Towards time-dependent wave packet tunnelling via complex Riccati equations

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Abstract. Since the discovery of tunnelling in the early days of quantum mechanics, there has been considerable interest in finding an effective method to determine the transmission of wave packets through a potential barrier. In this work, we combine the transfer matrix method, known from stationary tunnelling problems, with the construction of Gaussian wave packets via superposition of stationary states with the knowledge about the dynamics of generalized Gaussian-shaped coherent states in terms of complex Riccati equations. In the low-energy regime, this leads to an approximate analytical expression for the transmission probability and its dynamics. Extension to more general potential shapes appears straightforward.

1. Introduction
Tunnelling in physics is a typical quantum mechanical phenomenon describing a situation where a system with energy $E$ approaches a potential barrier of maximum height $V_0$. For $E < V_0$, a classical particle would be reflected into the region where it was coming from. For the quantum system, however, there is a finite probability for the system to surmount the barrier and to be found on the other side of it. This effect was first noticed in 1927 by Friedrich Hund [1] describing isomers of a molecule using a symmetric double-well potential. A first application was the explanation of alpha decay, given in 1928 by George Gamow [2]. Soon after, Max Born [3] realised that this effect was not restricted to nuclear physics but is a general quantum effect that applies to many physical systems. Since then, various fields of application were found, e.g., in solid-state physics and quantum chemistry. A variety of methods have also been developed to obtain the reflection and transmission probabilities. Some of them are based on stationary states using semi-classical approximations [4, 5, 6, 7, 8, 9], path integrals [10, 11] and many others (for reviews see, e.g., [12, 13]).

In textbooks, tunnelling is usually introduced in the context of the one-dimensional time-independent Schrödinger equation (SE). It is assumed that the quantum system approaches a potential step or barrier that can be modelled piecemeal by constant potentials. This is advantageous because as long as the energy of the system is larger than the potential, then
there are exact analytical solutions in the form of plane waves. They turn into exponentially-decaying or growing functions when the potential is larger than the energy. To find a solution that is valid in the entire space, i.e., in the regions before and after the barrier as well as inside it, the solutions in the different regions must fulfill certain continuity conditions at the borders where two regions meet. There, the wave functions and their first derivative must have the same value in both regions, leading to conditions for weighting factors that determine the contributions of the solutions in the different regions to the overall solution.

Tangible potentials, however, are not just rectangular steps or barriers. There are several ways of tackling the problem of potentials with different shapes. We mention one explicitly as it has some formal similarities with the time-dependent approach proposed by us in this paper. It is the so-called WKB–approximation, named after Gregor Wentzel [14], Hendrik Kramers [15] and Léon Brillouin [16] who developed it independently in 1926; sometimes extended to JWKB–approximation to include Harold Jeffreys [17] who found this method already three years earlier in a mathematical context. In this approach, the time-independent SE is rewritten as a complex, quadratically-nonlinear Riccati equation. Then, the real part of the function fulfilling this equation as well as its first derivative are neglected, leading to an approximate solution of the original SE in terms of the imaginary part of the Riccati variable that depends on the given potential. This method gives a reasonable approximation, providing certain conditions are fulfilled; in other cases, alternative methods are needed.

One alternative is to approximate a given potential by a sequence of rectangular potential barriers and repeat the above-mentioned boundary conditions at the borders between each set of two of these barriers. Depending on the shape of the original potential, many of these barriers might be needed. A more efficient fit with less “pieces” might be possible if barriers other than rectangular ones could be included, such as parabolic contributions; an aim of our approach.

The task gets even more difficult when looking at the time-dependent situation. As the above-mentioned plane-wave solutions of the time-independent SE are delocalized over the entire (one-dimensional) space, they are not well-suited to represent the physical situation that one actually has in mind. In the classical case, one would regard a well-localized particle that approaches the barrier and interacts with it. A quantum mechanical counterpart to the classical particle was already found by Schrödinger in 1926 [18] when he superimposed the stationary solutions of the SE for the harmonic oscillator to obtain a Gaussian-shaped wave packet with finite width and a maximum that moved like the corresponding classical particle. It can be shown that such Gaussian wave packets exist as an analytical solution for all time-dependent SEs when the Hamiltonian is at most quadratic (or bilinear) in position and momentum. However, in all cases except the one discussed by Schrödinger, also the width of the wave packet becomes time-dependent. This is also interesting for the tunnelling problem as the finite width of the wave packet shows that there is the probability of finding the quantum system in areas where the corresponding classical particle could not be at that time. Hence, the time-dependence of the wave packet width in connection with the tunnelling process is the main object of interest in our study.

However, this time-dependence of the width, and thus the shape of the wave packet, also means that the above-mentioned matching conditions at the boundaries between different regions become time-dependent.

In the literature, there are many attempts to solve or circumvent this problem. One way entails numerical simulations (see, e.g., [19, 20]) but they do not provide the information that could be obtained from an analytical approach, even if this is only an approximate one.

There are many other attempts; to get a general idea, see, e.g., [12, 13] and the literature cited there. An interesting one that apparently does not suffer some of the shortcomings others do uses a bipolar, counter-propagating wave decomposition [21, 22] that can also be applied to time-dependent wave packet dynamics [23].
In the following, we present a first step towards a description of time-dependent tunnelling (that could be extended to scattering) for arbitrary (one-dimensional) potentials by combining the above-mentioned plane wave formalism from the time-independent approach with the possibility of constructing Gaussian wave packets by superimposing these waves. We then make use of the fact that the parameters determining the dynamical properties of the Gaussians can be obtained in analytical form from a complex Riccati equation. In contrast with the JWKB approach, this Riccati equation depends on time, not on space, and we do not use an approximation but, instead, the exact analytical solutions of the Riccati equation.

In Section 2, a comprehensive analysis of the relationship between the complex variable of this Riccati equation, the quantum uncertainties and the classical equations of motion will be carried out. In Section 3, it is shown how the Gaussian wave packet for the free motion and the motion in a constant potential can be obtained using a superposition of plane wave solutions of the time-independent case. We also explain the particular choice of the superposition coefficients to guarantee our description of a situation where only tunnelling occurs, but there is no scattering of the wave packet at a barrier. In Sections 4 and 5, the results from the time-independent formalism for the step potential and the rectangular barrier are used and extended to our time-dependent wave packet formalism.

The aim of this procedure is to show that the relevant quantities, like reflection and transmission coefficients and corresponding probabilities, are essentially determined by the solution of the complex Riccati equation discussed in Section 2. This is finally outlined in Section 6 as well as possibilities to extend our approach to more general potential barriers, including sequences other than rectangular barriers.

Our results will be summarised in the conclusions, indicating limitations as well as hinting at prospective generalisations.

2. Time-dependent quantum systems and Riccati equation

In the time-independent case the SE possesses exact analytic solutions for the free motion ($V = 0$) and the constant potential ($V = V_0$), where both can be combined to form a step potential, a rectangular potential barrier, or a series of such barriers. In both cases ($V = 0$ and $V = V_0$), the solutions are given by plane waves that can be used to describe an incoming, a reflected and a transmitted part of the initial wave.

Also in the time-dependent case there are potentials that allow exact analytic solutions, this time in the form of Gaussian wave packets that exist for potentials that are at most quadratic in the position variable, i.e., the free motion, a linear in-/decreasing potential and an oscillator potential $V = \frac{1}{2}m\omega^2x^2$. In the latter case an analytic form of the parameters determining the evolution of the wave packet can be given for a constant frequency $\omega = \omega_0$ (i.e., the harmonic oscillator) and certain cases with time-dependent frequency, $\omega = \omega(t)$ (i.e., the parametric oscillator; see, e.g., [24]).

As already mentioned, the case of the harmonic oscillator wave packet was already considered by Schrödinger himself [18] shortly after he had published his first communications on wave mechanics. In the beginning, Schrödinger was very confident that similar stable wave packets could also be found, e.g., for the Coulomb problem [18], but already the free motion wave packet with its spreading width showed that this was not possible and finally favoured the probabilistic interpretation of the wave function. In any case, it became clear that both parameters of the Gaussian function, the maximum and the width, are in general time-dependent.

Taking this also into account one can formulate a general Gaussian ansatz for the solution of the time-dependent SE (with at most quadratic Hamiltonian) in the form

$$\psi(x,t) = N(t) \exp \left[ \frac{i}{\hbar} \left( \frac{m}{2}C \dot{x}^2 + \langle p \rangle \dot{x} + K(t) \right) \right], \quad (1)$$
where $C(t)$ is a complex time-dependent quantity that is connected with the wave packet width via $C_I = \frac{\hbar}{2m(x)}$ with $(\tilde{x}^2)(t) = \langle x^2 \rangle - \langle x \rangle^2 = \sigma_x^2$ being the mean square deviation in position space that is essentially the square of the width, $\tilde{x} = x - \langle x \rangle$ with $\langle x \rangle$ being the mean value of position, i.e., the classical trajectory, indicating that the maximum of the Gaussian function is at the position of the corresponding classical particle. The quantities $N(t)$ and $K(t)$ are purely time-dependent and not relevant for the dynamics of the two essential parameters.

The equations of motion for these parameters can easily be obtained inserting ansatz (1) into the time-dependent SE

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right\} \psi(x,t).$$

(2)

This leads to the Newtonian equation of motion for the maximum $\langle x \rangle(t) = \eta(t)$,

$$\ddot{\eta} + \omega^2(t) \eta = 0,$$

(3)

(for the parametric oscillator with the special cases of the harmonic oscillator, $\omega = \omega_0$, and the free motion, $\omega = 0$) and the complex Riccati equation

$$\dot{C} + C^2 + \omega^2(t) = 0$$

(4)

for the parameter connected with the wave packet width via its imaginary part $C_I(t)$.

Methods to solve this Riccati equation are well-known, but one gains further insight by rewriting this equation introducing a new variable $\alpha(t)$ that is defined via

$$C(t) = \frac{\dot{\alpha}}{\alpha} + i \frac{1}{\alpha^2(t)}$$

(5)

and is thus directly proportional to the wave packet width, as $\alpha(t) = \sqrt{\frac{2m}{\hbar(\tilde{x}^2)}} = \sqrt{\frac{2m}{\hbar}} \sigma_x$. Inserting (5) into (4) shows via the imaginary part of this equation that $C_R(t) = \frac{\dot{\alpha}}{\alpha}$, i.e., the relative change in time of the width. Therefore, for wave packets with time-dependent width the variable of the Riccati equation always is complex. The case of the harmonic oscillator solution with constant width is the special case where the Riccati equation possesses a particular solution that is constant and only exists, if the initial width of the wave packet is that of the ground state wave function of the stationary case; in all other cases, also the width of the harmonic oscillator wave packet oscillates (for details, see e.g. [25, 26]).

It is straightforward to show that position and momentum uncertainties can be expressed in terms of $C_R$ and $C_I$, or, $\alpha$ and $\dot{\alpha}$ as

$$\sigma_x^2 = \frac{\hbar}{2m C_I} = \frac{\hbar}{2m} \alpha^2$$

(6)

$$\sigma_p^2 = \frac{\hbar C_R^2 + C_I^2}{2 C_I} = \frac{\hbar}{2} \left( \alpha^2 + \frac{1}{\alpha^2} \right),$$

(7)

hence the absolute square of $C$ attains the form

$$|C|^2 = C_R^2 + C_I^2 = \frac{\dot{\alpha}^2 + \frac{1}{\alpha^2}}{\alpha^2} = \frac{1}{m^2} \sigma_p^2.$$

(8)

Inserting $C_I$ and $C_R$ in terms of $\alpha(t)$ into the real part of the Riccati equation (4) leads to

$$\ddot{\alpha} + \omega^2(t) \alpha = \frac{1}{\alpha^3}.$$

(9)
the so-called Ermakov equation. Solving this equation directly provides the time-dependence of the wave packet width. Further, this formulation yields the advantage that the dynamics of this quantum property can be traced back to the dynamics of the classical system\(^1\). It has been shown by Man’ko et al. [29, 30] that, knowing two linear independent solutions \(\eta_1\) and \(\eta_2\) of the classical equation of motion (3), the solution of equation (9) can be written as

\[
\alpha(t) = \sqrt{\frac{2m}{\hbar}} \left( \sigma_{\mathcal{P},0}^2 \eta_1(t) + \sigma_{x,0}^2 \eta_2(t) + 2\sigma_{x,0,p} \eta_1(t) \eta_2(t) \right)
\]

(10)

with \(\sigma_{x,0}^2 = \langle (x - \langle x \rangle)^2 \rangle(t = 0) = \langle x^2 \rangle(0) - \langle x \rangle^2(0)\), \(\sigma_{\mathcal{P},0}^2 = \langle (p - \langle p \rangle)^2 \rangle(t = 0) = \langle p^2 \rangle(0) - \langle p \rangle^2(0)\) and \(\sigma_{x,0,p} = \frac{1}{2} \langle [(x - \langle x \rangle)(p - \langle p \rangle)]_+ \rangle(t = 0)\), where \(\eta_1(t)\) is the classical trajectory and \([\quad , \quad \]_+ the anticommutator (for further details, see also [31, 25]). But also \(\eta_2(t)\) is defined by the Riccati equation (4) up to a constant of integration. This is connected with the fact that any Riccati equation can be linearized using a logarithmic derivative. In this case

\[
C(t) = \frac{\dot{\lambda}}{\lambda}
\]

(11)

with \(\lambda(t)\) being a complex variable fulfilling

\[
\dot{\lambda} + \omega^2(t)\lambda = 0,
\]

(12)

\(i.e., the classical equation of motion. It can be shown [32, 25, 26] that the imaginary part \(z(t)\) of \(\lambda\), when writing it in Cartesian coordinates as \(\lambda = u + iz\), is, up to a constant factor, identical with the classical trajectory,

\[
z = \frac{m}{\alpha_0 p_0} \eta(t).
\]

(13)

Furthermore, \(z\) and \(u\) are not independent of each other. This can be seen inserting definition (11) into the Riccati equation (4). From the imaginary part one obtains

\[
\dot{z}u - uz = 1,
\]

(14)

what allows to obtain \(u(t)\) simply via integration, if \(z(t)\) is known,

\[
u = -z \int_t^0 \frac{1}{z^2(t')} dt'.
\]

(15)

Therefore, \(u(t)\) is (up to a constant factor) the second solution \(\eta_2\) that is needed to obtain \(\alpha(t)\) via (10).

Writing \(\lambda(t)\) in polar coordinates as \(\lambda = \alpha e^{i\varphi}\), it can be shown [25, 26] that the amplitude \(\alpha\) is identical with \(\alpha\) defined in (5) and from the imaginary part of (4) one obtains the conservation law (14) now in the form

\[
\dot{\varphi} = \frac{1}{\alpha^2}.
\]

(16)

From the polar form immediately follows

\[
\lambda\lambda^* = \alpha^2 = u^2 + z^2,
\]

(17)

so knowing \(z(t)\) and \(u(t)\) also directly provides \(\alpha(t)\).

\(^1\) There are other approaches to describe the dynamics of generalized coherent states like those base on the Dirac-Frenkel variational method [27, 28]; but these are not applied here. As long as systems with exact analytical solutions are considered, they lead to the same result as our method.
The essence of this is that, up to initial conditions that have to be fixed, the complete dynamics of the quantum system can be obtained by solving the classical Newtonian equation of motion, because the connection between the different dynamical variables is provided via the complex Riccati equation (4). This might not be so spectacular in cases, where exact solutions of the Riccati or Ermakov equations are available, but, e.g., for parametric oscillators without analytic solutions this might be advantageous. In this case, still numerical solutions of the linear Newtonian equation can be obtained which, when fed into the above-described algorithm, are able to supply the information about the corresponding quantum mechanical uncertainties, responsible for the wave packet spreading and thus scattering and tunneling properties. The algorithm is sketched again in Figure 1.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Schematic representation of the connection amongst the complex Riccati equation and the dynamics of the maximum and width of a Gaussian wave packet.}
\end{figure}

One further aspect of this combined Newton–Ermakov system (3) and (9) shall be mentioned that will not be exploited in this approach, but may open another aspect how to tackle time-dependent problems of the kind under investigation.

Already, in 1880 Ermakov [33] had shown that by eliminating the frequency $\omega$ from equations (3) and (9), a dynamical invariant can be obtained that is still a constant of motion, even when for $\omega = \omega(t)$ the corresponding Hamiltonian no longer has this property. This so-called Ermakov invariant has the form

\[ I = \frac{1}{2} \left[ (\dot{\alpha} - \alpha \dot{\lambda})^2 + \left( \frac{\eta}{\alpha} \right)^2 \right] = \text{const.} \]  \tag{18} \]

It has been shown by Lewis [34] in a quantum mechanical context, i.e., replacing the momentum $m\dot{q}$ by the corresponding operator in position space, $\hat{p}_\text{op} = \frac{\hbar}{i} \frac{\partial}{\partial x}$, that one obtains a corresponding operator that has stationary solutions. It is possible to show that the problem of
a time-dependent SE can be transformed to the solution of this stationary problem [35, 36, 37], what, in principle, should allow to apply methods from time-independent quantum mechanics to time-dependent problems, in our case scattering and tunneling.

Last, but not least it should also be mentioned that the operator corresponding to the Ermakov invariant can be factorized in a similar way as the Hamiltonian operator of the harmonic oscillator can be factorized in terms of creation and anihilation operators. The factorization of the invariant leads to generalized creation and anihilation operators [38]

\[
a^{\dagger}(t) = -i\sqrt{\frac{m}{2\hbar}}\alpha \left( \frac{1}{m} \hat{p}_{op} - C^*x \right)
\]

(19)

\[
a(t) = i\sqrt{\frac{m}{2\hbar}}\alpha \left( \frac{1}{m} \hat{p}_{op} - Cx \right)
\]

(20)

that depend on the complex Riccati variable \(C(t)\) and allow to obtain generalized coherent states with time-dependent width in the same way as the minimum uncertainty coherent states are obtained by the usual creation and anihilation operators. These are obtained for \(\alpha = \alpha_0 = \) constant, i.e., \(C_R = \frac{\alpha}{\alpha}\) vanishes and \(C_I = \frac{1}{\alpha}\) turns into \(C_I = \frac{1}{\alpha_0} = \omega_0\). The generalized coherent states are again eigenstates of the (generalized) anihilation operator with corresponding complex eigenvalue. Whereas the Gaussian wave packet of the harmonic oscillator with constant width corresponds to the so-called frozen Gaussians (see Heller [39, 40, 41]), the generalized coherent states obtained using the general solutions of the complex Riccati equation could be called “thawed” Gaussian wave packets.

3. General coherent state tunneling

In the following sections, the tunnelling of a generalized coherent state, i.e., one with time-dependent width into a step potential and through a rectangular potential barrier of height \(V_0\) is discussed in the low energy regime, i.e., without scattering.

Low energy regime means the maximum of the initial momentum distribution of the incoming wave packet is much lower than an “effective momentum” that could be attributed to the barrier according to \(p_{\text{eff}} = \sqrt{2mV_0}\), indicating the classical momentum that must be exceeded to pass the barrier in the classical case. This is guaranteed by imposing an initial momentum mean value \(\langle p \rangle_0\) that is at most 1\% of \(p_{\text{eff}}\). Furthermore, we make sure that also the tail of the initial momentum distribution cannot come close to \(p_{\text{eff}}\) by restricting the width of the momentum distribution according to \(\frac{\sigma_{V0}}{\langle p \rangle_0} = 25\%\). A momentum distribution, adjusted accordingly, will be used to obtain the time-dependent wave packets by superposition of plane wave solutions.

These wave packets can be constructed as

\[
\psi(x,t) = \int A(p)\langle p|\psi_0\rangle \psi_p \exp \left[ \frac{i}{\hbar} \left( -\frac{p^2t}{2m} \right) \right] dp,
\]

(21)

where the coefficient \(A(p)\) is 1 for the incoming and r and for the respective reflected and transmitted wave packets. The function \(\psi_p\) defines the plane wave solutions, \(\psi_p = \frac{1}{\sqrt{2\pi\hbar}} \exp \left( +i\frac{px}{\hbar} \right)\) for the incoming and transmitted and \(\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp \left( -i\frac{px}{\hbar} \right)\) for the reflected contributions. The initial momentum distribution \(\langle p|\psi_0\rangle\) that provides the superposition coefficients is given by

\[
\langle p|\psi_0\rangle = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{a_0}{\hbar}} N_0 \exp \left[ \frac{i}{\hbar} \frac{ia_0}{2\hbar} \hat{p}_0^2 - \eta_0 p + \hbar K_0 \right],
\]

(22)

with \(\frac{a_0}{2\sigma_{V0}} = \frac{1}{2\sigma_{V0}}, \hat{p}_0 = p - \langle p \rangle_0\) and is shown for the above-mentioned restrictions in Figure 2.
4. Rectangular potential step

Before treating the rectangular barrier, the behaviour of a generalized coherent state colliding with a rectangular potential step of height $V_0$ at $x = 0$, shown in Figure 3, shall be studied in the low energy regime. In the stationary problem, the eigenfunctions are given by the superposition of an incoming (positive $p$-value) and a reflected (negative $p$-value) plane wave for $x < 0$ whereas, for $x > 0$, a decaying exponential function is taken into account (a function growing exponentially is discarded, as it does not allow normalization of the wave function):

$$\psi_p = \begin{cases} 
\exp \left( \frac{ipx}{\hbar} \right) + R \exp \left( - \frac{ipx}{\hbar} \right) & \text{for } x < 0 \\
B \exp \left( - \frac{\kappa x}{\hbar} \right) & \text{for } 0 < x,
\end{cases}$$

where $R$ and $B$ are complex-valued coefficients and $\kappa = \sqrt{2mV - p^2}$. Using the above-mentioned continuity conditions for the wave function and its derivative, one obtains

$$R = -1 + B,$$
$$B = \frac{2}{z},$$

where $z = 1 + \frac{\kappa}{p}$.

In the low energy regime these expressions can be simplified up to first order in $\sqrt{\epsilon}$, where $\epsilon = \frac{p^2}{2m}$, to yield

$$R = -1 - 2i \frac{1}{\sqrt{2mV}} p,$$
$$B = -2i \frac{1}{\sqrt{2mV}} p.$$

The wave function within the low energy approximation is therefore given by

$$\psi_p = \begin{cases} 
\exp \left( \frac{ipx}{\hbar} \right) - \exp \left( - \frac{i p x}{\hbar} \right) - 2i \frac{1}{\sqrt{2mV}} p \exp \left( - \frac{i p x}{\hbar} \right) & \text{for } x < 0 \\
-2i \frac{1}{\sqrt{2mV}} p \exp \left( - \frac{\sqrt{2mV}}{\hbar} x \right) & \text{for } 0 < x.
\end{cases}$$
The colliding wave packet is then obtained via Eq. (21), by integrating the wave function (28) with the initial momentum distribution (22), yielding

\[
\psi(x,t) = \begin{cases} 
\psi_{WP}(x,t; \eta_0, \langle p \rangle_0, \sigma_{x,0}) - \psi_{WP}(x,t; -\eta_0, -\langle p \rangle_0, \sigma_{x,0}) & \text{for } x < 0 \\
-2 \frac{1}{\hbar \sqrt{2mV}} \left( mC(x + \eta) - \langle p \rangle \right) \psi_{WP}(x,t; -\eta_0, -\langle p \rangle_0, \sigma_{x,0}) \exp \left[ -\frac{1}{2} \frac{\hbar}{mV} x \right] & \text{for } 0 < x.
\end{cases}
\]

As we can see from Figure 4(e), the contribution inside the potential step is by powers of ten smaller than outside and is therefore negligible.

5. Rectangular potential barrier

In this section, a rectangular barrier of height \( V_0 \) and width \( L \) is considered in the low energy region. For \( x < 0 \), the eigenfunctions of the stationary problem are again given by the superposition of an incoming and reflected plane wave, inside the barrier, \( 0 < x < L \), by a superposition of functions decaying and growing exponentially whereas, in the transmission region, \( L < x < \infty \), only a plane wave with positive \( p \)-value is considered; there is no wave coming from the right towards the barrier. In this case, \( \psi_p \) is given by

\[
\psi_p(x) = \begin{cases} 
\exp \left( \frac{ipx}{\hbar} \right) + R \exp \left( -\frac{ipx}{\hbar} \right) & \text{for } x < 0 \\
A \exp \left( \frac{\kappa x}{\hbar} \right) + B \exp \left( -\frac{\kappa x}{\hbar} \right) & \text{for } 0 < x < L \\
\tau \exp \left( \frac{ipx}{\hbar} \right) & \text{for } L < x.
\end{cases}
\]

The continuity conditions can then be written in matrix form for \( x = 0 \) as

\[
\begin{bmatrix} 1 & 1 \\ ip & -ip \end{bmatrix} \begin{bmatrix} 1 \\ R \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \kappa & -\kappa \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix},
\]

and for \( x = L \) as

\[
\begin{bmatrix} \beta & \frac{1}{\beta} \\ \kappa \beta & -\frac{\kappa}{\beta} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ ip & 0 \end{bmatrix} \begin{bmatrix} \gamma \tau \\ 0 \end{bmatrix},
\]

where \( \beta \doteq \exp \left( \frac{\kappa L}{\hbar} \right) \) and \( \gamma \doteq \exp \left( \frac{i\pi L}{\hbar} \right) \).

As shown in textbooks, (e.g., [42]), after matrix-inversion and matrix-multiplication, the transmission and reflection coefficients are obtained in the form

\[
\begin{cases} 
\frac{ip}{\hbar} \gamma \tau = \left( \frac{\pi^2}{\beta} - \frac{\pi^2}{\beta} \right) \frac{1}{2} \\
R = -\frac{1}{2} \frac{\hbar}{mV} \left( \beta - \frac{1}{\beta} \right) \frac{\pi}{4\kappa} \gamma \tau.
\end{cases}
\]

Considering again the low energy regime, one can take into account only terms up to first order in \( \sqrt{\frac{\pi}{V}} \), thus reducing the above expressions to

\[
\tau = -\frac{i\hbar}{mVL} p \exp \left( -\frac{pL}{\hbar} \right) \quad (34)
\]

\[
R = -\left( 1 + \frac{i\hbar}{mVL} p \right). \quad (35)
\]

As seen in the previous section, the contribution inside the barrier is smaller than outside by several powers of ten; therefore, it will be neglected in the following\(^2\).

\(^2\) At least for sufficiently small values of \( L \), also the contribution growing exponentially will be neglected.
Figure 4. Collision of the state (29) for $p_0 = 0.01\sqrt{2}$ and $\sigma_{p,0} = 0.0025\sqrt{2}$ with a potential step of height $V_0 = 1$ within the low energy regime, for four successive times: (a) $T = 0$, (b) $T = 50$, (c) $T = 100$ and (d) $T = 180$. Regarding the evanescent part of the wave packet inside the step, we only show in (e) the order of magnitude for the time $T = 100$ in order to ease the readability of the plots.
Therefore, the wave function \( \psi_p \) outside the barrier can be written as
\[
\psi_p = \begin{cases} 
\exp\left(\frac{i px}{\hbar}\right) - \exp\left(-\frac{i px}{\hbar}\right) - \frac{i \hbar}{mV_L} p \exp\left(-\frac{i px}{\hbar}\right), & \text{for } x < 0 \\
\frac{i \hbar}{mV_L} p \exp\left(i \frac{p}{\hbar}(x - L)\right), & \text{for } L < x.
\end{cases}
\] (36)

The wave packet solution is then again obtained by inserting the momentum distribution (22) and \( \psi_p \), as given now by (36), into (21). Integration then yields
\[
\psi(x, t) = \begin{cases} 
\psi_{WP}(x, t; \eta_0, \langle p \rangle_0, \sigma_x, 0) - \psi_{WP}(x, t; -\eta_0, -\langle p \rangle_0, \sigma_x, 0) \\
\frac{1}{mV_L} \left( mC(x + \eta) - \langle p \rangle_0 \right) \psi_{WP}(x, t; -\eta_0, -\langle p \rangle_0, \sigma_x, 0), & \text{for } x < 0 \\
\frac{1}{mV_L} \left( mC(x - L - \eta) + \langle p \rangle_0 \right) \psi_{WP}(x - L, t; \eta_0, \langle p \rangle_0, \sigma_x, 0), & \text{for } L < x.
\end{cases}
\] (37)

The reflection from, and transmission through, the barrier are depicted in Figure 5 for large times and narrow barriers with various widths of \( L \).

**Figure 5.** Collision of the state (37) for \( p_0 = 0.01\sqrt{2} \) and \( \sigma_{p,0} = 0.0025\sqrt{2} \) with a rectangular barrier of height \( V_0 = 1 \) within the low energy regime, for four different widths: (a) \( L = 0.05 \), (b) \( L = 0.01 \), (c) \( L = 0.0001 \). The wave packets of (a), (b) and (c) for large time \( T = 280000 \) are depicted in (d), (e) and (f), respectively. The widths in (a), (b) and (c) are not up to scale.
6. Transmission probabilities

So far, though our method allows one to obtain analytical expressions for the transmission and reflection of wave packets under the assumption of a low energy regime, it does not seem to provide much essentially new information about these processes. Our aim is to link these processes with the dynamics described by a complex Riccati equation. How this can be achieved will be shown subsequently.

The transmission coefficient $T$ can be obtained from

$$
T = \left( \frac{1}{mVL} \right)^2 \int_L^\infty \left| \frac{mC(x-L-\eta)}{x} \psi_{WP}(x-L,t;\eta_0,\langle p \rangle_0,\sigma_x) \right|^2 \, dx. \tag{38}
$$

For large times $t \gg 1$, the transmitted wave packet is practically to be found in the region $x \gg L$. As $L$ is then negligible compared to $\eta(t)$, as are the contributions of the wave packet near $L$, the lower limit of integration can be moved to minus infinity and in good approximation one gets

$$
T_{t \gg 1} = \int_{-\infty}^\infty \left( \frac{1}{mVL} \right)^2 \left| \frac{mC(x)}{x} \psi_{WP}(x-L,t;\eta_0,\langle p \rangle_0,\sigma_x) \right|^2 \, dx \tag{39}
$$

$$
= \left( \frac{1}{mVL} \right)^2 \int_{-\infty}^\infty \left| \frac{mC}{x} \psi_{WP}(x-L,t;\eta_0,\langle p \rangle_0,\sigma_x) \right|^2 \, dx
$$

what finally leads to

$$
T_{t \gg 1}(C,\langle p \rangle_0, V, L, m) = \frac{m^2|C|^2\sigma^2_x + \langle p \rangle_0^2}{(mVL)^2} \approx \frac{|C|^2\sigma^2_x}{(V_0L)^2} = \frac{\sigma^2_p(t)}{(mVL)^2}, \tag{40}
$$

taking into account that $\frac{\langle p \rangle_0^2}{m} \ll V_0$ and using equations (6-8).

This does not only show that the transmission probability decreases when mass $m$, barrier height $V_0$ and width of the barrier $L$ increase, but also that the probability increases with $\sigma^2_p(t)$, i.e., essentially when the quantum contribution to the kinetic energy mean value increases. Moreover, this now also provides the desired link to the Riccati (or equivalently Ermakov) equation, as $\sigma_p$ can be expressed in terms of $C(t)$ or $\alpha(t)$ according to equations (6-8).

Particularly for our generalized coherent states with $\hat{\alpha} \neq 0$, $\sigma_p(t)$ becomes explicitly time-dependent; and so does the transmission probability. At the same time, due to the nonlinearity of the Riccati equation, it can also be sensitive to the choice of the initial conditions, leading to qualitative changes in the dynamical behavior of $\sigma_p(t)$. If one takes into account potentials that are more general, not just constant ones, then it is possible to have even more variety in the dynamics. A step in this direction will be outlined next.

Our approach should certainly not only be applicable to the potential step and the rectangular barrier but to potential barriers of a more general shape. In the time-independent case, this situation can be described within the WKB-approximation. In the time-dependent case, we want to take an approach that approximates the given (smooth) potential better, the smaller their widths and the larger their number.

For this purpose, let us assume a potential barrier of range $L$ that can be described by a square integrable function $f(x)$ with positive local minima, as shown in Figure 6 (a),

$$
V(x) = \begin{cases} 
0 & \text{for } 0 < x < L, \\
\frac{f(x)}{} & \text{for } 0 < x < L.
\end{cases} \tag{41}
$$

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Then a grid of $N$ cells is imposed to discretize $V(x)$ in terms of rectangular barriers, as shown in Figure 6(b). Between each of these cells, the transfer matrices are determined at their interface, taking into account the continuity of the wave function and its first derivative. The reflection and transmission coefficients are then connected using the transfer matrix method\(^3\) described in [7, 8] via a product of transfer matrices $M_j$ between neighboring barriers according to

$$
\begin{bmatrix}
1 & r \\
0 & 1
\end{bmatrix} = \prod_{j=0}^{n} M_j(V_j, L, \epsilon) \begin{bmatrix}
\tau \\
0
\end{bmatrix},
$$

(42)

where $V_j$ denotes the height of the potential within the $j^{th}$ cell, i.e., $V(x) = V_j$ for cell and with $p$ being the momentum of the incident beam. To be consistent with the low energy restrictions applied in this paper, one can introduce the minimum value of the discretized barrier by $U = \min\{V_j\}$ and consider $\epsilon \ll U$. In the above-mentioned method, the matrix equation (42) can be inverted and the transmission coefficient obtained. After applying the low-energy approximation up to first order in $\sqrt{\epsilon} = \frac{p}{\sqrt{2mU}}$, this leads to a transmission coefficient of the form

$$
\tau = a + \frac{b}{\sqrt{2mU}}p,
$$

(43)

with $a, b \in \mathbb{C}$. So, after integration, this yields the wave packet

$$
\psi(x,t) = \frac{1}{V}(wC(t)(x-u) + d)\psi WP(x-L,t;\eta_0,\langle p \rangle_0,\sigma_x,0),
$$

(44)

where $w, u, d$ are real-valued quantities, provided the initial state is described by the wave packet (22). Pursuing the procedure outlined in the beginning of this section, the transmission probability for large times can be gained in the form

$$
T_{t \gg \frac{1}{C}, \langle p \rangle_0, V, L} = \frac{GC^2 + K}{V^2},
$$

(45)

with $G$ and $K$ real-valued.

This method can be refined by considering more barriers with smaller widths and taking into account further orders of $\sqrt{\epsilon} = \frac{p}{\sqrt{2mU}}$ to determine the transmission coefficient of the stationary case.

For a given shape of a potential barrier, it could be beneficial to (partially) replace the rectangular barriers in the sequence by barriers of a different shape. The advantage of the Gaussian wave packet approach lies in the exact analytical solutions for linearly-increasing and -decreasing as well as parabolic potentials (in addition to the constant potentials) that might fit the shape of a given potential (at least locally) better than the rectangular barriers. The difference between the above potentials is simply given by the equations of motion for the maximum and the width of the wave packets.

Consider, again, the low-energy regime. The dynamics of the width is essentially the core and, as pointed out above, is determined by the solutions of the respective Riccati equations. For this approximation, constant and linear potentials yield the same result concerning the dynamics of the width as only terms quadratic in $x$ contribute to the Riccati equation. However, the situation changes when the energy approaches the height of the barrier where the classical equations of motion start contributing to the transmission.

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\(^3\) In these approaches, unlike in the ones described by Bremmer [4] and M. Berry [6] inspired by optical problems, no multiple reflections are taken into account at the boundaries of the potential barriers.
Figure 6. (a) Schematic representation of a barrier, of width $\frac{7}{\sqrt{2}}$, given by $V(x) = 1 - x(x - \frac{7}{\sqrt{2}})$. (b) Discretized version of the previous barrier, by means of a grid of 10 equally wide cells.

7. Conclusion

In this paper we present the first steps on our way to the description of the process of wave packet tunnelling through an arbitrarily shaped potential barrier. The starting point is the dynamics of Gaussian wave packets that are exact analytic solutions of the time-dependent SE with at most quadratic Hamiltonian. The dynamics of such wave packets is completely determined by the time-dependence of two parameters, its maximum and its width. For the tunnelling process, particularly the latter is of importance. The dynamics of the width is essentially determined by a complex nonlinear Riccati equation. It can also be shown how this dynamics is linked to the corresponding classical equations of motion. Furthermore, the variable of the Riccati equation can be used to construct generalized creation and anihilation operators that allow to obtain coherent states with time-dependent width, also called “thawed” Gaussian wave packets, in the usual way.

In the next step the stationary tunnelling problem for a potential step and a rectangular potential barrier were discussed in terms of plane wave solutions using the transfer matrix method to obtain the reflection and transmission coefficients for these cases. The link to the Gaussian wave packets is provided by the possibility to construct these by superimposing the plane wave solutions with appropriate momentum dependent superposition coefficients. In order to assure that we describe essentially only the tunnelling process, no scattering, our discussion is restricted to the low-energy regime by choosing the momentum distribution accordingly. The transmission probability for the wave packets can be given in good approximation by an analytical expression depending on the Riccati variable $C(t)$ and a few parameters characterizing the system and the potential barrier. In particular, due to the time-dependence of $C(t)$, also this probability is time-dependent.

To extend this method to more general potentials a method is used that approximates a given smooth potential by a sequence of rectangular potential barriers [8] or linear de-/increasing ones [7]. This situation can be described formally by taking the product of the transfer matrices for each of the barriers. As mentioned in Section 6, concerning the dynamics of the wave packet width, constant and linear potentials lead to the same Riccati equation for the width, so the discussion of the rectangular barrier in Section 5 is sufficient for both cases. Also for the sequence of potential steps, the transmission probability can be expressed in terms of the Riccati variable $C(t)$. 
An advantage of the Riccati approach is that the formulation is the same for constant, linear and quadratic potentials, only the solutions of the respective Riccati equations and thus the time-dependence of the wave packet width vary. Therefore, for certain potential shapes it might be advantageous to locally approximate them by parabolic (or inverse parabolic) potentials. However, caution should be taken in the case of parabolic potentials. In our derivation, for the rectangular potential, we exploited the fact that the wave packet can be constructed by superposition of the stationary solutions, in this case plane waves. In the parabolic case, the stationary solutions are Hermite polynomials multiplied by a Gaussian function (with constant width). These also can be superimposed to a Gaussian wave packet, using adequate superposition coefficients, but it still has to be analyzed if the transfer matrix formalism can be taken over without modifications.

For practical applications it also has to be taken into account that real quantum systems are not isolated in absolute vacuum, but interacting with an environment at finite temperature, thus introducing effects like dissipation of energy and irreversibility of the dynamics. An advantage of our Riccati formalism is, that it can be adapted to this situation with very little modifications. There are various approaches for the description of open dissipative quantum systems. One kind of methods uses an effective description of the environment, i.e., only the effect of the environment on the system of interest and the corresponding changes in the dynamics and energetics of the system are taken into account, but no individual degrees of freedom of the environment are considered explicitly. This can lead to nonlinear modifications of the time-dependent SE. Some of these approaches lead to unphysical results, but there are also those that do not suffer these problems [43,44,45,25]. In this case, there also exist Gaussian wave packets as exact analytical solutions whose maximum follows the classical equation of motion including a linear velocity dependent friction force. Important for our purpose is that the dynamics of the width is again determined by a complex Riccati equation with the only difference of an additional linear term. This modification, however, can lead to interesting qualitative changes like occurrence of bifurcations [46,47]. For the case of constant potentials, also modified plane wave solutions exist that can be superimposed to provide the Gaussian wave packet solution [48], however now with time-dependent coefficients. So it seems promising that for this kind of potentials the formalism developed in this paper can be extended to include dissipative environmental effects. Concerning dissipation in parabolic potentials, the same applies as mentioned above for the conservative case.

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