

Time delays and space shifts for almost monochromatic wave packets after quantum reflection

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Abstract. The time delay of an almost monochromatic wave packet can be defined unambiguously via the energy derivative of the phase of the amplitude defining the superposition of stationary states making up the wave packet. We illustrate how this concept, originally formulated by Eisenbud and Wigner in the context of scattering theory, can be applied to quantum reflection by the nonclassical region of a long-ranged attractive potential tail. We pay special attention to the case of a wave packet incident from the near side of the nonclassical region and interpret the results with the help of regularized step potentials.

1. Introduction

An expression for time delay in particle scattering was formulated by Eisenbud and Wigner more than fifty years ago [1]. The prescription of Eisenbud and Wigner involves the energy derivative of the phase of the scattering matrix, and it is well defined and unambiguous for wave packets which are almost monochromatic. The concept can be transferred from the scattering problem to other processes involving time; the scattering matrix must then be replaced by the appropriate energy-dependent amplitude describing the process.

In this contribution we apply the formula of Eisenbud and Wigner to wave packets subjected to quantum reflection by the nonclassical region of an attractive potential tail, as typically occurs beyond the close region of a few atomic units in the interaction of atoms and molecules with each other and with surfaces. After a brief review of the Eisenbud-Wigner time delay in Sect. 2, its application in connection with quantum reflection is described in Sect. 3. The choice of reference waves affects the phase of the quantum reflection amplitude and hence the interpretation of the time delays obtained, as discussed in Sect. 4. In Sect. 5 we focus on quantum reflection of a wave packet incident from the near side of the nonclassical region of the potential tail, and in Sect. 6 we interpret the results with the help of regularized potentials in which the singular attractive potential at positive distances is smoothed to a deep constant value at negative distances.

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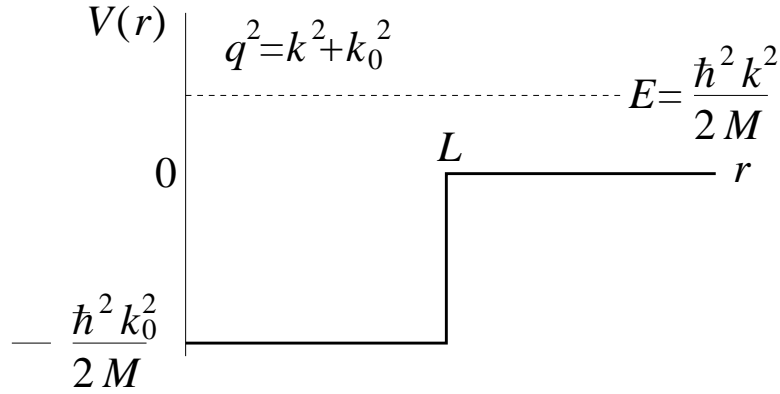


Figure 1. Sharp potential step at $r = L$

2. Eisenbud-Wigner time delay

Consider a rightward-travelling free-particle wave packet,

$$\psi(r, t) = \int_{-\infty}^{\infty} \tilde{\psi}(k') \psi_{k'}(r, t) dk', \quad \psi_{k'} = e^{i[k'r - \omega(k')t]}, \quad \omega(k) = \frac{\hbar k^2}{2M}. \quad (1)$$

If the amplitude function $\tilde{\psi}(k')$ is sufficiently narrowly peaked around a (positive) wave number k , then the wave packet moves to the right with little spreading at the *group velocity*

$$v_g = \frac{d\omega}{dk}, \quad (2)$$

which here is given by $v_g = v_\infty = \hbar k/M$. A wave packet centred around r_0 at time t_0 will be centred around $r = r_0 + v_\infty(t - t_0)$ at a later time t . If the wave packet is modulated by an amplitude function $A(k') = |A(k')| e^{i\phi(k')}$,

$$\psi(r, t) = \int_{-\infty}^{\infty} \tilde{\psi}(k') A(k') \psi_{k'}(r, t) dk', \quad (3)$$

then at time t it will be centred around

$$r = r_0 + v_\infty(t - t_0) - \frac{d\phi}{dk} \quad (4)$$

if it was centred around r_0 at time t_0 . Compared to the free wave packet defined without the amplitude $A(k')$, the wave packet (3) lags behind by a space shift Δr which translates into a time delay $\Delta t = \Delta r/v_\infty$ for a particle travelling with velocity v_∞ ,

$$\Delta r = \frac{d\phi}{dk}, \quad \Delta t = \frac{\Delta r}{v_\infty} = \hbar \frac{d\phi}{dE}, \quad E = \frac{\hbar^2 k^2}{2M}. \quad (5)$$

The expressions (5) were originally derived by Eisenbud and Wigner [1] for partial wave scattering, where the relevant amplitude is the partial wave S -matrix $e^{2i\delta}$, so $\phi(k) = 2\delta(k)$. They are readily transferred to other situations, e.g. the reflection of a particle incident from the right by a sharp potential step at a distance L from the origin, as illustrated in Fig. 1. Solving the Schrödinger equation with the boundary conditions

$$\psi \stackrel{r \leq L}{\approx} \frac{T}{\sqrt{\hbar q}} e^{-iqr}, \quad \psi \stackrel{r \geq L}{\approx} \frac{1}{\sqrt{\hbar k}} \left(e^{-ikr} + R(k) e^{+ikr} \right) \quad (6)$$

gives the reflection amplitude $R(k)$ and the space and time shifts as

$$R(k) = \frac{k - q}{k + q} e^{-2ikL}, \quad \Delta r = -2L, \quad \Delta t = -2L \frac{M}{\hbar k}. \quad (7)$$

The k -independent space shift $-2L$ describes the fact that the reflected wave is generated at the point $r = L$ and hence is advanced by the distance $2L$ with respect to the free wave travelling to $r = 0$ and back; the time shift in (7) expresses the corresponding time *gain* (negative time delay) for a particle travelling with the velocity $\hbar k/M$.

3. Application to quantum reflection by attractive potential tails

Reflection by the sharp step in Fig. 1 is a typical example of “quantum reflection”, i.e., classically forbidden reflection by a nonclassical region in coordinate space in the absence of a classical turning point. Nonclassical regions in coordinate space occur where the condition for validity of the WKB approximation,

$$|Q(r)| \ll 1, \quad Q(r) = \frac{1}{16\pi^2} \left[2\lambda_k \lambda_k'' - (\lambda_k')^2 \right], \quad (8)$$

is poorly fulfilled. Here $\lambda(r) = 2\pi\hbar/p(r) = 2\pi\hbar/\sqrt{2M[E - V(r)]}$ is the local de Broglie wave length. For attractive potential tails more singular than $-1/r^2$, the “badlands” or “quantality function” $Q(r)$ usually has its maximum absolute value near the point r_E , where the absolute value of the potential is equal to the total energy, $|V(r_E)| = E$ [2; 3]. For homogeneous potential tails,

$$V_\alpha(r) = \frac{C_\alpha}{r^\alpha} = -\frac{\hbar^2}{2M} \frac{(\beta_\alpha)^{\alpha-2}}{r^\alpha}, \quad (9)$$

this characteristic position is given by

$$r_E = \beta_\alpha (k\beta_\alpha)^{-2/\alpha}, \quad (10)$$

and semiclassical approximations become increasingly valid not only for $r \rightarrow \infty$, but also on the near side of r_E for $r \rightarrow 0$.

Quantum reflection amplitudes have been calculated [2–7] for various attractive potential tails by solving the Schrödinger equation with the boundary conditions defined in terms of stationary monochromatic waves for $r \rightarrow \infty$, see Fig. 2,

$$\psi(r) \stackrel{r \rightarrow 0}{\approx} \frac{T}{\sqrt{p(r)}} e^{-\frac{i}{\hbar} \int^r p(r') dr'}, \quad \psi(r) \stackrel{r \rightarrow \infty}{\approx} \frac{1}{\sqrt{\hbar k}} \left(e^{-ikr} + R e^{-ikr} \right). \quad (11)$$

The boundary condition for small distances corresponds to incoming waves, which is conveniently expressed in terms of inward-travelling WKB waves in the semiclassical region on the near side of r_E . The Schrödinger equation for quantum reflection corresponds to the that for s -wave scattering, and the analogy is highlighted by expressing the amplitude $R(k)$ for quantum reflection in terms of a complex phase shift δ ,

$$R(k) = |R(k)| e^{i\phi(k)} = -e^{2i\delta(k)}, \quad |R| = e^{2\Im(\delta)}, \quad \phi = \pi + 2\Re(\delta). \quad (12)$$

The near-threshold behaviour of R can be derived via an adaptation of the effective-range formalism of ordinary scattering theory to incoming boundary conditions on the near side of the nonclassical region [7],

$$\delta(k) \stackrel{k \rightarrow 0}{\approx} -k(\bar{a} - ib) + \frac{1}{3}(k\Lambda)^3. \quad (13)$$

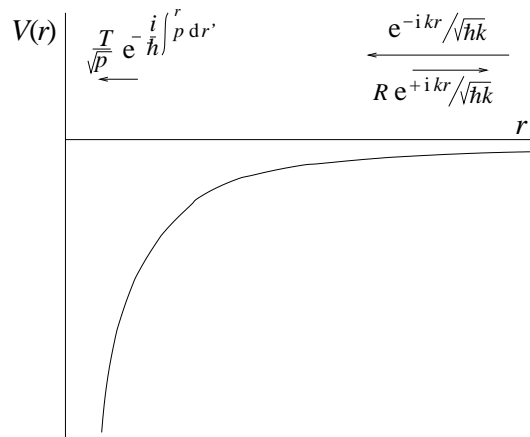


Figure 2. Schematic illustration of quantum reflection by an attractive potential tail with monochromatic incoming and reflected waves as reference waves beyond the nonclassical region.

The “threshold length” b determining the leading deviation of the quantum reflection probability from unity is well defined for all potentials falling off faster than $-1/r^2$ asymptotically. The “mean threshold length” \bar{a} determining the leading near-threshold behaviour of the phase of R is a well defined finite number only for potentials falling off faster than $-1/r^3$. The last term on the right-hand side of (13) exists in the given form only for potentials falling off faster than $-1/r^5$.

Away from threshold, semiclassical approximations rapidly become more accurate, and the amplitude for quantum reflection assumes a form typical of classically forbidden processes in smooth potentials [8; 9], $R(k) \stackrel{k \rightarrow \infty}{\sim} e^{-\mathcal{B}S/\hbar}$, where S is some typical classical action of the system, e.g. $\hbar k r_E$, with the characteristic distance r_E defined after Eq. (8). For homogeneous potential tails (9), (10), $k r_E = (k\beta_\alpha)^{1-2/\alpha}$ and

$$R(k) \stackrel{k \rightarrow \infty}{\sim} e^{-\mathcal{B}(k\beta_\alpha)^{1-2/\alpha}}, \quad \mathcal{B} = B - iD. \quad (14)$$

This behaviour was confirmed for the modulus of $|R|$ in [2], where an explicit expression is given for the dimensionless parameter B as a function of the power α .

Table 1 lists the values of the parameters b , \bar{a} and Λ for homogeneous potential tails (9) in units of β_α . The parameter Λ is a real multiple of the *complex scattering length* $\bar{a} - ib$ for homogeneous potentials. The last row shows the values of the dimensionless parameter B determining the “high”-energy behaviour of the quantum reflection probabilities (14).

For potential tails falling off faster than $-1/r^3$, the space shift Δr defined by (5) tends to a finite limit at threshold, namely $-2\bar{a}$ according to (13). This implies that the quantum reflected wave propagates as a free wave reflected at the point $r = \bar{a}$ rather than at $r = 0$. The near-threshold behaviour of the time correspondingly is $\Delta t \stackrel{k \rightarrow 0}{\sim} -2\bar{a}M/(\hbar k)$, which diverges at threshold, simply because the slow free particle takes so long to traverse the distance from $r = \bar{a}$ to $r = 0$ and back. At higher energies, the phase of R becomes proportional to $-k r_E$, so the energy dependence of the phase shift is that of the characteristic distance r_E , see (10). Note, however, that the coefficient is not simply 2, so the time delay is only proportional, but not equal, to that of a classical free particle reflected at $r = r_E$ rather than at $r = 0$ [4; 6]. The phase ϕ of the quantum reflection amplitude and the resulting space shift Δr are shown for homogeneous potential tails (9) as functions of $k\beta_\alpha$ in Fig. 3.

Table 1. Threshold length b , mean scattering length \bar{a} and the parameter Λ of Eq. (13) for homogeneous potential tails (9). The last row shows the values of the dimensionless parameter B determining the “high”-energy behaviour of the quantum reflection probabilities (14).

α	3	4	5	6	7	∞
b/β_α	π	1	0.6313	0.4780	0.3915	$\pi/(\alpha-2)$
\bar{a}/β_α	—	0	0.3645	0.4780	0.5389	1
$\Lambda/(\bar{a}-ib)$	—	—	—	1	0.6496	$2.1265/(\alpha-2)$
B	2.2405	1.6944	1.3515	1.1202	0.9545	$2\pi/\alpha$

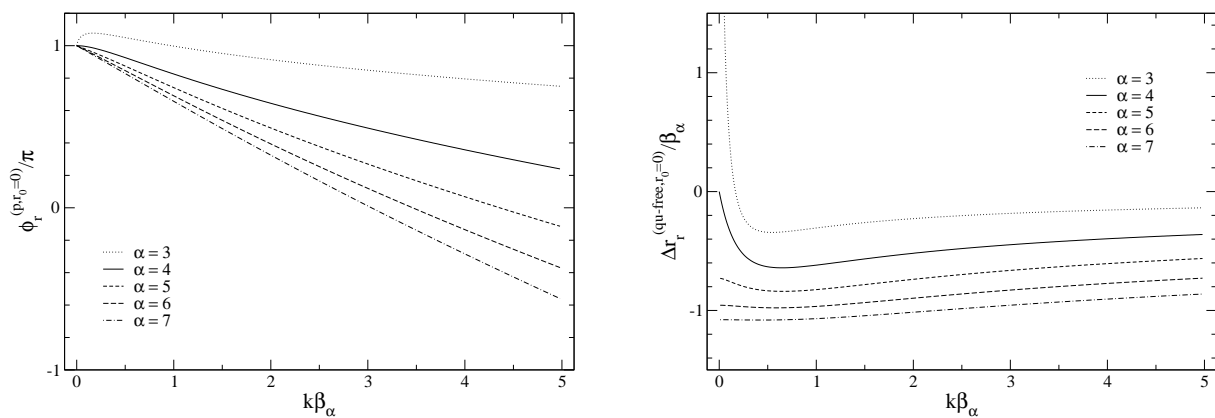


Figure 3. The left-hand panel shows the phase of the quantum reflection amplitude as function of k for homogeneous potential tails (9); the right-hand panel shows the resulting space shifts Δr as defined in (5)

4. Choice of reference waves

Instead of using plane waves (i.e. monochromatic waves) for reference as in (11), we can also use WKB waves,

$$\psi \stackrel{r \rightarrow \infty}{\equiv} \frac{1}{\sqrt{p(r)}} \left[-e^{\frac{i}{\hbar} \int_{r_0}^r p(r') dr'} + R^{(\text{WKB}, r_0)} e^{+\frac{i}{\hbar} \int_{r_0}^r p(r') dr'} \right]. \quad (15)$$

Reference to WKB waves does not imply any approximation of the quantum reflection amplitudes; applicability of the WKB approximation away from the nonclassical region is a necessary condition for an unambiguous decomposition of the quantum wave into incoming, reflected and transmitted parts. The probability $|R|^2$ for quantum reflection does not depend on whether WKB waves or monochromatic waves are used for reference, but the phase of R depends on this choice and also on the point of reference of the WKB integrals, which is called r_0 in (15) and sets a zero in the phase of the WKB wave functions [6]. For this reason, we keep the labels “WKB” and r_0 as superscripts on the quantum reflection amplitude.

When the reference waves are WKB wave functions as in (15), the derivatives of the phase of the reflection amplitude define space and time shifts relative not to free-particle motion, but to the motion of classical particles under the accelerating influence of the potential. E.g., the momentum and energy derivatives of the phase $\phi^{(\text{WKB}, r_0)}$ of $R^{(\text{WKB}, r_0)}$ in (15) describe the space and time shifts of the quantum reflected wave relative to a classical particle reflected at the point

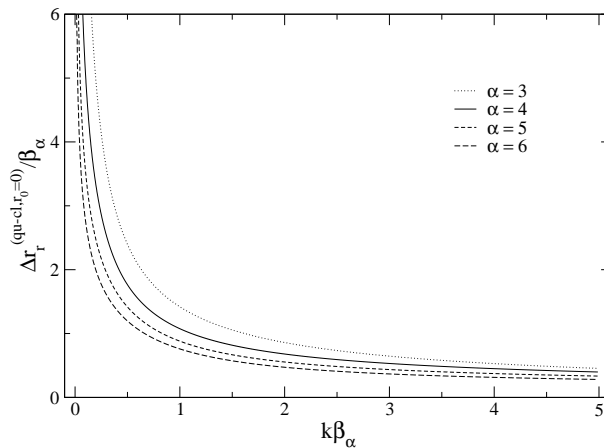


Figure 4. Space shifts $\Delta r^{(\text{qu-cl}, r_0=0)}$ expressing the delay of the quantum reflected wave relative to the classical accelerated particle for homogeneous potential tails (9).

of reference r_0 ,

$$\frac{d\phi^{(\text{WKB}, r_0)}}{dk} = \Delta r^{(\text{qu-cl}, r_0)}, \quad \hbar \frac{d\phi^{(\text{WKB}, r_0)}}{dE} = \Delta t^{(\text{qu-cl}, r_0)}. \quad (16)$$

The point of reference r_0 in the above expression is arbitrary, and we can remove this arbitrariness by fixing r_0 to an appropriate value, e.g. $r_0 = 0$. The phase of the reflection amplitude defined via the boundary conditions (15) diverges for $r_0 \rightarrow 0$, because the phases of the WKB waves diverge in this limit, but the space and time shifts stay well defined, because

$$\begin{aligned} \Delta r^{(\text{qu-cl}, r_0 \rightarrow 0)} &= \Delta r^{(\text{qu-free}, r_0=0)} + \Delta r^{(\text{free-cl}, r_0=0)}, \\ \Delta t^{(\text{qu-cl}, r_0 \rightarrow 0)} &= \Delta t^{(\text{qu-free}, r_0=0)} + \Delta t^{(\text{free-cl}, r_0=0)}. \end{aligned} \quad (17)$$

In (17) the superscript “qu-free” denotes the space and time shifts of the quantum reflected wave relative to the free wave, which were discussed in the previous section. The superscript “free-cl” denotes the space and time shifts of the free wave or particle relative to the classical particle moving under the accelerating influence of the potential and reflected at r_0 , and these shifts are defined classically and remain finite in the limit $r_0 \rightarrow 0$. For homogeneous potential tails (9),

$$\Delta r^{(\text{free-cl}, r_0=0)} = 2r_E \tau(\alpha), \quad \Delta t^{(\text{free-cl}, r_0=0)} = \Delta r^{(\text{free-cl}, r_0=0)} / v_\infty, \quad (18)$$

with r_E given by (10) and $\tau(\alpha) = \Gamma\left(\frac{1}{2} + \frac{1}{\alpha}\right) \Gamma\left(1 - \frac{1}{\alpha}\right) / \sqrt{\pi} \approx 1$ [4]. Note that the time *gain* of the quantum wave relative to the free particle is smaller than the time delay of the free particle relative to the classical particle; in terms of space shifts:

$$-\Delta r^{(\text{qu-free})} < \Delta r^{(\text{free-cl})} \Rightarrow \Delta r^{(\text{qu-cl})} = \Delta r^{(\text{qu-free})} + \Delta r^{(\text{free-cl})} > 0. \quad (19)$$

Although the dominantly negative space shifts shown in Fig. 3 indicate that the quantum reflected wave returns sooner than the free wave (except for $\alpha = 3$ and very small energies), the quantum reflected wave is always *delayed* relative to *classical* particle subjected to the accelerating influence of the attractive potential tail. The corresponding positive space shifts are illustrated in Fig. 4.

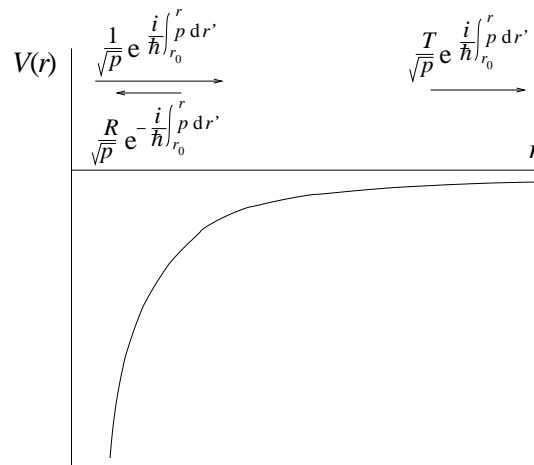


Figure 5. Schematic illustration of near-side quantum reflection in an attractive potential tail

5. Near-side quantum reflection

Since there is a semiclassical region on the near side of the nonclassical region, one can also study the quantum reflection of particles which initially move outward and are reflected back without managing to traverse the nonclassical region, the “badlands”, see Fig. 5. Since the potential depends strongly on r at small distances, incoming and reflected waves are appropriately represented by WKB waves, and the Schrödinger equation has to be solved with the following boundary conditions:

$$\psi \stackrel{r \rightarrow 0}{\equiv} \frac{1}{\sqrt{p(r)}} \left[e^{\frac{i}{\hbar} \int_{r_0}^r p(r') dr'} + R_{\text{ns}}^{\text{WKB}, r_0} e^{-\frac{i}{\hbar} \int_{r_0}^r p(r') dr'} \right], \quad \psi \stackrel{r \rightarrow \infty}{\equiv} \frac{T_{\text{ns}}}{\sqrt{p(r)}} e^{\frac{i}{\hbar} \int_{r_0}^r p(r') dr'}. \quad (20)$$

The quantum reflection amplitude (as also the transmission amplitude) is labelled with the subscript “ns” in (20), in order to distinguish these amplitudes for incidence from the near side from the conventional amplitudes defined via the boundary conditions (11). According to well known reciprocity relations, the probabilities $|R|^2$ for reflection and $|T|^2$ for transmission do not depend on the direction of incidence, nor on whether monochromatic waves or WKB waves are used for reference. However, the phase of the quantum reflection amplitude does depend on the direction of incidence, on the choice of reference waves and on the point of reference r_0 .

Since the reference waves are WKB wave functions, the energy derivative of the phase of the reflection amplitude in (20) defines the time shift relative to a classical particle incident from small r values and reflected at the point of reference r_0 ,

$$\hbar \frac{d\phi_{\text{ns}}^{(\text{WKB}, r_0)}}{dE} = \Delta t_{\text{ns}}^{(\text{qu-cl}, r_0)}. \quad (21)$$

It turns out to be useful to define a related space shift for a free particle moving with constant velocity v_∞ ,

$$\Delta r_{\text{ns}}^{(\text{qu-cl}, r_0)} = v_\infty \Delta t_{\text{ns}}^{(\text{qu-cl}, r_0)} = \frac{d\phi_{\text{ns}}^{(\text{WKB}, r_0)}}{dk}, \quad (22)$$

even though particle motion is not asymptotically free on the near side.

Again we can remove the arbitrariness in the choice of reference point r_0 by taking the limit $r_0 \rightarrow 0$. The phase of the reflection amplitude in (20) diverges in this limit, but the derivatives

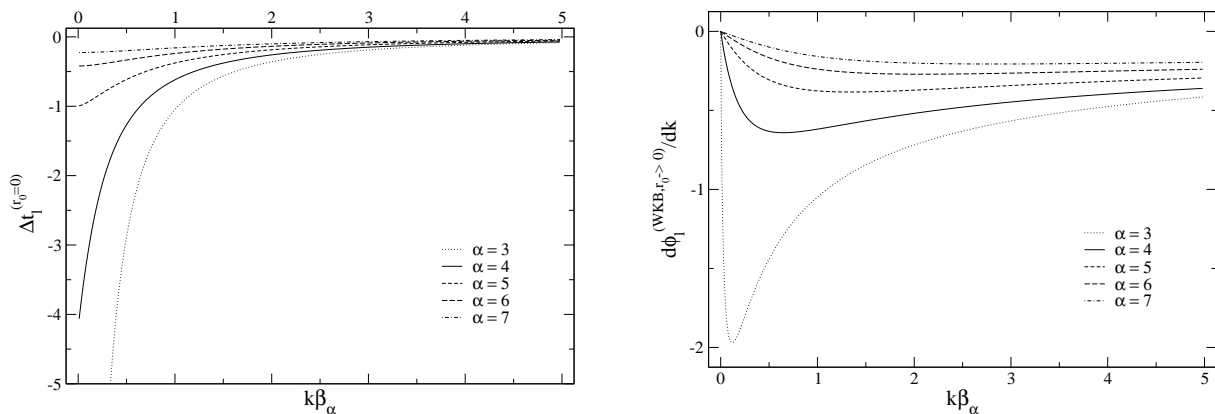


Figure 6. Time shifts (21) and k -derivative (22) for near-side quantum reflection in the limit $r_0 \rightarrow 0$.

of the phase with respect to E or k remain finite, so the time and space shifts (21), (22) remain well defined for $r_0 \rightarrow 0$. The results for homogeneous potential tails (9) are shown in Fig. 6

A striking feature of Fig. 6 is, that the time and space shifts are all negative. These shifts refer to the delay of the quantum reflected wave relative to a classical particle starting from the near-side classical region and reflected at the point of reference r_0 . In the limit $r_0 \rightarrow 0$ this means, that the quantum reflected wave is reflected faster than instantaneously. To understand the origin of this apparent paradox, it is important to remember that the Eisenbud-Wigner formula (5) applies for almost monochromatic wave packets, with a momentum distribution sharply peaked around a given finite value. The (small) momentum spread Δk of a (free) wave packet at large distances is related to an energy spread $\Delta E = \hbar k \Delta k / M$, which is independent of the position of the wave packet. At smaller distances the local wave number is r -dependent and $k(r)$ becomes very large as the potential assumes large negative values. The corresponding momentum spread must thus become very small for constant ΔE , so the uncertainty of the wave packet in coordinate space becomes larger and larger as it enters the near-side classical region at small distances. It is actually impossible to construct a wave packet well localized on the near side of the nonclassical region which also fulfills the condition “almost monochromatic” as assumed in the application of the Eisenbud-Wigner formula. In order to nevertheless reach a meaningful interpretation of the results in this section, we study regularized potential steps in which the attractive potential tail is smoothly continued to a large negative constant value for negative distances r .

6. Interpretation via regularized potentials

We replace the homogeneous potential (9) by the regularized potential

$$V_\alpha(r; a) = -\frac{\hbar^2(\beta_\alpha)^{\alpha-2}}{2M} \begin{cases} (r^\alpha + a^\alpha)^{-1} & \text{for } r \geq 0, \\ a^{-\alpha} & \text{for } r < 0. \end{cases} \quad (23)$$

The potential now has the constant value $-\hbar^2 q_0^2 / (2M)$, $q_0^2 = (\beta_\alpha)^{\alpha-2} / a^\alpha$, for negative r values, and we can define the near-side reflection amplitude conventionally using plane, i.e. monochromatic waves,

$$\psi \stackrel{r \leq 0}{=} \frac{1}{\sqrt{\hbar q}} \left[e^{iqr} + R_{\text{ns}}^{(p, r_0)} e^{-iqr} \right], \quad \psi \stackrel{r \rightarrow \infty}{=} \frac{T_{\text{ns}}^{(p, r_0)}}{\sqrt{\hbar k}} e^{ikr}, \quad q = \sqrt{k^2 + q_0^2}. \quad (24)$$

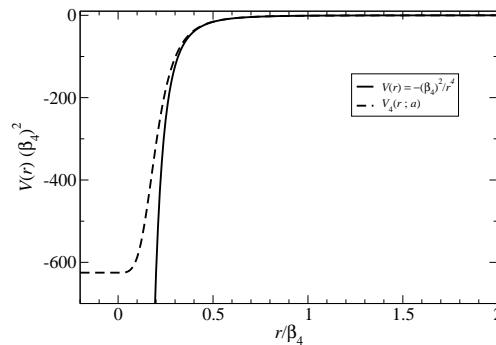


Figure 7. Smoothed potential (23) for $\alpha = 4$ and a “smoothing length” $a = 0.2\beta_4$.

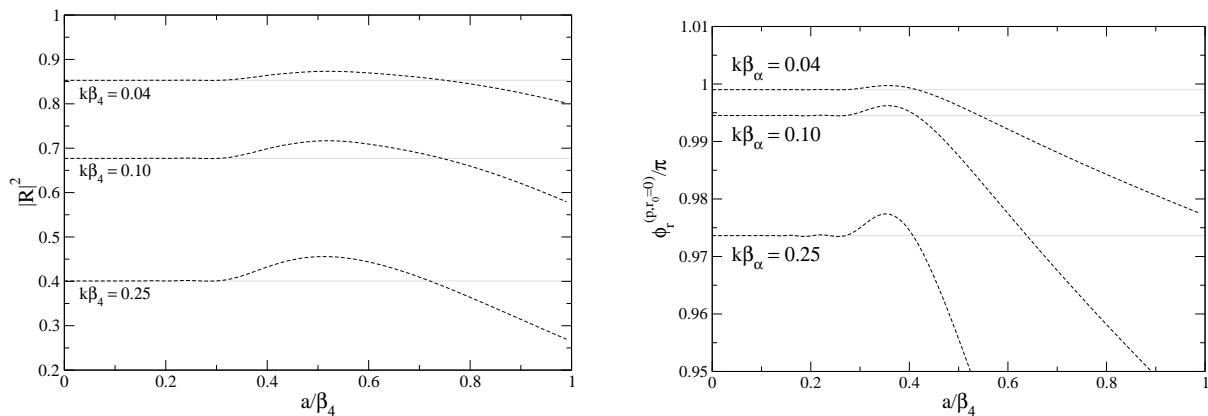


Figure 8. Quantum reflection probabilities (left-hand panel) and phase of the quantum reflection amplitude (right-hand panel) for incidence from negative r values to the smoothed potential step (23) as functions of the smoothing length a for various total energies $E = \hbar^2 k^2 / (2M)$. The straight horizontal lines show the corresponding result for near-side quantum reflection by the singular homogeneous potential (9) with $\alpha = 4$.

The phase $\phi_{\text{ns}}^{(p, r_0)}$ of the reflection amplitude is now well defined for $r_0 = 0$, but it depends, as does the reflection probability $|R|^2$, on the choice of smoothing length a . Figure 8 shows, for $\alpha = 4$, how $|R|^2$ and $\phi_{\text{ns}}^{(p, r_0=0)}$ depend on a in (23) for various total energies $E = \hbar^2 k^2 / (2M)$. At energies for which the quantum reflection probabilities are still appreciable, the results for the smoothed potential are very close to the results obtained for near-side quantum reflection by the singular homogeneous potential (9) (straight horizontal lines) when a/β_4 is smaller than about 0.25.

The results obtained in the previous section are thus essentially unaffected by the smoothing of the potential for appropriately small smoothing lengths. This is confirmed in Fig. 9, where the time delay for near-side quantum reflection is plotted as a function of energy. The solid line shows the result obtained for a singular homogeneous potential (9), $\alpha = 4$, as already shown as one of the curves in the left-hand panel of Fig. 6. The dashed line, which is hardly distinguishable from the solid line, shows the result obtained with the smoothed potential (23) for a smoothing length $a = 0.2\beta_4$. The negative time delay seems to indicate, that the quantum

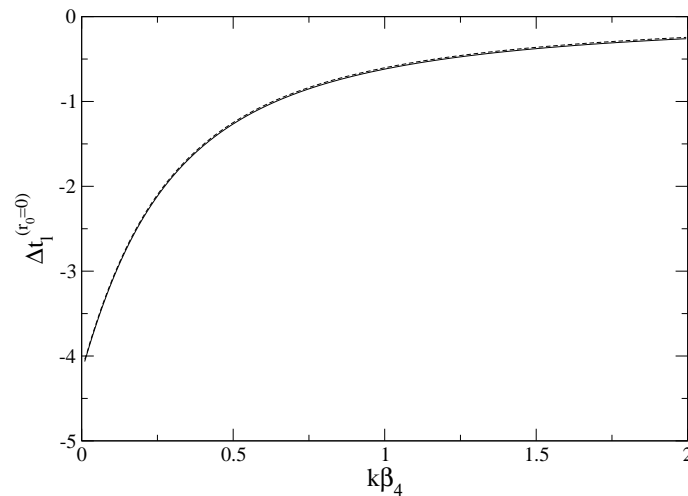


Figure 9. Time shift for near-side quantum reflection. The solid line shows the result obtained for a singular homogeneous potential (9), $\alpha = 4$. The dashed line shows the result obtained with the smoothed potential (23) for a smoothing length $a = 0.2\beta_4$.

reflected part of an almost monochromatic wave packet incident from negative r values returns earlier than the same wave packet after total reflection at $r = 0$, even though the potential step lies wholly beyond $r = 0$ at positive r values.

The apparent paradox is resolved when considering that the quantum reflected wave packet has a smaller amplitude than the totally reflected free wave packet (incident from the left), and that the “boost” it receives is very small compared to the large spread of the almost monochromatic wave packet. This is illustrated in Fig. 10, showing a typical example of a quantum reflected wave packet compared to a wave packet totally reflected at $r = 0$. The initial Gaussian wave packet

$$\psi(r; t = 0) = (\beta\sqrt{\pi})^{-1/2} e^{iqr} \exp\left(-\frac{(r - r_{\text{in}})^2}{2\beta^2}\right) \quad (25)$$

starts at $r_{\text{in}} = -15\,000\beta_4$ in the potential (23) with $\alpha = 4$ and $a = 0.2\beta_4$ corresponding to a step depth $q_0^2 = (25)^2/(\beta_4)^2$. The width parameter is $\beta = 6\,000\beta_4$, corresponding to a momentum spread given by $\Delta q = 1/(6\,000\beta_4)$. The mean initial energy $E = \hbar^2 k^2/(2M)$ is chosen to lie just above threshold, $k = 0.1/\beta_4$, which implies a mean wave number $q = q_0 + 0.0002/\beta_4$ on the down-side of the step. The momentum spread on the up-side of the step, which is relevant for the transmitted part of the wave packet, is given by $\Delta k = (q/k)\Delta q \approx 1/(24\beta_4)$.

The space shift of the quantum reflected wave on the down-side of the step is

$$\Delta r_{\text{ns}} = \frac{\hbar q}{M} \Delta t_{\text{ns}}^{(\text{qu-free}, r_0=0)} \quad (26)$$

and is equal to $-78\beta_4$ in this example according to the Eisenbud-Wigner formula. The shift in the maximum of the quantum reflected wave packet is near $-76\beta_4$ and is barely visible in Fig. 10, because it is so small compared to the large spatial spread of the quantum reflected wave packet. Its probability density at the front edge (moving towards larger negative r values) is never larger than for the totally reflected free wave. Reducing the spatial spread of the incident

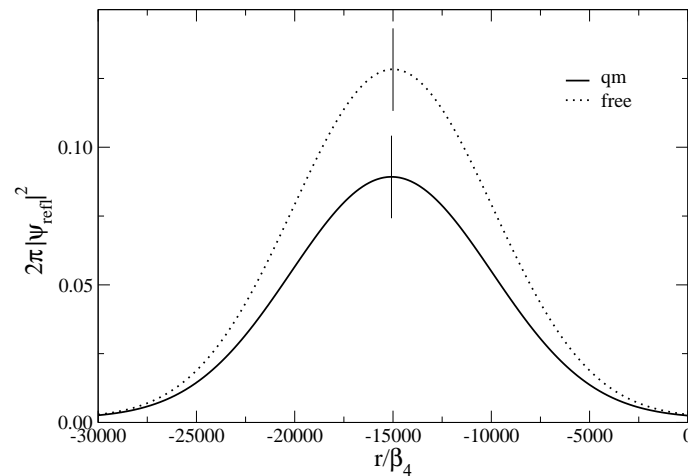


Figure 10. Quantum reflected wave packet in a smoothed potential step (23) with $\alpha = 4$ and $a = 0.2\beta_4$ corresponding to a step depth $q_0^2 = (25)^2/(\beta_4)^2$. The incident Gaussian wave packet with width parameter $6000\beta_4$ started at $r_{\text{in}} = -15000\beta_4$ with mean momentum $\hbar q$, $q = q_0 + 0.0002/\beta_4$ corresponding to a mean wave number $k = 0.1/\beta_4$ for large positive r -values. The solid line shows the quantum reflected wave packet after twice the time the incident wave needed to reach $r = 0$, i.e. passing its initial position on the way back. The dotted line shows the returning wave packet after total reflection at $r = 0$ without any influence of the potential at positive r values. The “boost” meaning negative space shift of the maximum of the quantum reflected wave packet is $-76\beta_4$ while the value given according to the Eisenbud-Wigner formalism by (26) is $-78\beta_4$.

wave packet increases the distortion of the quantum reflected part, and we never see an “acausal advance” of a part of the quantum reflected wave packet due to the potential beyond $r = 0$.

7. Summary

The Eisenbud-Wigner definition of time delay is unambiguous for almost monochromatic wave packets. For quantum reflection in an attractive potential tail, the time delay and the related space shift are *negative* (except for $-1/r^3$ potentials at very low energies). The maximum of the quantum reflected wave returns sooner than that of a free wave reflected at $r = 0$. This time gain is, however, too small to compensate the time delay of the free particle relative to the classical particle accelerated by the attractive potential. The quantum reflected wave is delayed relative to the classical accelerated particle.

For near-side quantum reflection, the Eisenbud-Wigner formula predicts a boost in the reflected wave: a wave packet incident from the left seems to be reflected faster than instantaneously. This boost is still present when the singular attractive potential tail is smoothed to a large negative constant value for $r < 0$; the maximum of the reflected wave packet actually returns sooner than that of the free wave packet. However, due to the reduced amplitude of the reflected wave packet and the smallness of the boost, we see no apparent violation of causality.

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