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# Delayed broadening in reflectionless scattering

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**Abstract.** The factorisation method is used to analyse the motion of wavepackets in symmetric, confining, one-dimensional reflectionless potentials. We calculate the quantal time advance and compare it to the classical limit. It is proven that the broadening of wavepackets is delayed when they move over the potential well.

## 1. Introduction

The quantum mechanical motion of a particle in a given potential is a rather general problem. It is well known that a comparison between the quantal motion and the corresponding classical motion is difficult in the following sense: almost every wavepacket will split into a reflected and a throughgoing part when scattered at a potential. Therefore, the classical concept of a particle moving in a certain direction cannot be applied to the quantal motion in an arbitrary potential. Reflectionless potentials, however, do not disperse wavepackets by breaking them into two or more pieces. This property of reflectionless potentials makes it easier to compare quantal and classical motion.

There is no general technique to find analytic solutions of the time-dependent Schrödinger equation. In some cases, however, the factorisation method (Infeld and Hull 1951) can be a tool to find such time-dependent solutions analytically. There is another technique, the Darboux method (Darboux 1882), which is closely related to the factorisation method, and which was recently investigated in great detail by Sukumar (1985), Gaveau and Schulman (1986), Englefield (1987) and Humi (1987).

When it comes to physics, the complete set of time-dependent solutions is used for working out (Crandall 1983) the time-dependent propagator of the Schrödinger equation. Another quantity of interest is the quantal time advance which has been guessed (Crandall and Litt 1983) to be always less than its classical analogue. Surprisingly enough, the dispersion of wavepackets which move in reflectionless potentials has not been investigated in the literature.

The motivation for writing this paper is due to three new and, as we hope, interesting results:

(i) whenever the factorisation method works, the propagator can be determined in a straightforward way (§ 2);

(ii) the quantal time advance can exceed the classical value (§ 3); and

(iii) the broadening of wavepackets is always delayed in comparison with a free motion (§ 4).

The last result is the most important one, because it means that reflectionless potentials transfer some coherence to every wavepacket as it moves over the potential.

  

## 2. Time-dependent propagator

In order to apply the factorisation method to the time-dependent Schrödinger equation we proceed in the following way: we decompose the Hamiltonian $H$ into a pair of adjoint time-independent operators $l$, $l^+$ in the following manner:

$$H = l^+ l + E_0 \tag{1}$$

where $E_0$ is a constant. Then the Schrödinger equation for $\psi$,

$$\mathrm{i}\hbar\dot{\psi} = H\psi \tag{2}$$

is equivalent to the following set of equations:

$$l^+\varphi = \psi \tag{3}$$

$$l\psi = \mathrm{i}\hbar\dot{\varphi} - E_0\varphi. \tag{4}$$

Eliminating $\psi$ from this set of equations, we obtain the Schrödinger equation for $\varphi$:

$$\mathrm{i}\hbar\dot{\varphi} = (ll^+ + E_0)\varphi. \tag{5}$$

As usual, the dot denotes the derivative with respect to time.

A frequently discussed example is obtained by choosing

$$l = \frac{1}{\sqrt{2m}}(\mathrm{i}p + \hbar\beta \tanh \beta x) \tag{6}$$

where $p$ is the one-dimensional momentum operator. One also chooses $E_0 = -(\hbar\beta)^2/2m$ and finds that $\varphi$ satisfies the Schrödinger equation for a free particle. At the same time $\psi$ is a solution of the Schrödinger equation with the Hamiltonian $H = p^2/2m + V$, where $V$ is the following reflectionless potential (Gaveau and Schulman 1986, Crandall and Litt 1983):

$$V = -\frac{\hbar^2}{2m}\frac{2\beta^2}{\cosh^2 \beta x}. \tag{7}$$

Reflectionless potentials have been treated in detail in the literature. It is known that there exists exactly one symmetric, reflectionless potential for a given finite set of bound-state energies (Schonfeld *et al* 1980). Furthermore, algorithms have been found to compute such potentials. Quigg and Rosner (1981) used such algorithms to construct reflectionless approximations to confining potentials.

In the following we restrict ourselves to normalisable states $\psi$ and $\varphi$ since we are interested in the dynamics of (normalisable) wavepackets. Let us consider the case where $l$ is given by equation (6). From equation (3) we find that $\varphi$ can be expressed uniquely in terms of $\psi$ because the homogeneous equation $l^+\varphi = 0$ only has solutions $\varphi \sim \cosh(\beta x)$ which cannot be normalised and which, therefore, do not contribute to the mapping of $\psi$ on $\varphi$. In other words, for normalisable wavepackets equation (3) can be inverted at any time $t_0$

$$\varphi(t_0) = b^+\psi(t_0) \tag{8}$$

and the operator $b^+$ exists. Since we know the time-dependent propagator $P_0(t, t_0)$ for a free particle, we can calculate the time evolution of $\varphi(t)$:

$$\varphi(t) = P_0(t, t_0)\varphi(t_0). \tag{9}$$

By means of equation (3) we then express $\psi(t)$ in terms of $\varphi(t)$.

There is, however, one normalisable eigenstate $\psi_0$ of $H$ such that $l\psi_0 = 0$. As shown by Infeld and Hull (1951),

$$\langle x|\psi_0\rangle = (\beta/2)^{1/2}(\cosh \beta x)^{-1} \tag{10}$$

is the (only) bound state of $H$ with energy $E_0 = -(\hbar\beta)^2/2m$. By use of equation (4) we can determine the state $\varphi_0$ which corresponds to $\psi_0$. The result is $\langle x|\varphi_0(t)\rangle = c\exp(-\mathrm{i}E_0 t/\hbar)$, where $c$ is undetermined. Because of equation (5), such a state is not normalisable except for $c = 0$. Since we consider normalisable states only, we conclude that $\psi_0$ will be mapped on the null state of the free-particle problem. We therefore must treat $\psi_0$ separately by projecting $\psi_0$ out of $\psi$. Instead of equation (8) we then have

$$\bar{\varphi}(t_0) = b^+(1 - |\psi_0\rangle\langle\psi_0|)\psi(t_0). \tag{11}$$

From equations (3), (8), (9) and (11) we obtain

$$\psi(t) = l^+ P_0(t, t_0) b^+(1 - |\psi_0\rangle\langle\psi_0|)\psi(t_0) + \psi_0\langle\psi_0|\psi(t_0)\rangle \exp[-\mathrm{i}(E_0/\hbar)(t - t_0)]. \tag{12}$$

The second term in equation (12) describes the time evolution of the $\psi_0$ component of $\psi$. We are now in a position to write down the propagator of the Schrödinger equation (2):

$$P(t, t_0) = l^+ P_0(t, t_0) b^+(1 - |\psi_0\rangle\langle\psi_0|) + |\psi_0\rangle\langle\psi_0| \exp[-\mathrm{i}(E_0/\hbar)(t - t_0)]. \tag{13}$$

In coordinate representation we have

$$P_0(x, t|x', t_0) = \left(\frac{m}{2\pi\mathrm{i}\hbar(t - t_0)}\right)^{1/2} \exp\left(-\frac{m(x - x')^2}{2\mathrm{i}\hbar(t - t_0)}\right) \tag{14}$$

and

$$\langle x|b^+(1 - |\psi_0\rangle\langle\psi_0|)|x'\rangle = (1/\hbar)(m/\beta)^{1/2}[\mathrm{e}^{+\beta x}\Theta(x' - x) - \mathrm{e}^{-\beta x}\Theta(x - x')]\psi_0(x') \tag{15}$$

where $\Theta(x)$ is the unit step function. Inserting (14) and (15) into the coordinate representation of (13) leads to the result of Crandall and Litt (1983) who obtained the propagator by summing explicitly over the complete set of eigenstates of $H$. Figure 1 summarises graphically the method of how to determine the 'difficult' propagator $P$ in terms of the known propagator $P_0$.

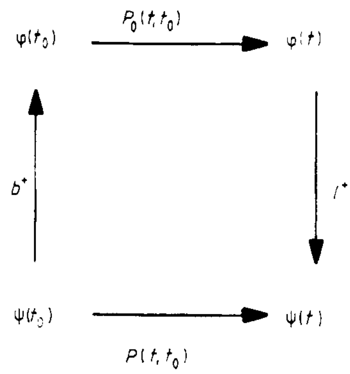


**Figure 1.** Construction scheme for the propagator $P(t, t_0)$: instead of going directly from the lower left to the lower right corner, a more convenient bypass can be found by means of the factorisation method (13). For simplicity the diagram represents the case where the initial wavepacket has no overlap with the bound state: $\langle\psi_0|\psi(t_0)\rangle = 0$.

## 3. Time advance of the mean position

In this section we investigate the properties of a wavepacket $\psi$ moving in the potential $V$ (equation (7)). The Schrödinger equation then becomes

$$\mathrm{i}\hbar\dot{\psi}=\left(\frac{p^2}{2m}-\frac{\hbar^2}{2m}\frac{2\beta^2}{\cosh^2\beta x}\right)\psi. \tag{16}$$

The Hamiltonian of equation (16) is factorised by (3) and (4), with $l$ from equation (6). Inserting (6) into (3) yields

$$\psi=(1/\sqrt{2m})(-\mathrm{i}p+\hbar\beta\tanh\beta x)\varphi. \tag{17}$$

Any solution of the time-dependent free-particle Hamiltonian will be transformed through (17) to a solution of (16).

In the following we assume

$$\langle\varphi|\varphi\rangle=1. \tag{18}$$

From the last two equations we see that $\langle\psi|\psi\rangle$ is time independent but not normalised to unity. The expectation value of an operator $L$ calculated for a wavepacket $\psi$ is given by

$$\langle L\rangle=\frac{\langle\psi|L|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{19}$$

From equation (17) it follows that the wavepacket $\psi$ behaves like a free particle far away from the potential $V$. Asymptotically we have

$$\psi=-A\varphi \qquad \text{for } \beta x\ll-1 \tag{20}$$

$$\psi=A^+\varphi \qquad \text{for } \beta x\gg+1 \tag{21}$$

with

$$A=(1/\sqrt{2m})(\mathrm{i}p+\hbar\beta). \tag{22}$$

We see that the asymptotic limit (21) can be obtained from (20) by a unitary transformation

$$U=-A^+A^{-1}. \tag{23}$$

With the same reasoning as in § 2 we can show that the inverse to $A$ exists, if again only normalised solutions are allowed. Far away from the reflectionless potential we can evaluate all expectation values by using equations (20) and (21). For example, we obtain

$$\langle p^n\rangle=\frac{1}{2m}\frac{1}{\langle\psi|\psi\rangle}\int_{-\infty}^{+\infty}\mathrm{d}x\,\varphi^*(x,t)(p^{n+2}+\hbar^2\beta^2p^n)\varphi(x,t). \tag{24}$$

A free particle has the property

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty}\mathrm{d}x\,\varphi^*(x,t)p^n\varphi(x,t)=0. \tag{25}$$

Therefore $\langle p^n \rangle$ is a conserved quantity for $|\beta x| \gg 1$. This means that $\langle p^n \rangle$ assumes the same value in front of and behind the scatterer.

Let

$$\tilde{\varphi}(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x\, \varphi(x, t) \exp(-\mathrm{i}kx)$$

vanish for $k \leqslant 0$, i.e.

$$\tilde{\varphi}(k, t) = 0 \qquad \text{for } k \leqslant 0. \tag{26}$$

Equation (26) corresponds to a situation where all momentum components of $\varphi(x, t)$ move from the left to the right. From equation (20) it then follows that $\psi$ is incident from the left, too. At a great distance from the scatterer the Ehrenfest theorem (see, e.g., Merzbacher 1961) tells us that $\langle \ddot{x} \rangle = 0$. In elastic scattering the asymptotic expectation value $p_\infty = \langle p \rangle$ ($n = 1$ in (24)) is a conserved quantity. Integrating $\langle \ddot{x} \rangle = 0$ twice with respect to time yields

$$\langle x \rangle = p_\infty t/m + x_0 \tag{27}$$

where $x_0$ is an integration constant, which will be different in the two asymptotic domains $\beta x \gtrless 1$. According to equation (20) we can write

$$\langle x \rangle_{\text{incident}} = \frac{\langle \varphi | A^+ x A | \varphi \rangle}{\langle \psi | \psi \rangle} \tag{28a}$$

whereas from (21) we have

$$\langle x \rangle_{\text{scattered}} = \frac{\langle \varphi | A x A^+ | \varphi \rangle}{\langle \psi | \psi \rangle}. \tag{28b}$$

Subtracting the two equations yields

$$x_{0,\text{scattered}} - x_{0,\text{incident}} = \frac{\hbar^2 \beta}{m \langle \psi | \psi \rangle}. \tag{28c}$$

The time advance $\tau$ is the amount of time by which the mean position of the scattered wavepacket $\psi$ is ahead of its freely evolved counterpart ($\beta = 0$). In the asymptotic region $\beta x \gg 1$ we obtain from (28$c$)

$$\tau = \frac{\beta \hbar^2}{p_\infty \langle \psi | \psi \rangle}. \tag{29}$$

Expression (29) is, in the case of equation (7), equivalent to equation (4.7) of Crandall and Litt (1983).

As an example of (29) we consider a wavepacket $\psi(x, 0)$ given in terms of $\varphi(x, 0)$. At $t = 0$, the initial state $\varphi$ is chosen to have the coordinate representation

$$\varphi(x, 0) = \left( \frac{2\alpha}{\pi} \right)^{1/2} \frac{1}{[1 - \mathrm{i}\alpha(x + d)]^2}. \tag{30}$$

Here $d$ is sufficiently large to make sure that the particle starts from the far left at $t = 0$. In the $k$ representation the initial wavefunction (30) is

$$\tilde{\varphi}(k, 0) = \frac{2}{\sqrt{\alpha}} \frac{k}{\alpha} \mathrm{e}^{-k/\alpha} \Theta(k)\, \mathrm{e}^{+\mathrm{i}kd}. \tag{31}$$

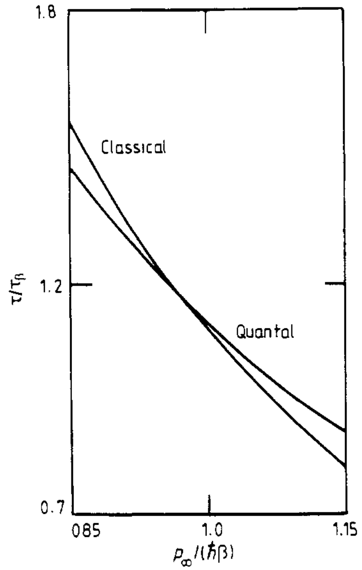


**Figure 2.** Comparison between the quantal time advance $\tau$ of a wavepacket (30) and the classical time advance $\tau_{\mathrm{class}}$ of a particle moving in the $\cosh^{-2}\beta x$ potential. The reference time is $\tau_\beta = m/\hbar\beta^2$.

Equation (31) obeys equation (26). All momentum components of the wavepackets $\varphi$ and, because of (20), also of $\psi$ move from the left to the right. The time advance $\tau$ and the expectation value $p_\infty$ are given by

$$\tau = \frac{4}{3}\frac{m}{\hbar}\frac{\beta}{\alpha}\frac{1}{5\alpha^2+\beta^2} \tag{32}$$

$$p_\infty = \tfrac{3}{2}\hbar\alpha\frac{5\alpha^2+\beta^2}{3\alpha^2+\beta^2}. \tag{33}$$

The time advance $\tau_{\mathrm{class}}$ of a classical particle moving in the potential $V$ (equation (7)), and having the same incident momentum $p_\infty$ as the wavepacket, follows from the classical equations of motion:

$$\tau_{\mathrm{class}} = \frac{m}{\beta p_\infty}\ln\left(1+\frac{2\hbar^2\beta^2}{p_\infty^2}\right). \tag{34}$$

Figure 2 compares the classical time advance with the quantal expression. We see that there exists a region where

$$\tau_{\mathrm{class}} < \tau. \tag{35}$$

Equation (35) shows that the conjecture of Crandall and Litt (1983), $0<\tau<\tau_{\mathrm{class}}$, does not hold true in general.

## 4. Time delay of the uncertainty product $\Delta x \Delta p$

A measure of the broadening of a wavepacket is the product of the uncertainties in the position and the momentum. In general, wavepackets contain momenta $k$ having different signs and running in opposite directions. This leads to dispersion which we do not want to deal with. We therefore let $\tilde{\psi}(p, t)=0$ for $p \leqslant 0$. In this case the wavepackets $\psi$ move from the left to the right.

We consider now symmetric reflectionless potentials $V(x)=V(-x)$, with asymptotic values $V(\pm\infty)=0$. These potentials are uniquely determined by their bound-state energies (Quigg and Rosner 1981)

$$\begin{aligned} &E_0 < E_1 < \ldots < E_{N-1} < 0 \\ &E_j = -(\hbar^2/2m)\beta_j^2 \qquad \text{for } j=0,1,\ldots,N-1. \end{aligned} \tag{36}$$

Far away from the scattering potential the wavepacket $\psi$ corresponds to a free particle. The initial wavepacket is connected with the scattered wavepacket by the transmission coefficient $T(p)$ (Deift and Trubowitz 1979, Crandall and Litt 1983)

$$T(p)=\exp(\mathrm{i}\Phi(p))=\prod_{j=0}^{N-1}\frac{p+\mathrm{i}\hbar\beta_j}{p-\mathrm{i}\hbar\beta_j}. \tag{37}$$

Now assume that the particle has been scattered and moves freely again. Then the Ehrenfest theorem for $(\Delta x)^2$ and $(\Delta p)^2$ can be used together with equation (20) to determine $\Delta x \Delta p$ for $t \to \infty$. The calculation is similar to the calculation of $\langle x\rangle$ in the preceding section. The result is

$$\Delta x \Delta p = 2(E_\infty - p_\infty^2/2m)[(t-t_1)^2+t_2^2]^{1/2} \tag{38}$$

with $E_\infty = \langle H\rangle$. The integration constants $t_1$, $t_2$ of the scattered wavepacket differ from those of the freely evolved facsimile of the initial wavepacket. Hence, for $t\to\infty$ the uncertainty product of the scattered wavepacket lags a time $t_\Delta = t_{1,\text{scattered}} - t_{1,\text{incident}}$ behind the freely evolved wavepacket. Because of (24) and (25) the uncertainty $\Delta p$ is the same for the scattered and for the freely evolved wavepackets. In order to calculate $t_\Delta$ it is useful to determine $(\Delta x)^2_{\text{scattered}} - (\Delta x)^2_{\text{incident}}$. This task is simplified by going into the momentum representation and by taking into account equation (37); it means that for any operator $L$ the relation $\langle L\rangle_{\text{scattered}} = \langle \mathrm{e}^{-\mathrm{i}\Phi(p)} L\, \mathrm{e}^{\mathrm{i}\Phi(p)}\rangle_{\text{incident}}$ holds true. After some algebraic manipulations and by noting (38) we get

$$t_\Delta = \frac{\hbar}{2}\frac{1}{(E_\infty - p_\infty^2/2m)}\langle (p-p_\infty)(\Phi'(p)-\Phi'(p_\infty))\rangle. \tag{39}$$

The expectation value in (39) can be evaluated both with the incident and with the scattered wavepacket. This fact is due to (37). In the case of very long monoenergetic wavepackets we have $E_\infty \to p_\infty^2/2m$ and l'Hôpital's rule must be applied to (39). By means of (37) we can show that the derivative of $\Phi$ with respect to $p$, $\Phi'(p)$, increases monotonically with $p \geqslant 0$. Using this property, it is easy to see that $t_\Delta$ is always a positive quantity.

For the purpose of illustration, let us take the previously discussed wavepacket (30), scattered by the potential (7). We then obtain

$$t_\Delta = 8\frac{m}{\hbar}\alpha\beta\frac{1}{15\alpha^4+12\alpha^2\beta^2+\beta^4}. \tag{40}$$

$t_\Delta$ vanishes for $\alpha=0$ and $\alpha\to\infty$, and has a maximum for $\alpha=\beta/\sqrt{15}$. In figure 3 the asymptotic values of the uncertainty product, equation (38), are plotted for the incident wavepacket (i) and the scattered wavepacket (s). The scattering at the potential causes

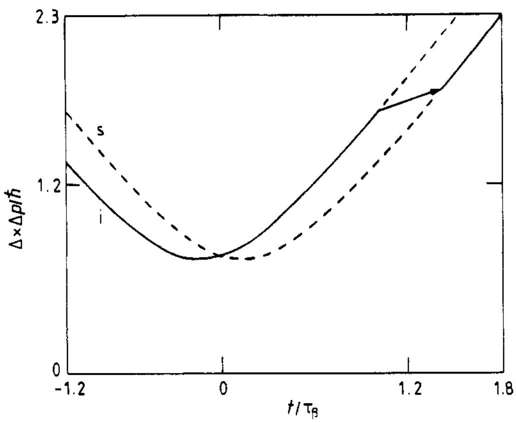


**Figure 3.** Asymptotic behaviour of the uncertainty product $\Delta x \Delta p$, plotted for a wavepacket moving in the $\cosh^{-2} \beta x$ potential. The asymptote i refers to the incident wavepacket and the asymptote s refers to the scattered wavepacket. As in figure 2 we have used the wavepacket (30) with $\alpha = \beta$. The change from i to s is schematically indicated by an arrow, and it occurs when the wavepacket passes through the potential.

the change from curve i to curve s. We conclude that the broadening of the uncertainty product is reduced as long as the wavepacket passes through the scattering region.

In this context let us make a few remarks about one-dimensional crystals ($V(x) = V(x-L)$), where delayed broadening is also possible. A maximum delay of the broadening will occur if there is a $k$ interval where the energy $E(k)$ depends linearly on $k$

$$E(k) = \hbar(k-k_0)v \qquad \text{for } k_1 \leqslant k \leqslant k_2. \tag{41}$$

Then, Bloch waves $\psi_k(x, t)$ with $k$ values in the interval $k_1 \leqslant k \leqslant k_2$ can be used to construct wavepackets which move through the crystal. From the properties of the Bloch waves we derive the following relation for such wavepackets:

$$\psi(x-L, t-L/v) = \exp(-ik_0 L)\psi(x, t). \tag{42}$$

Equation (42) means that these special wavepackets move as coherent states (Perelomov 1986) through the crystal. Their motion is unbounded, in contrast to the motion described by the usual coherent Glauber state (Glauber 1963a, b) in a harmonic potential.

In the real world we have to deal with three dimensions. Let us consider a three-dimensional superlattice (see Kelly and Weisbuch (1986) for example), which we assume to be homogeneous in the $y$ and $z$ directions with $V(x, y, z) = V(x)$. If $V(x)$ is the same periodic potential as discussed above, then the broadening of wavepackets will be delayed in the $x$ direction. In the $y$ and $z$ directions there will be the usual broadening of a free motion—unless we apply a static homogeneous magnetic field in the $x$ direction. In this case the magnetic field will make both $\Delta y \Delta p_y$ and $\Delta z \Delta p_z$ an oscillating function of time. Under these circumstances a three-dimensional wavepacket can propagate along the magnetic field direction with little (or even no) broadening.

## 5. Conclusion

Equation (17) relates a time-dependent solution $\psi(x, t)$ of the reflectionless Schrödinger equation to a time-dependent solution $\varphi(x, t)$ of the free Schrödinger equation. Starting from this relation we derived the general expression (29) for the quantal time advance. By means of an example we demonstrated that the quantal time advance is not always less than the classical time advance, as surmised in the literature (Crandall and Litt 1983).

In order to gain insight into the quantum mechanical motion we studied the time evolution of the uncertainty product $\Delta x \Delta p$. For a free particle this uncertainty product diverges for $t \rightarrow \infty$, because then the corresponding free wavepacket has completely dispersed. We found that the increase of the uncertainty product $\Delta x \Delta p$ of an asymptotically free wavepacket is delayed relative to the free (zero-potential) motion. This delay happens as the wavepacket moves over the potential well. We also showed that coherent non-dispersing wavepackets can move through crystals, if the energy $E(k)$ depends linearly on $k$ in some finite $k$ interval.

The results of this paper could be useful in the context of quantum transport. For example, a superlattice (Kelly and Weisbuch 1986) made by many reflectionless potentials in a row would help fast electrons to stay ballistic for a longer time.

## Acknowledgments

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