Time dependence of quantum entanglement in the collision of two particles

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Abstract
We follow the emergence of quantum entanglement in a scattering event between two initially uncorrelated distinguishable quantum particles interacting via a delta potential. We calculate the time dependence of the Neumann entropy of the one-particle reduced density matrix. Using the exact propagator for the delta potential, we derive an approximate analytic formula for the asymptotic form of the two-particle wavefunction which is sufficiently accurate to account for the entanglement features of the system.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Quantum entanglement has become an important research topic in modern physics, not only because it exhibits the striking differences from classical concepts, but also because it is widely considered now as the fundamental resource in quantum information theory. Although the first famous paradox connected with entanglement [1] was presented in the context of observables with continuous values, the specific entanglement properties of such systems [2–5] are less explored than those with discrete, e.g., spin states.

Recent studies of continuous variable quantum systems focus on the emergence of bipartite entanglement in a scattering event of two interacting distinguishable quantum particles, which have no initial correlations [6–11]. Since this is a fundamental process in quantum physics, it is important to explore how it generates quantum entanglement. Some general features of this process were identified in [12, 13]. References [14, 8, 10] considered specific models on the scattering of ultracold atoms trapped in a harmonic potential well. Important results on the entanglement of colliding particles, modeled by Gaussian wave packets and interacting with different finite-range potentials, were published in [15, 6, 11, 7, 16, 13].
In this work, we consider the explicit time dependence of entanglement in a quantum mechanical model of a collision process with a continuous spectrum, which itself creates entanglement during the interaction between two particles that were independent in the beginning. To be specific, we assume a non-relativistic one-dimensional motion with an attractive or repulsive delta potential between the particles. The evolution of the process is described by the explicit solution of the time-dependent Schrödinger equation. Although this problem has been considered previously, here we derive analytic expressions for the post collision behavior that incorporates the spread of the individual wave packets, using the exact propagator for the delta potential [17, 18]. To quantify the entanglement, we use the Neumann entropy [19] and show how it is built up during the collision. The asymptotic value of the entropy is then obtained from our analytic expression of the long time limit of the time-dependent two-particle wavefunction. This study may find an application, e.g., in the experimental analysis of collision and recollision of atomic fragments following a laser-induced dissociation [20].

2. Interaction of two particles via a delta potential

The Hamiltonian of the system is written in terms of the position and momentum operators of the particles as

\[ H_{12} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} - V_0 \delta (X_1 - X_2). \]  

For an attractive (repulsive) interaction, we have here \( V_0 > 0 \) (\( V_0 < 0 \)). We introduce, as usual for two-body problems, the operators

\[ X_0 = \alpha_1 X_1 + \alpha_2 X_2, \quad P_0 = P_1 + P_2 \]  

\[ X = X_1 - X_2, \quad P = \alpha_2 P_1 - \alpha_1 P_2 \]  

resulting in a sum of two independent Hamiltonians corresponding to the center-of-mass motion and the relative motion

\[ H_{12} = H_0 + H, \quad H_0 = \frac{P_0^2}{2m}, \quad H = \frac{P^2}{2\mu} - V_0 \delta (X). \]  

Here, \( m = m_1 + m_2 \) is the total mass of the particles, \( \alpha_i = m_i/m \) and \( \mu = m_1 m_2 / (m_1 + m_2) \) is the reduced mass of the system. In the center-of-mass reference frame, the expectation value of \( P_0 \), the total momentum of the particles, is zero and the natural coordinate system is the one which has its origin in the expectation value of the center-of-mass operator \( X_0 \). Then, \( \langle P_0 \rangle = 0 \) and \( \langle X_0 \rangle = 0 \) for all times. We shall proceed using coordinate wavefunctions and assume that initially the particles are described by a product of the normalized Gaussians

\[ \Psi(x_1, x_2, t = 0) = \psi_1(x_1)\psi_2(x_2) \]  

\[ = \frac{(\alpha_1 \alpha_2)^{1/4}}{\sqrt{\pi}} e^{-\alpha_1 (x_1 + a_1)^2/2\sigma^2} e^{ia_1 x_1} e^{-\alpha_2 (x_2 + a_2)^2/2\sigma^2} e^{ia_2 x_2} \]  

localized at distant points around \( -a_1 = -\alpha_2 a \) and \( a_2 = \alpha_1 a \) as required by \( \langle X_0 \rangle = 0 \). From \( \langle P_0 \rangle = 0 \), we also have \( -k_2 = k_1 = q \). In terms of the center of mass and relative coordinates \( x_0 \) and \( x \), this wavefunction takes the form

\[ \Psi(x_1, x_2, t = 0) = \Phi(x_0, x, t = 0) = \psi_1(x_0)\psi_2(x), \]
where
\[ \varphi_{0}(x_{0}) = \sigma^{-1/2} \pi^{-1/4} e^{-x_{0}^{2}/2\sigma^{2}}. \] (8)
\[ \varphi_{1}(x) = (\alpha/\sigma)^{1/2} \pi^{-1/4} e^{-\alpha^{2}(x+\alpha t)^{2}/2\sigma^{2}} e^{i\alpha t}. \] (9)
are the normalized functions of \( x_{0} \) and \( x \), respectively, \( \alpha = a_{1} + a_{2} \) is the mean value of the distance between the particles and \( \sigma^{2} = a_{1}a_{2} = \mu/m \).

The separability of the wavefunction in terms of the coordinates \( x \) and \( x_{0} \) is due to the specific choice of the initial wavefunction [15, 6, 16, 13, 12], where the variances of the positions of the individual particles \( (\Delta X)^{2} \) obey \( m_{1}(\Delta X_{1})^{2} = m_{2}(\Delta X_{2})^{2} \). In a more general case, one has a double sum of products of arbitrary basis functions in the new variables, which could still be transformed into a single sum in the Schmidt bases of the respective spaces (see equation (16)). As implied by the linearity of the Schrödinger equation, the time evolution of the initial state could then be obtained by solving the problem for each term in the sum.

The time dependence of the wavefunctions in the coordinates \( x_{0} \) and \( x \) are determined by \( H_{0} \) and \( H \) independently, and they can be given by the respective propagators. For the free motion of the center of mass, this is well known
\[ K_{m}^{0}(x_{0}, y_{0}, t) = \left( \frac{m}{2\pi i\hbar} \right)^{1/2} \exp\left[ im(x_{0} - y_{0})^{2}/2\hbar t \right], \] (10)
which yields the usual spreading Gaussian wave packet according to
\[ \Phi_{m}(x_{0}, t) = \int K_{m}^{0}(x_{0}, y_{0}, t) \varphi_{0}(y_{0}) \, dy_{0} \]
\[ = N_{m} \exp \left[ -x_{0}^{2}/2(\sigma^{2} + i\hbar t/m) \right], \] (11)
where \( N_{m} = \pi^{-1/4}(\sigma + i\hbar t/m\sigma)^{-1/2} \). The propagator for the delta-potential Hamiltonian is more complicated but still can be obtained in a closed form. For the attractive case \( (V_{0} > 0) \), the propagator has been derived in [17, 18], while it turns out that the result is valid for both signs of the potential and is given by
\[ K(x, y, t) = K_{m}^{0}(x, y, t) + \frac{g}{2} e^{-u^{2}|x-y|^{2}/\beta^{2}} \exp \left( -i\hbar t/\beta^{2} \right) \operatorname{erfc}(u), \] (12)
where
\[ g = \frac{\mu V_{0}}{\hbar^{2}}, \quad \beta = \frac{i\hbar}{2\mu}, \quad u = \frac{|x| + |y|}{\sqrt{2i\hbar t/\mu}} - g\sqrt{i\hbar t/2\mu}. \] (13)
The time dependence of the relative wavefunction can now be given as
\[ \Phi_{r}(x, t) = \int K(x, y, t) \varphi_{r}(y) \, dy \] (14)

It is not possible to determine \( \Phi_{r}(x, t) \) in a closed form given its initial value by (9); we have to rely on numerical integration but a very good approximate formula, valid for large times, will be given below in section 4.

In order to consider the entanglement of the particles, one makes the substitution corresponding to (2) and obtains a function of \( x_{1} \) and \( x_{2} \):
\[ \Psi(x_{1}, x_{2}, t) = \Phi_{r}(x_{0}, t) \Phi_{r}(x, t) = \Phi_{r}(\alpha_{1}x_{1} + \alpha_{2}x_{2}, t) \Phi_{r}(x_{1} - x_{2}, t). \] (15)
which is not a separable state in the original coordinates \( x_{1} \) and \( x_{2} \) any more. The above-mentioned approximation for \( \Phi_{r}(x, t) \) will enable us to treat \( \Psi(x_{1}, x_{2}, t) \) analytically and explicitly consider the entanglement involved in it.
3. Reduced density operator and entanglement

In order to quantify the entanglement in the state in (15), one uses a measure that characterizes how much an actual two-particle wavefunction is different from a single product of two one-particle wavefunctions. In the context of quantum mechanics, this was first formulated by Neumann [19], based on the Schmidt decomposition [21] theorem. It states that for a square-integrable function \( \Psi(x_1, x_2, t) \) of two variables, there exist a set of functions \( \phi_k(x_1, t) \) and \( \psi_k(x_2, t) \) which both form an orthonormal (but not necessarily complete) set in their respective Hilbert spaces, such that \( \Psi \) can be written as a single sum of their products:

\[
\Psi(x_1, x_2, t) = \sum_k \sqrt{p_k(t)} \phi_k(x_1, t) \psi_k(x_2, t).
\]

The actual values of the \( p_k \)s are the simultaneous eigenvalues of the reduced density operators \( \hat{\rho}_1 \) and \( \hat{\rho}_2 \) describing either of the two subsystems defined by the hermitian kernel

\[
\hat{\rho}_1(x_1', x_1, t) = \int \Psi^*(x_1', x_2, t) \Psi(x_1, x_2, t) \, dx_2
\]

for system 1 and similarly for system 2. As shown in [19, 21] in more detail, \( \hat{\rho}_1 \) and \( \hat{\rho}_2 \) have a complete set of square-integrable eigenfunctions forming a basis \( \phi_k(x_1) \), \( \psi_k(x_2) \), respectively, such that the corresponding eigenvalues \( p_k \) are identical. The \( p_k \)s are nonnegative and form a discrete set, the sum of which is equal to unity. This also implies that the multiplicity of a positive eigenvalue must be finite.

For quantifying entanglement, it is natural to use the measure of randomness of the discrete probability distribution given by the \( p_k \)s in the Schmidt sum. Statistical physics tells us that this is best characterized by \( S = -\sum_k p_k \ln p_k \), which is just the Neumann entropy belonging to the reduced density operator for each of the particles

\[
S(t) = -\text{Tr}[\hat{\rho}_1(t) \ln \hat{\rho}_1(t)] = -\text{Tr}[\hat{\rho}_2(t) \ln \hat{\rho}_2(t)].
\]

In order to calculate \( S \), one has to find the nonzero eigenvalues \( p_k \) that shall be time dependent during the collision.

Figure 1 shows the numerical results about the time dependence of the quantum entanglement during the collision process using atomic units. We plot the Neumann entropy versus time in nine cases: the mass ratios are 1:1, 1:2 and 1:10, and the ratios of the initial momentum \( q \) to the potential strength parameter \( |g| \) are 1:2, 1:1 and 2:1. It is clearly seen that the maximal degree of the entanglement is reached shortly after the classical collision time \( t_c = \mu a/\hbar q \). On increasing the momentum or the mass ratio, the degree of the maximal entanglement decreases. The asymptotic value of the Neumann entropy, however, depends only on the value of \( q/|g| \). Among the cases shown in figure 1, the ratio \( q/|g| = 1 \) leads to the highest asymptotic entanglement. These features will be explained by the analytic results derived below. We note that the peaks appearing around the classical collision time are similar to those in [14], where a system of two equal mass particles bound in a harmonic trap has been considered. An important feature in our result is that—independent of its asymptotic value—the entanglement around the classical collision time instant is increased with decreasing the relative momentum. This can be explained by the longer interaction time between the particles in the case of a slower relative motion. That is the reason why the sequence of the maxima of the entropies in the case of different values of momenta differs from the sequence of the asymptotic values: the latter is determined by the ratio of \( q/|g| \).
0.5
0.55
0.6
0.65

Figure 1. Time dependence of the quantum entanglement during the collision process. We plot the Neumann entropy (18), computed numerically, versus time in nine cases. For solid curves (a)–(c) \[ \frac{q}{|g|} = 2, t_c = 0.5 \]; for dotted curves (d)–(f) \[ \frac{q}{|g|} = 1, t_c = 1 \]; for dashed curves (g)–(i) \[ \frac{q}{|g|} = \frac{1}{2}, t_c = 2 \]. For curves (a), (d) and (g) (blue online), \[ m_1 = m_2 = 1 \]; for curves (b), (e) and (h) (green online), \[ m_1 = 1, m_2 = 2 \]; for curves (c), (f) and (i) (red online), \[ m_1 = 1, m_2 = 10 \]. The inset shows curves (a)–(c) zoomed into the peak region. We use atomic units and the other parameters are \[ V_0 = -10, a = 10, \sigma = 1/2 \] in all cases.

4. Approximate propagator and entropy for long times

The time evolution of the relative wavefunction, i.e. the second factor in (14) cannot be given in a closed form. We find an approximate analytical formula for the relative wavefunction and entropy using certain approximations for the propagator given by (12).

The assumption that initially the particles are localized in a large distance from each other means that \( \varphi_r(y) \) is different from zero only around \( -a \ll 0 \); therefore, the contribution to the integral in (14) for \( y > 0 \) can be neglected and \( |y| \) can be replaced by \( -y \) in the propagator (12). Setting \( v = \hbar q/\mu \), which is the mean velocity of the relative wave packet, we can consider the asymptotic behavior of the system for times much larger than \( t_c = a/v \), which is the time instant of the corresponding classical collision. We can then use the asymptotic approximation [22]: \( \exp(a^2) \text{erfc}(u) = (\sqrt{\pi} u)^{-1}(1 - u^{-2}/2 + O(u^{-4})) \), valid for large values of \( u \). Keeping only the first term here, we then have

\[
K = (4\pi \beta)^{-1/2} \exp \left[ -\frac{(x - y)^2}{4\beta} \right] + \frac{8\sqrt{\beta}}{\sqrt{\pi} (|x| - y - 2g\beta)} \exp \left[ -\frac{(|x| - y)^2}{4\beta} \right].
\]

The reduced (one-particle) density matrix in the form of equation (17) cannot be calculated from the propagator (19) analytically. Therefore, we simplify it further by replacing the \( x \) and \( y \) variables of the propagator with the classical initial and final coordinate values, \( y = -a \).
and $|x| = |-a + hqt/\mu|$, in the prefactor of the exponential of $K_i$, but keeping the position dependence in the rapidly oscillating phase factor. This approximation is similar to the usual one in scattering theory and yields the propagator

$$K(x, y, t) = (4\pi \beta)^{-1/2} \left[ \exp \left( -\frac{(x-y)^2}{4\beta} \right) \right] + \left( \frac{|-a + hqt/\mu + a}{i\hbar g/\mu} - 1 \right)^{-1} \exp \left( -\frac{|x-y|^2}{4\beta} \right).$$

(20)

Due to the presence of $|x|$ in the exponential of the second term, the integral (14) with the function $q_i(y)$ from (9) will split into two distinct Gaussians: one centered around $x = -a + vt$, that corresponds to the forward scattered wave, while the other around $a - vt$ that yields the reflected wave. In this way, we get the following asymptotic form of the relative propagator:

$$K(x, y, t) = \sqrt{\frac{\mu}{2\pi i\hbar t}} \left( c_+ \exp \left( \frac{i\mu(x-y)^2}{2\hbar} \right) + c_- \exp \left( \frac{i\mu(x+y)^2}{2\hbar} \right) \right),$$

(21)

where $c_- = \left( \frac{|-a + vt + |a|}{i\hbar g/\mu} - 1 \right)^{-1}, c_+ = 1 + c_-$. It is easy to check that for times larger than $v/a$, these amplitudes coincide with the plane wave transmission and reflection coefficients for a delta potential with wave number $q$, which is the mean value of $k$ in the initial relative state

$$\lim_{t \to \infty} c_+ = T(q) := q/(q - ig), \quad \lim_{t \to \infty} c_- = R(q) := ig/(q - ig).$$

(22)

The great advantage of the approximate form in (21) is that it allows one to proceed entirely analytically and determine the total wavefunction as well as the final value of the entanglement entropy in the system in a closed form. This is due to the emergence of the Gaussian-type integrals in (14), which leads us to the approximate relative wavefunction

$$\Phi_i(x, t) = T(q)\phi_+(x, t) + R(q)\phi_-(x, t),$$

where

$$\phi_\pm(x, t) = N\sqrt{\alpha} \exp \left[ -\frac{\alpha^2(\pm x + a - vt)^2}{2(\sigma^2 + i\hbar t/m)} \right].$$

(24)

The total two-particle wavefunction is now obtained with equation (15) and after some algebra, we obtain the result

$$\Psi(x_1, x_2, t) = [T(q)\Phi_1(x_1, t)\Phi_2(x_2, t) + R(q)\Phi_1(-x_1, t)\Phi_2(-x_2, t)]$$

(25)

with

$$\Phi_j(\xi, t) = N_j\alpha_j^{1/4} \exp \left[ -\frac{\alpha_j^2(\xi - u_j t + a_j)^2 + i\gamma_j(\xi, t)}{\sigma_j^2} \right]$$

(26)

and

$$\gamma_j(\xi, t) = \frac{\hbar t}{m\sigma_j^2}[a_j(a_j + \xi)^2 - \alpha_j^2a_j^2/2] + \sigma_j^2[2(a_j + \xi) - vt/2].$$

(27)

Here, $a_1 = a_2a, a_2 = a_1a$, while $\sigma_j^2/\alpha_j = (\sigma^2 + \hbar^2 l^2/\alpha^2 m^2)/\alpha_j$ describes the spreading of the respective wave packets, and $u_j = \hbar q/m_j$ are the velocities of the particles in the corresponding classical problem. Expression (25) is the required approximation of the Schmidt decomposition consisting of two terms.

Figure 2 compares $\Phi_1(x_1, t)$ and $\Phi_1(-x_1, t)$ to those two eigenstates of the numerically computed one-particle density matrix, which belong to the two largest eigenvalues. The sum of these two largest eigenvalues is almost 1 (ca 1–10$^{-7}$), i.e. these are the only dominant eigenstates in the numerical Schmidt decomposition. The time instants are chosen to be in the asymptotic region of time evolution. We quantify the quality of the approximation by
Figure 2. Comparison of the asymptotic analytical formula of the Schmidt decomposition, equation (25), with the numerical method for the case of (a) $m_1 = m_2 = 1, q = |g|, t = 4c$, corresponding to curve (d) in figure 1, and (b) $m_1 = 1, m_2 = 10, q = 2|g|, t = 2c$, corresponding to curve (c) in figure 1. We plot the absolute value of the two eigenstates of the one-particle density matrix belonging to the two largest eigenvalues, obtained numerically, with black points (on the right-hand side) and gray points (on the left-hand side). The solid black and gray curves are the absolute values of $\Phi_1(x_1, t)$ and $\Phi_1(-x_1, t)$ functions, respectively; see equation (26). We use atomic units and the parameters are $V_0 = -10, a = 10, \sigma = 1/2$.

the magnitude of the overlap integral between $\Phi_1$ and the numerically computed eigenstate. This quantity is 0.9975 in the case of figure 2(a) both for the transmitted and the reflected components. In the case of figure 2(b), the magnitude of the overlap integral is 0.9999 for the transmitted component, and it is 0.9998 for the reflected component. These cases show that $\Phi_1$ very well approximates the corresponding eigenstate of (17). Both the increase of the mass ratio and the increase of the relative momentum increase the accuracy of the analytic approximation (25). The larger mass ratio yields a larger relative velocity of the particles, that is why the separation of the packets is larger in figure 2(b).
The asymptotic value of the entropy of the entangled state (25) is
\[
S = -|T(q)|^2 \ln |T(q)|^2 - |R(q)|^2 \ln |R(q)|^2 \\
= - \left( \frac{q^2}{q^2 + g^2} \ln \frac{q^2}{q^2 + g^2} + \frac{g^2}{q^2 + g^2} \ln \frac{g^2}{q^2 + g^2} \right).
\]
(28)

The entanglement will be maximal for \( q = |g| \), i.e., for the center-of-mass momenta with
\(-p_2 = p_1 = \mu |V_0|/\hbar\) and has the value \( \ln 2 \). This explains why we have a larger entanglement for \( m_2 = 10m_1 \), when this condition is almost satisfied.

5. Conclusions

We have followed the emergence of the entanglement of two colliding particles that are independent initially and thus their wavefunction is a product state. In the case of the delta interaction potential and Gaussian initial states, we have found an approximate analytic expression for the final entangled state, which is in good agreement with numerical results based on the exact propagator. Let us note that the wavefunction \( \Psi(x_1, x_2, t) \) is a kind of an EPR state [1] in its original sense, i.e., in the coordinate space of two entangled particles. In [1], however, the state considered is given by a highly singular delta function, while here \( \Psi(x_1, x_2, t) \) is square integrable during the whole process and has an especially simple asymptotic form.

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