass, $A$ the amplitude of the potential oscillation, $k_0$ its the wavenumber and $\Theta$ the Heaviside function, with $t_{on}$ and $t_{off}$ the times of turning on and off of the potential, respectively.

We note that the time-dependent Hamiltonian of Eq. (2) has the same form of the one used to describe the scattering of an electron by a standing light wave. Such an interaction has been widely studied both from the theoretical and the experimental points of view[16] [17] [18] [19], beginning with the the original work by Kaptiza and Dirac[15]. In the literature, the standing light electromagnetic potential is taken as a superposition of two counterpropagating travelling waves of identical frequency and the characteristic times of the scattering process are assumed to be much longer than the period of the wave. As a consequence, the approximation of time-average Hamiltonian can be used, thus leading to the so-called ponderomotive potential oscillating in space[16] [19].

Some peculiar aspects of the interaction between the electron and the sinusoidal wave can be understood by analyzing the dynamics of the single-particle wavefunction in the momentum representation $\phi(k, t)$, the latter being the Fourier transform of the real-space wave function $\psi(x, t)$, with $k = p/\hbar$. At the initial time, $\phi(k, t_0)$ is given by a Gaussian wavepacket with a mean dispersion $1/\sigma$ centered around $k_{in} = p_{in}/\hbar$. Let us now introduce the wavefunction $\varphi(k, t)$ in the interaction picture

$$\phi(k, t) = \exp\left(-\frac{i\hbar k^2}{2m} t\right) \varphi(k, t).$$

(3)

Its time evolution can be evaluated by inserting Eq. (3) into the Schrödinger equation of the system, whose Hamiltonian is given in Eq. (2) for $t_{on} \leq t \leq t_{off}$. Straightforward calculations lead to the following recurrence relation[18] [19]:

$$\frac{\partial}{\partial t} \varphi(k, t) = -\frac{A}{2\hbar} \exp\left[i\left(\frac{\hbar k_0}{m} - \frac{\hbar k^2}{2m}\right) t\right] \varphi(k - k_0, t)$$

$$+ \frac{A}{2\hbar} \exp\left[-i\left(\frac{\hbar k_0}{m} + \frac{\hbar k^2}{2m}\right) t\right] \varphi(k + k_0, t).$$

(4)

This represents the dynamical equation for $\varphi(k, t)$ due to the interaction between the particle and the sinusoidal potential. The two terms appearing in the rhs of the Eq. (4) have a clear physical meaning: the interaction with a potential oscillating in space allows
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Figure 1. (a) Square modulus of the single-electron wave function $\psi(x)$ at the initial time. The inset shows the square modulus of its Fourier transform $\phi(k,0)$. (b) Top panel: square modulus of the electron wave function $\psi(x)$ (dashed line) at $t=1.3$ ps, for a pulse duration $\Delta\tau_1=0.1$ ps. Bottom panel: same as top for $\Delta\tau_2=0.2$ ps. In both cases $t_{on}=1$ ps. (c) Comparison of the square modulus of the two electrons wavefunctions at $t=2.8$ ps, i.e. after the pulse, for $\Delta\tau_1$ (dashed line) and $\Delta\tau_2$ (dotted line). The inset displays their Fourier transforms. In these numerical calculations we have taken $m=2.91 \times 10^{-31}$ Kg, $\sigma=10$ nm, $k_0=0.46$ nm, $k_{in}=0.205$ nm and $A=6.11$ meV. They are the physical parameters which could describe electron transport in low dimensional semiconductor structures. Note the logarithmic scale, adopted for clarity.

Under some specific conditions, approximate analytical solutions of Eq. (4) can be obtained[17, 18, 19]. However, for the sake of generality, we face the problem numerically by solving the time-dependent Schrödinger equation for the electron real-space wavefunction by means of a Crank-Nicholson finite difference scheme. In Fig. 1 we report the square modulus of the wavefunction $\psi(x,t)$ given in Eq. (1) at three different time steps and for two different pulse lengths $\Delta\tau = t_{off} - t_{on}$, namely $\Delta\tau_1=0.1$ ps and $\Delta\tau_2=0.2$ ps. In both cases the sine potential is turned on at $t_{on}=1$ ps. The sinusoidal potential is included in the time evolution of the system for the duration $\Delta\tau$ of the

the particle to change its momentum by an integer number of $\pm \hbar k_0$. This consideration will turn out to be fundamental to explain our results.
pulse. From panel (b) we observe that shortly after $t_{off}$ the wavepacket is not described by a smooth function anymore, but exhibits rapid oscillations. Their appearance can be ascribed to the instantaneous potential switching off giving rise to a large energy uncertainty. However such oscillations are less pronounced at longer times owing to the natural spreading of the wavefunction. The latter results to be split in three peaks, as can be seen from panel (c). In order to understand this behaviour we need to analyze the dynamics of the momentum wave function $\phi(k, t)$, whose square modulus, after the pulse of sinusoidal potential, shows three peaks (see the inset of panel (c) of Fig. 1): one is still centered in $k_{in}$, while the other two are centered in $k_{in} + k_0$ and $k_{in} - k_0$. This suggests us that, for the sinusoidal pulses of length $\Delta \tau_1$ and $\Delta \tau_2$, the particle is scattered by the potential and its momentum can be possibly increased or decreased by $\hbar k_0$, in perfect agreement with the prediction of Eq. (4). Specifically, the $\Delta \tau$ used in this work can be considered sufficient to induce a variation of $\hbar k_0$ in the electron momentum, while the transfer of larger multiples of $\hbar k_0$ has a very small probability, as revealed by the negligible amplitude of the corresponding peaks in the momentum representation (not included in Fig. 1).

Thus, for pulses of duration $\Delta \tau_1$ and $\Delta \tau_2$, the splitting of the wavefunction into three peaks after $t_{off}$, has an immediate physical interpretation. The central peak gives the free evolution of the electron with momentum $p_{in}$ while the other two describe the single-particle free dynamics with momentum $p_{in} + \hbar k_0$, the “accelerated component” and $p_{in} - \hbar k_0$, the “reflected component”. For both pulse lengths the peak corresponding to the acceleration is smaller than the one giving the reflection. This asymmetry can be related to the form of the dynamical equation for the momentum wave function $\phi(k, t)$ given in the Eq. (4). Here, the two terms describing the addition and the subtraction of the momentum $k_0$ contain the factors $\exp[-i (\hbar k_0 \bar{m} + \hbar k_0^2/2m) t]$ and $\exp [i (\hbar k_0 \bar{m} - \hbar k_0^2/2m) t]$: the former oscillates in time more rapidly than the latter and therefore its integration gives a smaller contribution to $\phi(k, t)$.

3. Electron-electron entanglement

We now focus on the entanglement created in a two-electron scattering. The two particles interact via the Coulomb repulsion and are subject to a sinusoidal pulse, as described in the previous section. Since the entanglement formation in 1D- and 2D-scattering events between two unbound and/or trapped particles has been recently investigated [5, 6, 20], it appears of interest to study the building up of quantum correlations in such systems when a time-dependent external potential is introduced.

Here, the two interacting particles run in opposite directions along a 1D structure. The external sinusoidal potential is switched on at $t_{on}$ and for a time interval $\Delta \tau$. The Hamiltonian of the system reads

$$H(x_a, x_b) = H_{on-off}(x_a) + H_{on-off}(x_b) + \frac{e^2}{\epsilon \sqrt{(x_a - x_b)^2 + d^2}} (5)$$
where $H_{on-off}$ is the single-particle Hamiltonian given in Eq. (2), $\epsilon$ is the dielectric constant and $d$ represents the cut-off of the Coulomb interaction.

The two carriers have the same spin (up) and are obviously indistinguishable, so that the quantum state describing the system is given by

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|\psi\phi\rangle - |\phi\psi\rangle) |\uparrow\uparrow\rangle,$$

(6)

where both the wavefunctions corresponding to the states $|\psi\rangle$ and $|\phi\rangle$ are of the type defined in Eq. (1). The initial spread of the wavepackets and the distance between their centers are such that the Coulomb energy of the system is negligible at initial time. In Eq. (6) the ket $|\uparrow\rangle$ indicates spin up state.

To obtain the system evolution we solve the time-dependent Schrödinger equation for the two-particle wavefunction of Eq. (6). Once the real-space wavefunction is found at a given time step, we compute the two-particle density matrix $\rho = |\Psi\rangle\langle\Psi|$ and from the latter we calculate the one-particle reduced density matrix $\rho_r$ by tracing over the degrees of freedom of one of the two electrons. $\rho_r$ is then used to evaluate the entanglement. In fact, it is well known that for a two-fermion system a good correlation measure is given by the von Neumann entropy of $\rho_r$ [20, 21]:

$$\varepsilon = -\text{Tr}[\rho_r \ln \rho_r] = \sum_{i=1} |z_i|^2 \ln |z_i|^2,$$

(7)

where $|z_i|^2$ are the eigenvalues of the matrix $\rho_r$.

As in the previous section, we consider pulses 0.1 ps and 0.2 ps long. This implies that each of the two carriers can gain or lose $\hbar k_0$ in its momentum and the corresponding wavefunction splits into three peaks. In Fig. 2 and 3 we report the time evolution of the entanglement for $\Delta\tau_1 = 0.1$ ps and $\Delta\tau_2 = 0.2$ ps respectively, for different values of $t_{on}$, i.e. the time at which the pulse is switched on. Since the electron-electron interaction builds up quantum correlations in a limited time interval (roughly corresponding to the width of the entanglement peak when no pulse is present: the solid line in Fig. 2 and 3) it is clear that by choosing different $t_{on}$ one means to consider cases with the potential pulse taking place before ($t_{on} = 0$), during ($t_{on} = 0.4$ and $t_{on} = 0.7$), and after ($t_{on} = 0.9$) the scattering.

At the initial time, the von Neumann entropy is equal to $\ln 2$. This value is related to unavoidable quantum correlations due to the exchange symmetry and it does not represent a manifestation of a genuine entanglement [20, 21].

In absence of pulse, the entanglement increases while the two electrons are approaching each other, it has a maximum when the centers of the two wave packets are at the minimum distance, and finally drops again to the initial value once the electrons get far apart. In this case, due to the small thickness of the quantum wire, the effective Coulomb interaction between the electrons is sufficient to cause a complete reflection of the two particles and the corresponding Gaussian wave packets are reconstructed with opposite momenta, as can be seen from the top panel of Fig. 4.

‡ The values of the physical parameters used in the calculation refer to a 1D scattering model in a silicon quantum wire of width $d$, but the results obtained are representative of a more general behaviour.
Figure 2. Entanglement vs. time for different initial times of the pulse $t_{on}$. Here the pulse duration is $\Delta \tau_2 = 0.2$ ps. At the initial time the two electrons have the same kinetic energy $E_k = 10$ meV corresponding to $|k_{in}| = 0.290$ nm$^{-1}$ and are described by two wavepackets with mean dispersion $\sigma = 10$ nm moving in opposite directions. The filled circle on the curves indicate the four different $t_{on}$ times. The inset shows the stationary values of the entanglement as a function of $t_{on}$.

Figure 3. Same as Fig. 2 with a pulse duration $\Delta \tau_1 = 0.1$ ps.
When the two particles are subject to a pulsed sinusoidal potential, the entanglement dynamics depends strictly upon the details of the potential switching on and off. For example, for $\Delta t_2 = 0.2 \text{ ps}$ and $t_{on} = 0 \text{ ps}$, the peak of the entanglement is lower than the one found with no pulse. This is a consequence of the interaction with the sine-like potential that splits the wave function of each particle before the effect of the Coulomb potential becomes significant. Thus, the two reflected components will not take part into the scattering process and will not contribute to the entanglement formation (see Fig. 4). After the peak, for $t_{on} = 0.4 \text{ ps}$ the entanglement does not vary significantly with time, while in the case $t_{on} = 0$ it appears to increase. Such a difference can be ascribed to the fact that the splitting of the wavefunction can be or be not completed when the Coulomb interaction gets its maximum value.

For the last two cases of Fig. 2, $t_{on} = 0.7 \text{ ps}$ and $t_{on} = 0.9 \text{ ps}$, the time evolution of the entanglement turns out to be quite peculiar. After the peak (due to the Coulomb scattering) the entanglement exhibits the same decrease as in the case without pulse, up to $t_{on}$, when the pulse is switched on. At the latter time, the wave function describing each electron is almost entirely reflected and splits in various peaks, as described above. Two of these, namely the components “reflected” by the pulse, propagate in opposite directions and approach each other. As a consequence, Coulomb interaction becomes...
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effective again and gives rise to a second increase of the entanglement.

We report in Fig. 3 the results for $\Delta \tau_1 = 0.1$ ps showing a behaviour similar to the previous case, with few, through significative, differences. Specifically, for $t_{on} = 0$ ps we observe that the entanglement shows a peak higher than the one found in absence of the pulse. This behavior is different from the one found for $\Delta \tau_2$ and can be ascribed to the diverse way of splitting of the two particle wavefunction in the two cases, as described in Sec. 2. Nevertheless we note that for $t_{on} = 0.7$ ps, after the peak (as high as the one found in absence of the external pulse) the entanglement decreases until $t_{on}$ and then slowly increases, in qualitative agreement with the results obtained for $\Delta \tau_2$.

Some time after the Coulomb interaction and the pulse, the entanglement reaches a stationary value. This value is displayed in the insets of the Fig. 2 and 3 as a function of $t_{on}$. We observe that the largest final entanglement is always found when $t_{on} = 0$. In this case the wave functions split before the scattering and both the “accelerated” components of the electron and the central peaks, interact strongly during the Coulomb scattering.

Taking into account the results obtained in absence of pulse, we can therefore assume that the stationary values of the entanglement depend upon the transmission in the scattering event: they are greater for greater transmission probability of the particles. This is in qualitative agreement with the results of the theoretical investigations on the entanglement dynamics in scattering events in 1D semiconductor structures [7, 22].

4. Summary and conclusions

The growing interest in the entanglement phenomena [1, 2, 5, 6, 9, 10, 11] led us to analyze the electron-electron entanglement dynamics of a two-particle scattering in a study model that has important applicative perspectives but whose simplicity makes it of general interest. In particular, the appearance of quantum correlations between two colliding electrons is a direct consequence of their mutual Coulomb repulsion during the scattering event, while the external periodic potential represents a mean to tailor the electron-electron interaction and to localize the particles. We stress that the equations of motion of the system under study are the same that describe the scattering of electrons by a standing laser wave [16, 17, 18, 19], where the particles can change their momentum by an integer multiple of $\hbar k_0$, with $k_0$ the wave vector of the real-space modulation of the potential. Our single-particle time-dependent simulations show directly how the momentum gain or loss is affected by the switching-on time of the sinusoidal potential. In particular the use of pulses in the range of few tenths of picoseconds leads to a variation of a single $\hbar k_0$ quantum in the momentum of the particle.

The issues described above allowed us to explain the entanglement behavior in a two-electron scattering and our two-particle simulations gave a direct insight on the origin of the correlations. In fact, we showed that the non-separability of the two-particle state is mainly originated by the splitting of the spatial wave function brought
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about by the interaction with the potential pulse. As a matter of fact, our results show that the two particles get more correlated for longer pulses while entanglement dynamics depends closely upon the time of turning on of the potential. Moreover, the time of the entanglement formation, i.e. the time at which the entanglement reaches its stationary value, is strictly related to the time of the initial switching-on of the sinusoidal potential. On the other hand, the final value of the entanglement depends upon the ratio between the transmitted and the reflected components of the wave function\[7, 22\]. We stress that the above finding shows that the final entanglement will be maximum for the specific system parameters that maximize the splitting of the wave function after the scattering.

Finally, we note that the simplicity of the model here investigated makes it of general interest. In this spirit we think that our results can be valid guidelines to analyze some phenomena related to the appearance of quantum correlations in various physical systems and have important applicative perspectives. The use of a sinusoidal potential could provide a way to produce and control the electron decoherence due to carrier-carrier collision in low-dimensional semiconductor structures. Moreover our model could be viewed as a prototype system to study the building up of quantum correlations into electron transport assisted by surface acoustic waves through quantum wires since they are modelled as a sinusoidal travelling electric potential which traps the carriers in its moving minima. The results shown here could also be helpful to investigate the entanglement formation in the collision event of ions trapped in quasi 1D-structures and subject to a laser pulse.

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