On Wave-Packets Dynamics

Learning notes

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Abstract

These are working notes on wave-packets: their construction, behaviour and dynamics. Wave equations in classical and quantum physics are often linear. In such cases, wave-packets – linear combinations of solutions corresponding to different frequencies or energies – are themselves solutions of the wave equation, and may possess useful properties such as normalisability, localizability etc. They also tend to exhibit the motion occurring in quantum systems in a way that corresponds to classical concepts. These notes deal with the free motion and potential scattering of wave-packets, almost always in one dimension $\mathbb{R}^1$.

The basic theory here is (very) well known. Indeed, the quantum dynamics is essentially trivial, because we are considering only motion under a Hamiltonian that is constant in time. This means that we never have to solve the time-dependent Schrödinger equation (TDSE) directly; the solutions of the TDSE are simply linear combinations of energy eigenstate multiplied by the standard dynamical phase factor, which is what I mean by the term wave-packet. The fun part comes with a set of numerical calculations on simple models that demonstrate in great detail how wave-packet dynamics actually works. In these models, the wave-packets are always built from plane waves, because that fits the simple systems considered. But the basic theory applies to wave-packets constructed from energy eigenstates of any kind, depending on the system.

Contents

1 Classical wave-packets

1.1 The wave equation

Consider the following partial differential equation governing the behaviour of a field $A(x,t)$ - we work only in $\mathbb{R}^1$ here:

$$\frac{\partial^2 A}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} \tag{1.1}$$

This would be the wave equation of classical electromagnetic theory, for example. There are many other wave equations in classical physics [1]. The solutions are obviously waves:

$$A(x,t) = Ne^{i(kx-\omega t)} \tag{1.2}$$

where the frequency is related, through the wave equation, to the wavelength by

$$\omega = \omega(k) = ck \tag{1.3}$$

This plane wave moves with speed $c = \omega/k$ relative to the positive x-direction (in the sense that planes of equal phase – points of equal phase in this $\mathbb{R}^1$ case – move at this speed). One says that the *phase velocity* is ω/k.

Because the wave equation is linear, we know that a linear combination of the plane wave solutions is also a solution of the wave equation. In the next section we construct and examine such a linear combination – a wave-packet.

1.2 Properties of classical wave-packets

Working in $\mathbb{R}^1$, take a wave-packet of general shape:

$$A(x,t) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} dk\, a(k) e^{i(kx-\omega(k)t)} \tag{1.4}$$

Remember that here the frequency $\omega(k)$ is a function of k because $A(x,t)$ is a solution of some wave equation that relates ω and k.

The normalisation $\int dx|A|^2 = 1$ (or, equivalently, $\int dk|a(k)|^2 = 1$) implies that A has the dimensions $(length)^{-1/2}$ (and that a has the dimensions $(length)^{1/2}$). We also want $a(k)$ to be peaked at $k = k_0$ with a k-width of l^{-1}, say. If we introduce a dimensionless function $f(q)$ of a dimensionless variable q such that $f(q)$ is peaked at $q = 0$ and $f(q) \ll 1$ *when* $|q| > 1$, then we can write

$$a(k) = Cf\big((k-k_0)l\big)$$

where C is some overall amplitude scale with dimensions $(length)^{1/2}$ that allows us to assume that $f(q)$ is of order 1. If we take $f(q)$ to be normalised in the sense that $\int dq f^2 = 1$, then it is easy to

show that normalisation of $A(x,t)$ implies that $C = I^{1/2}$. Thus our canonical normalised form for the envelope function is

$$a(k) = I^{1/2} f\big((k - k_0)I\big) \tag{1.5}$$

For example, if we take the standard normalised Gaussian form (see Appendix A) for $f(q)$

$$f(q) = \pi^{-1/4} e^{-q^2/2} \tag{1.6}$$

then

$$a(k) = \left(\frac{I}{\pi^{1/2}}\right)^{1/2} e^{-(k-k_0)^2 I^2/2} \tag{1.7}$$

Thus (1.4) becomes

$$A(x,t) = \left(\frac{I}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} dk f\big((k - k_0)I\big) e^{i(kx - \omega(k)t)}$$

or, using the dimensionless variable $q = (k - k_0)I$,

$$A(x,t) = e^{i(k_0 x - \omega(k_0)t)} (2\pi I)^{-1/2} \int_{-\infty}^{\infty} dq\, f(q) e^{iqx/I} e^{-i(\omega(k_0 + q/I) - \omega(k_0))t} \tag{1.8}$$

We now look explicitly at the time evolution, ie the motion, of this wave-packet.

1.2.1   At t=0
From (1.8), we have

$$A(x,0) = e^{ik_0 x} (2\pi I)^{-1/2} \int_{-\infty}^{\infty} dq f(q) e^{iqx/I}$$
$$= e^{ik_0 x} I^{-1/2} F(x/I) \tag{1.9}$$

where the (dimensionless) Fourier transform of $f(q)$ is

$$F(\xi) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq\, f(q) e^{iq\xi} \tag{1.10}$$

Equation (1.9) says that at $t = 0$ the wave-packet is a plane wave $e^{ik_0 x}$ whose amplitude varies in space as $F(x/I)$. Because we postulated the characteristics described above for $f(q)$, we can say that the amplitude function $F(\xi)$ will be peaked at $\xi = 0$ with width ~1 in the sense that $F(\xi)$ will be of order 1 and

$$F(\xi) \ll 1 \ when \ |\xi| > 1 \tag{1.11}$$

Moreover, if $f(q)$ is normalised, so is $F(\xi)$:

$$\int_{-\infty}^{\infty} dq \left| f(q) \right|^2 = 1 = \int_{-\infty}^{\infty} d\xi \left| F(\xi) \right|^2 \tag{1.12}$$

For example, the Gaussian form (1.6) for $f(q)$ gives $F(\xi) = \pi^{-1/4} e^{-\xi^2/2}$ (see Appendix A). The amplitude function $F(x/l)$ in (1.9) is thus peaked at $x = 0$ and has width $\sim l$. Hence the standard picture:
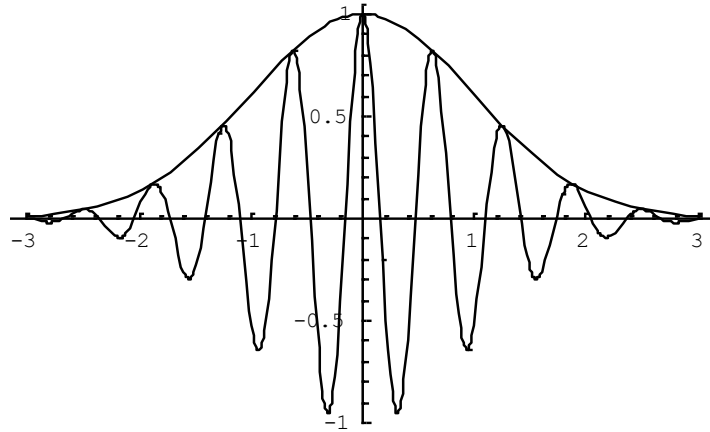
> **Note 1:**
>
> *It's easy to show that for the following wave-packet*
>
> $$A(x,t) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dk\, a(k) e^{i\left(k(x-x_0) - \omega(k)(t-t_0)\right)} \tag{1.13}$$
>
> *we get*
>
> $$A(x, t = t_0) = l^{1/2} e^{ik_0(x-x_0)} F\left((x - x_0)/l\right)$$
>
> *So this means that a wave-packet of the form (1.13) is localised at position $x = x_0$ at time $t = t_0$.*

1.2.2   For t>0

Now we have to know the function $\omega(k)$. Note, from (1.8) that if ω is independent of k the wave-packet does not move at all; it just sits at $x = 0$ oscillating up and down with frequency ω[1]. Since we know that wave-vectors near k_0 are important in the integral (1.8), we make a Taylor expansion of $\omega(k)$ around k_0:

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[1] Recall that in band theory a completely flat band means no hopping. But energy bands are a quantum, not classical, concept. The connection is just the wave equation in the two cases – see section 2.1.

$$\omega(k) = \omega_0 + v_0(k - k_0) + w_0(k - k_0)^2 + \dots \tag{1.14}$$

where

$$\omega_0 = \omega(k_0)$$

$$v_0 = \left.\frac{d\omega(k)}{dk}\right|_{k=k_0} \tag{1.15}$$

$$w_0 = \left.\frac{1}{2}\frac{d^2\omega(k)}{dk^2}\right|_{k=k_0}$$

If we take only the linear term in (1.8) we get

$$A(x,t) \sim A^{(1)}(x,t) = (2\pi l)^{-1/2} e^{i(k_0 x - \omega_0 t)} \int_{-\infty}^{\infty} dq\, f(q) e^{iq(x - v_0 t)/l}$$

$$= l^{-1/2} e^{i(k_0 x - \omega_0 t)} F\big((x - v_0 t)/l\big) \tag{1.16}$$

Thus $A^{(1)}(x,t)$ has a phase function $e^{i(k_0 x - \omega_0 t)}$ representing a plane wave moving with speed ω_0/k_0 relative to the $+x$ direction and an amplitude function that is the same in shape as at $t = 0$ but now centred at $x = v_0 t$. So the wave-packet moves with the *group velocity* v_0 relative to the x-direction and maintains its width l. There's no wave-packet spreading in this linear approximation.

Now if we put in the quadratic term in (1.14) we get

$$A(x,t) \sim A^{(2)}(x,t) = (2\pi l)^{-1/2} e^{i(k_0 x - \omega_0 t)} \int_{-\infty}^{\infty} dq\, f(q) e^{-iw_0 q^2 t/l^2} e^{iq(x - v_0 t)/l}$$

$$= l^{-1/2} e^{i(k_0 x - \omega_0 t)} F'\big((x - v_0 t)/l\big) \tag{1.17}$$

where $F'(\xi)$ is the Fourier transform of the modified amplitude function

$$f'(q) = f(q) e^{-iw_0 q^2 t/l^2} \tag{1.18}$$

The effect of this is as follows:

- the phase function becomes $e^{i(k_0 x - \omega_0 t + \varphi(t))}$; it still represents a plane wave but there is an additional phase contribution coming from F'.

- The amplitude function diminishes in time and its width increases – wave-packet spreading – but it still moves with speed v_0.

These statements can be checked analytically for a Gaussian wave-packet (see Appendix A). In particular, the modified x-width has the form [1]

$$l'(t) = \left(l^2 + 4w_0^2 t^2 / l^2\right)^{1/2}$$

In summary:

- If ω is independent of k, the wave-packet doesn't move at all;

- If ω is linear in k (as per light), the wave-packet moves with the usual group velocity and maintains a constant width;

- If ω is non-linear in k (as per electrons - see section 2.1), the wave-packet moves with the usual group velocity and spreads out as t increases away from 0 (in either direction).

> ### Note 2: Stationary phase
>
> *This motion of the wave-packet (ie of the maximum in the amplitude function) can be obtained directly from* (1.4) *using the **stationary phase** idea [3]. If $a(k)$ is peaked around k_0 then the maximum value of the integral will be reached when, in the region around k_0, the phase in the exponential varies slowly. So maxima are associated with points where the phase is stationary:*
>
> $$\frac{d}{dk}(phase)\Big|_{k_0} = \frac{d}{dk}\big(kx - \omega(k)t\big)\Big|_{k_0} = 0$$
>
> *In this way we predict the maximum amplitude to be at* $x = \dfrac{d\omega(k)}{dk}\Big|_{k_0} t = v_0 t$.

2   Quantum wave-packets

2.1   The time-dependent Schrödinger equation

The time-dependent Schrödinger equation (TDSE) governing the evolution of a wave function $\psi(x,t)$ is

$$i\frac{\partial \psi}{\partial t} = \mathcal{H}\psi \tag{2.1}$$

For free particles the Hamiltonian contains only kinetic energy and we have

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} \tag{2.2}$$

We know that the solutions of (2.2) are plane waves:

$$\varphi_k(x,t) = Ne^{i(kx-\varepsilon t)} \tag{2.3}$$

where

$$\varepsilon = \varepsilon(k) = \frac{1}{2}k^2 \tag{2.4}$$

Compare (2.3) and (2.4) with the classical analogues (1.2) and (1.3). The only difference is in the dispersion laws $\varepsilon(k)$ and $\omega(k)$: the classical dispersion is linear in k because its wave equation contains the second partial derivative in time, while the quantum dispersion is quadratic in k because the TDSE contains the first partial derivative in time. However, both the classical wave equation and the TDSE are linear and so, following section 1.2, we can construct a free particle quantum wave-packet

$$\psi(x,t) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dk\, a(k) e^{i(kx - \varepsilon(k)t)} \tag{2.5}$$

This linear combination is clearly a solution of the TDSE, which in turn means that all the properties of classical wave-packets described in section 1.2 also apply to the free particle quantum wave-packet. In particular, we see that since $\varepsilon(k)$ is certainly not linear in k the wave-packet spreading described in 1.2 is an inherent phenomenon for free particle quantum wave-packets. Indeed, as shown in section 3.2, it is a very strong effect.

Note 3:

Right at the outset there is an important point here about normalisation. A plane wave is not itself normalisable – hence the subtleties of normalising stationary states in a continuous spectrum (see [2], [3], [4]). In this sense, they can't represent physically realisable states. A wave-packet such as that given by (2.5), however, is certainly normalisable:

$$\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, a(k) \int_{-\infty}^{\infty} dk'\, a^*(k') e^{-i(\varepsilon(k) - \varepsilon(k'))t} \int_{-\infty}^{\infty} dx\, e^{i(k-k')x}$$

$$= \int_{-\infty}^{\infty} dk\, a(k) \int_{-\infty}^{\infty} dk'\, a^*(k') e^{-i(\varepsilon(k) - \varepsilon(k'))t} \delta(k - k') = \int_{-\infty}^{\infty} dk\, |a(k)|^2$$

There's no problem about choosing envelope functions such that $\int_{-\infty}^{\infty} dk\, |a(k)|^2 = 1$. Thus wave-packets like this can be taken to describe realisable states of electrons

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More generally, we consider motion under a Hamiltonian $\mathcal{H}(x)$. The Hamiltonian can depend on time (the most interesting cases really: forced dynamics) but here we suppose that it is time-independent and therefore has energy eigenfunctions and eigenvalues $\varphi_q(x)$ and ε_q:

$$\mathcal{H}(x)\varphi_q(x) = \varepsilon_q \varphi_q(x) \tag{2.6}$$

The label q stands for all the quantum numbers needed to specify an energy eigenvalue, discrete or continuous. When we integrate over q, we mean integrate over the continuous spectrum and/or sum over the discrete spectrum [3], [4].

We can now make an immediate generalisation of (2.5) and write the canonical form of a wave-packet for a system with a time-independent Hamiltonian:

$$\psi(x,t)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}dq\,a(q)\varphi_q(x)e^{-i\varepsilon_q t} \tag{2.7}$$

2.2   Density and current

Consider a wave packet of the following form (compare (1.8):

$$\psi(x,t)=e^{i(k_0 x-\varepsilon(k_0)t)}(2\pi l)^{-1/2}\int_{-\infty}^{\infty}dq\,f(q)e^{iqx/l}e^{-i(\varepsilon(k_0+q/l)-\omega(k_0))t} \tag{2.8}$$

The corresponding density is

$$\rho(x,t)=|\psi(x,t)|^2$$
$$=\frac{1}{2\pi l}\int dq\int dq'\,f^*(q)f(q')e^{-i(q-q')x/l}e^{i(\varepsilon(p/l+k_0)-\varepsilon(p'/l+k_0))t} \tag{2.9}$$

Let's evaluate this using the expansion (1.14), replacing the classical frequency $\omega(k)$ by the quantum eigenvalue $\varepsilon(k)$ of course, stopping at the linear term:

$$\rho^{(1)}(x,t)=\frac{1}{2\pi l}\int dq\int dq'\,f^*(q)f(q')e^{-i(q-q')(x-v_0 t)/l} \tag{2.10}$$

Thus we can write, using (1.10),

$$\rho^{(1)}(x,t)=l^{-1}\left|F\big((x-v_0 t)/l\big)\right|^2 \tag{2.11}$$

in agreement with (1.16). For the Gaussian wave packet defined by (1.6) or (1.7) we find the explicit form

$$\rho^{(1)}(x,t)=l^{-1}e^{-(x-v_0 t)^2/l^2} \tag{2.12}$$

The current associated with a wave function $\psi(x,t)$ is

$$j(x,t)=\frac{1}{2i}\left\{\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}-\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}\right\}$$
$$=\mathcal{I}m\left(\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right) \tag{2.13}$$

Evaluating this using (1.14) and stopping at the linear term again, we find

$$j^{(1)}(x,t)=k_0 l^{-1}\left|F\big([x-v_0 t]/l\big)\right|^2=k_0\rho^{(1)}(x,t) \tag{2.14}$$

Now if ρ and j are calculated from a wave function that is an exact solution of the Schrödinger equation, then (see [3], [4]) they must satisfy the continuity equation

$$\frac{\partial\rho(x,t)}{\partial t}+\frac{\partial j(x,t)}{\partial x}=0 \tag{2.15}$$

But if one calculates the density and current from an approximate wave function, then the continuity equation is not automatically satisfied (and charge may not be conserved). Indeed, for the Gaussian wave packet, the linear approximations (2.12) and (2.14) yield

$$\frac{\partial \rho^{(1)}}{\partial t} = \frac{2v_0}{l^3}\left(x - v_0 t\right)e^{-(x-v_0 t)^2 / l^2}$$

$$\frac{\partial j^{(1)}}{\partial x} = -\frac{2k_0}{l^3}\left(x - v_0 t\right)e^{-(x-v_0 t)^2 / l^2}$$

In general, of course, $v_0 = \dfrac{d\varepsilon(k)}{dk}\bigg|_{k_0} \neq k_0$ and so continuity is violated.

3   Wave-packet dynamics in free space

Section 2 describes essentially all the theory needed to discuss the motion of wave-packets in free space (at least those constructed from plane waves – which could be one definition of free space here). But to make it all real, here are some results of a numerical evaluation of the dynamical equation (2.5). For details of the calculations see [5].

The amplitude function in (2.5) was taken to be a Gaussian of k-width l^{-1} peaked at $k = k_0$:

$$a(k) = e^{-(k-k_0)^2 l^2 / 2}$$

The energy vs k dispersion relation was taken to be a 2nd order polynomial:

$$\varepsilon(k) = \alpha k + \beta k^2$$

The group velocity and width functions appearing in the Taylor expansion of $\varepsilon(k)$ about k_0 and defined in (1.15) are thus

$$v_0 \equiv \frac{d\varepsilon(k)}{dk}\bigg|_{k_0} = \alpha + 2\beta k_0, \quad w_0 \equiv \frac{1}{2}\frac{d^2\varepsilon(k)}{dk^2}\bigg|_{k_0} = \beta$$

Of course, for proper plane waves, we should take $\alpha = 0$, $\beta = 1$. But it's useful for exhibiting the wave-packet spreading phenomenon to give ourselves more freedom in the dispersion relation. For all the calculations in this section, we'll choose a dispersion relation such that the group velocity is equal to 2.

3.1   Motion
The following figure shows the simple motion of a wave-packet in time using a linear dispersion relation.

Dynamics of Plane-Wave-Packets

Linear dispersion relation: energy = 2*k
l   = 0.5
k0 = 1.0
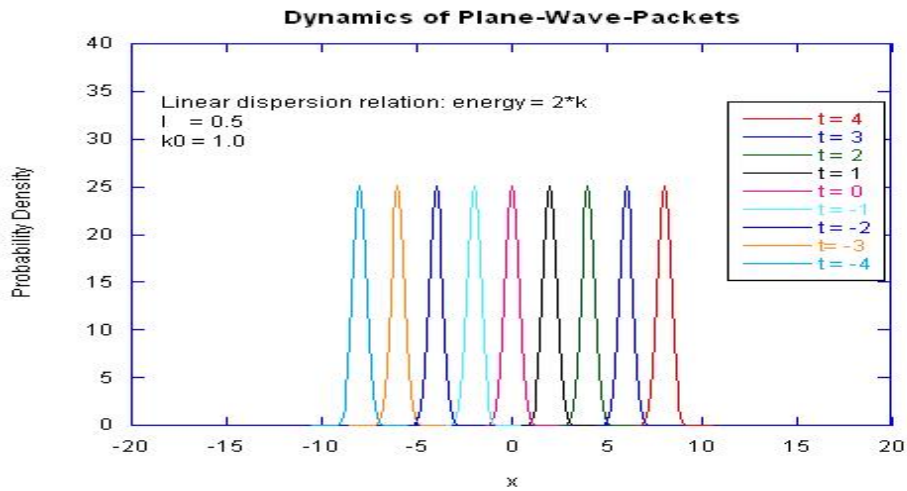
The wave-packet just moves from left to right with a speed of 2 and maintains its shape and length as it moves.

3.2   Wave-packet spreading

This picture shows exactly the same calculation but with a polynomial dispersion relation.

Dynamics of Plane-Wave-Packets

Polynomial dispersion relation: energy = 1.5*k + 0.25*k*k
l   = 0.5
k0 = 1.0
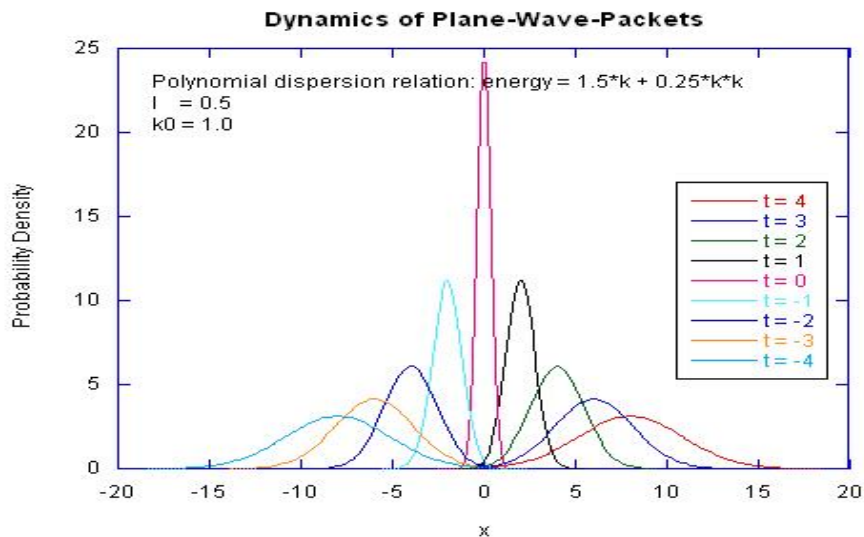
Again, the wave-packet moves from left to right with a speed of 2 but now its shape spreads out quite dramatically as time increases away from $t = 0$. This effect is even more pronounced if we use a pure quadratic dispersion relation:

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Dynamics of Plane-Wave-Packets
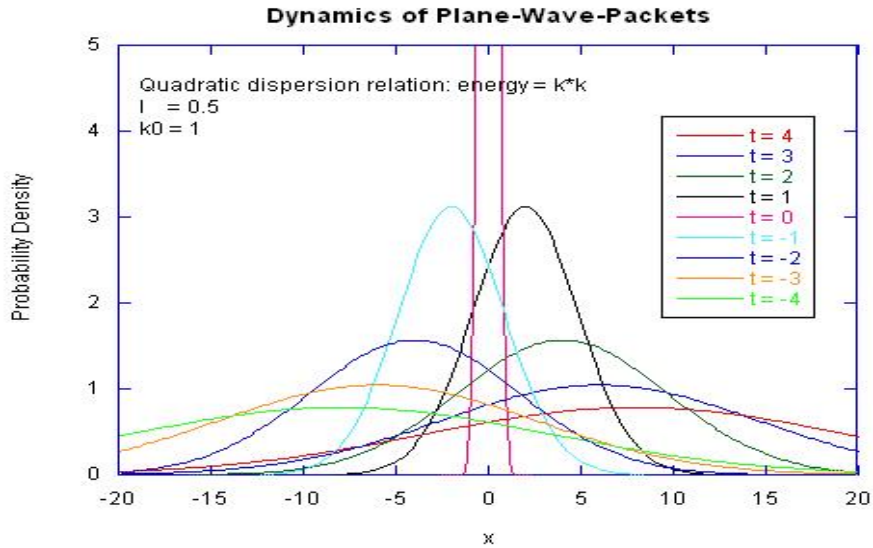
Note that at $t = 0$, the wave-packet is independent of the dispersion relation.

4   Scattering of wave-packets in $\mathbb{R}^1$

In an illuminating calculation, Cohen-Tannoudji et al [3] treat the scattering of a wave-packet by a potential step. Their method is really a general one for describing wave-packet dynamics in a static potential. First, you solve for the stationary states of the static potential and construct a wave-packet

$$\psi(x,t) = (2\pi)^{-1/2} \int dk\, g(k) \phi_k(x) e^{-i\varepsilon_k t} \tag{4.1}$$

involving the wave functions $\phi_k(x)$ and eigenvalues ε_k of the stationary states and an envelope function which confers the required properties on the wave-packet (eg moving to the right with a certain speed, whatever) – compare the general wave-packet form (2.7). The stationary states will generally be a continuum (or nearly so), but certainly don't need to be plane waves. Indeed, in the case of scattering by a potential step the stationary states are the full solutions as worked out in Landau & Lifshitz [2] and every other quantum mechanics book by matching plane wave solutions with different wave vector on either side of the step. Then, to see the dynamics you just let the above wave-packet evolve in time, ie just evaluate it at different times. You don't have to solve the time-dependent Schrödinger equation because the wave-packet is automatically such a solution.

In this way, Cohen-Tannoudji et al start off their wave-packet at some negative x moving towards the step at the origin. When the wave-packet reaches the step its structure becomes complex, with interferences all over the place, but after more time elapses it evolves into a reflected wave-packet (and a transmitted wave-packet if its energy is above the step). Interesting things like time-delays in the scattering can be analysed in this way. It's rather magical – all this complex dynamics is *embedded in the stationary states*, and it emerges via the wave-packet equation (4.1).

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Cohen-Tannoudji et al actually produce their analysis by using the stationary phase method to estimate the location of the wave-packet maximum as a function of time. They get a long way by this means, but it's irresistible to do a numerical evaluation like that of section 3 for this square barrier problem. Again, this makes it all real and it also provides a fully time-dependent description of a very simple but not completely trivial scattering problem.

We start this by recalling the standard theory of the stationary states for the square barrier potential in $\mathbb{R}^1$.

4.1   The time-independent scattering problem

The potential looks like this:
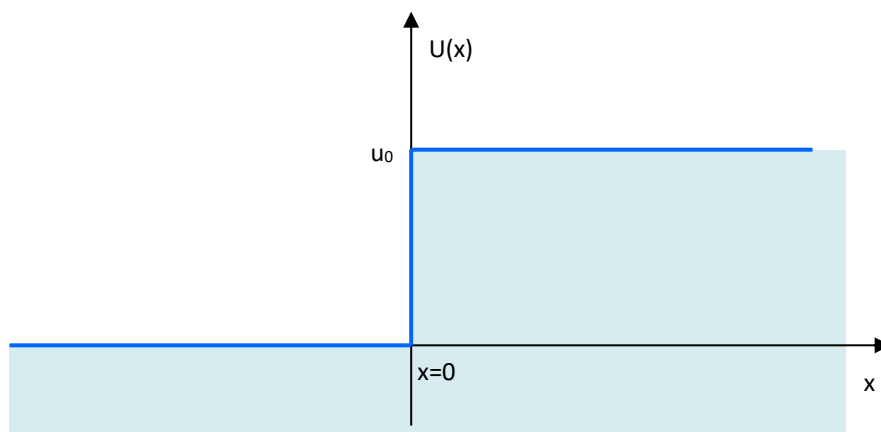
The height of the barrier at $x = 0$ is u_0 - we sometimes write this as $\kappa_0 \equiv \sqrt{u_0}$. We want to find the stationary state wave-function corresponding to a given energy. As in all the textbooks (see [2], [3]), we write this in terms of plane waves:

$$\phi_k(x) = (1 - \theta(x))\{e^{ikx} + A(k)e^{-ikx}\} + \theta(x)B(k)e^{i\bar{k}x} \tag{4.2}$$

with

$$k = \sqrt{\varepsilon}$$
$$\bar{k} = \sqrt{\varepsilon - u_0} = \sqrt{k^2 - \kappa_0^2} \tag{4.3}$$

The first term in (4.2) is valid for $x < 0$, the second for $x > 0$. Since we want to describe a wave incident on the barrier from the left, we have omitted a right-to-left travelling component in the region $x > 0$. We also choose to normalise the state such that the coefficient of the left-to-right travelling (incident) wave in region $x < 0$ is 1. As an aside (almost), note that the formula for $\bar{k}$, the wave-vector in the region $x > 0$, has a branch point at $\varepsilon = u_0$ in the complex ε plane. Since $\bar{k}$ can certainly be imaginary, it's necessary to make sure in a real calculation that it stays on the correct sheet. This is what it should look like:

Square Barrier Scattering; kbar
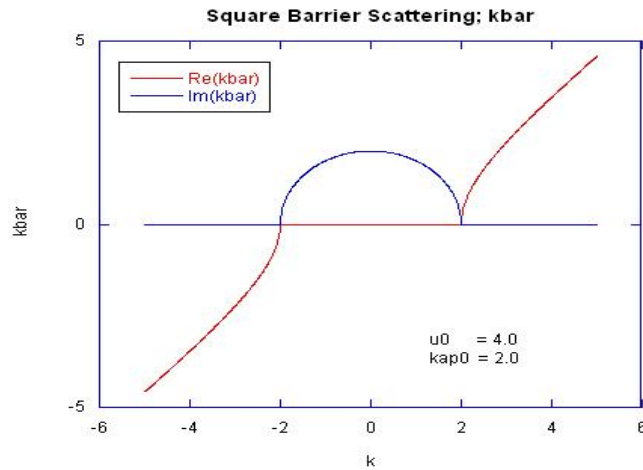
The standard calculation to match the two pieces of the wave-function smoothly across $x = 0$ gives these results for the scattering amplitudes:
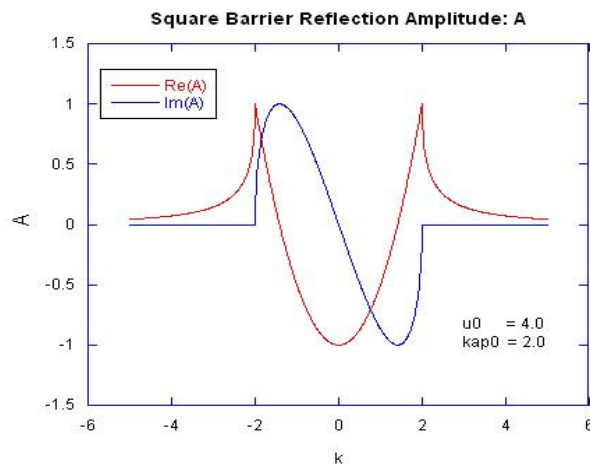
$$A(k) = \frac{k - \bar{k}}{k + \bar{k}}$$

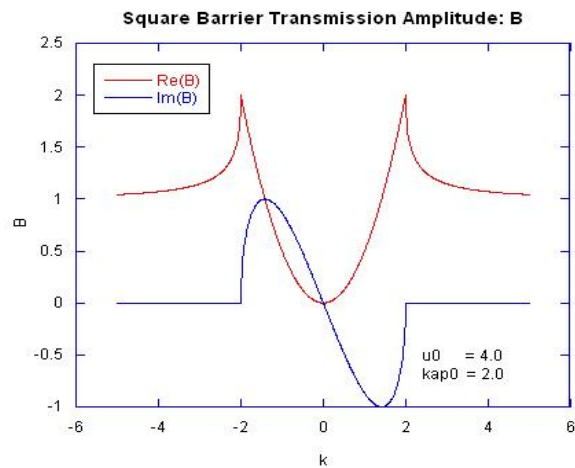$$B(k) = \frac{2k}{k + \bar{k}}$$

(4.4)

For obvious reasons, the coefficient A represents the amplitude for reflection and B that for transmission. Note that

$$1 + A(k) = B(k)$$

Clearly the imaginary parts of A and B are the same. Numerical evaluations of the scattering amplitudes are given below:

Square Barrier Reflection Amplitude: A

Square Barrier Transmission Amplitude: B

These pictures demonstrate that for energies below the barrier, the amplitudes are complex. This implies that for $\varepsilon < u_0$ reflection is accompanied by a phase shift related to the phase of A. The next picture gives the modulus and phase of A (with a little care taken to remove jumps of π in the phase, corresponding to zeroes of the real part of A):


Square Barrier Reflection Amplitude: A
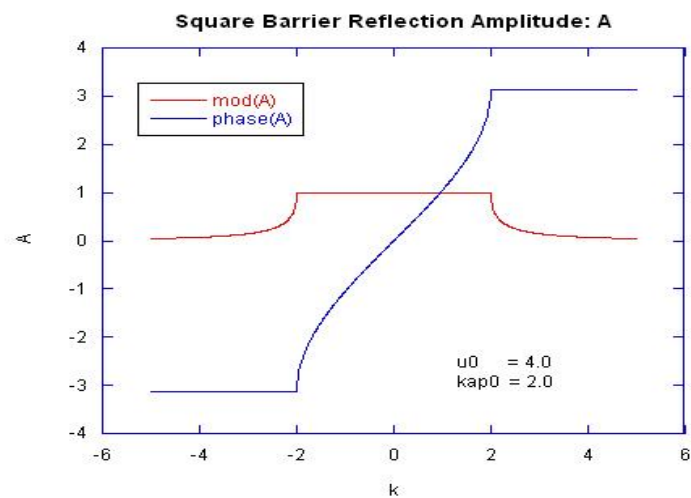
This phase shift produces a time-delay of the reflected wave, as we shall see in section 4.2.1.

Finally we show two calculations of the full wave-function in (4.2), first for an energy below the barrier:

Square Barrier: Stationary State Wave-Function
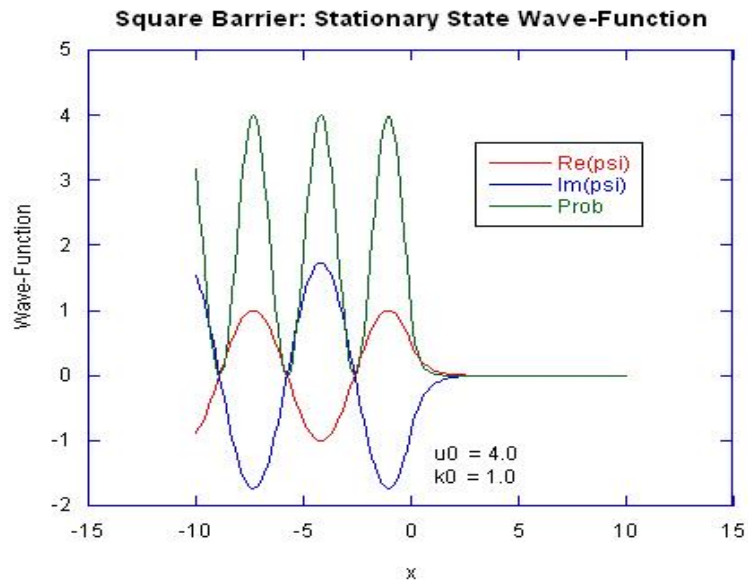
and second for an energy above the barrier:

Square Barrier: Stationary State Wave-Function
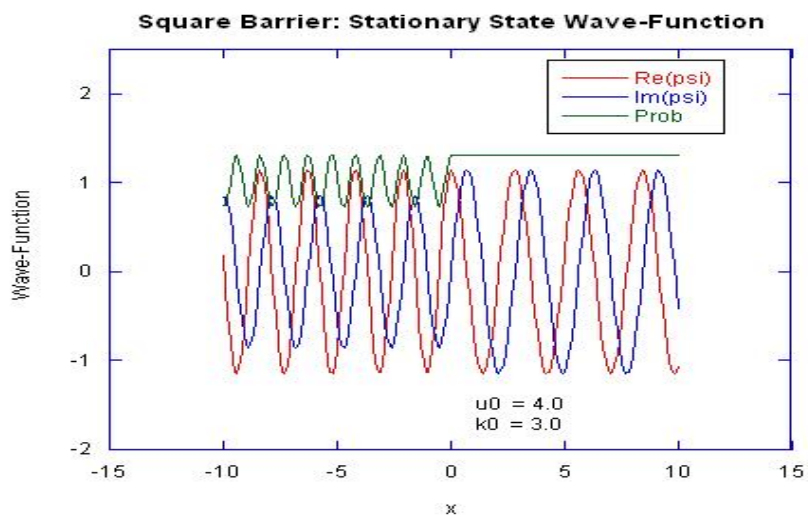
Clearly these functions are smoothly continuous at $x = 0$, and show the expected characteristics. We now use these wave-functions to construct a wave-packet with which to see the dynamics of scattering explicitly in time.

4.2   Wave-packet dynamics

We can now use the stationary states just discussed to build a wave-packet whose motion we want to follow. The wave-packet is given by equation (4.1) in which we insert the wave-functions given by (4.2). The quadrature in (4.1) is carried out by just the same methods as in section 3 – see [6] for details. Note that the wave-packet is constructed so as to arrive at the barrier at $t = 0$.

4.2.1 Total reflection

We first consider the case where $k_0^2 < \kappa_0^2 = u_0$. Here we expect no significant transmission into the region $x > 0$. The figure below shows results for a wave-packet with a linear dispersion law.

Wave-Packet incident on a Square Barrier at x = 0
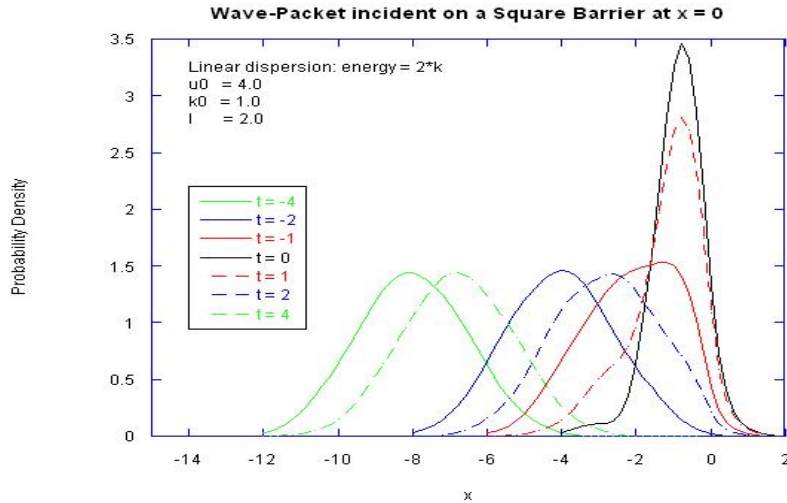
Reflection does indeed happen! When $t < 0$, the wave-packet moves from left to right. As it approaches the barrier, it becomes compressed (because it cannot penetrate far into the region $x > 0$. It is then reflected – for times $t > 0$ it moves from right to left – but the reflected wave is suffers a time delay manifested in the above figure by the observation that the peak of the wave-packet at time t occurs at a position displaced by a distance $v_0 \tau_W$ from its position at time $-t$ on the inward journey. This confirms the expectation outlined in section 4.1 above. To see this, write the reflected wave-packet as follows:

$$\varphi_R(x,t) = \int dk\, g(k) A(k) e^{-i(kx + \varepsilon_k t)}$$
$$= \int dk\, g(k) |A(k)| e^{-i(kx + \varepsilon_k t - \theta(k))}$$

where we've separated the reflection amplitude into its modulus and phase $\theta(k)$. The stationary phase condition is thus

$$\frac{d}{dk}\left(kx + \varepsilon(k)t - \theta(k)\right)\Big|_{k_0} = 0$$
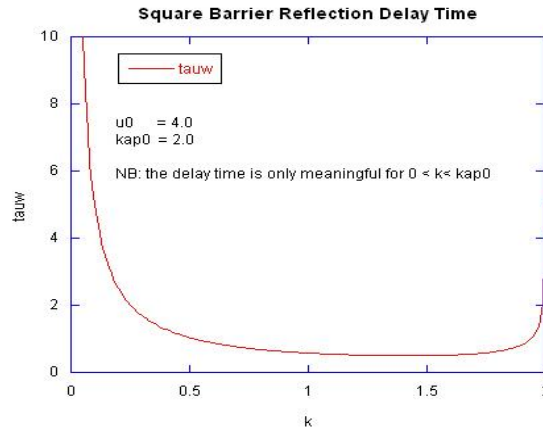
which we can write as follows:

$$x = -v_0\left(t - \tau_W\right)$$

with

$$v_0 = \left.\frac{d\varepsilon(k)}{dk}\right|_{k_0}$$

$$\tau_W = \left.\frac{d\theta(k)}{dk}\right|_{k_0} \bigg/ \left.\frac{d\varepsilon(k)}{dk}\right|_{k_0}$$

The following figure shows the time-delay corresponding to the above calculations of the reflection amplitude.

How does all this actually work in the k-quadrature (4.1)? Clearly, for times $t < 0$ the reflected and transmitted components of the wave-functions for different wave-vectors cancel out while the incident wave components add up constructively within a certain range of x, just as they do for wave-packets in free space. For times $t > 0$, on the other hand, the situation is the reverse: the incident components cancel out while the reflected components add up constructively. This is basis of the stationary phase argument.

The following figure shows the same calculations, but now using a polynomial dispersion law. The story is the same, but now wave-packet spreading takes place within the scattering process.
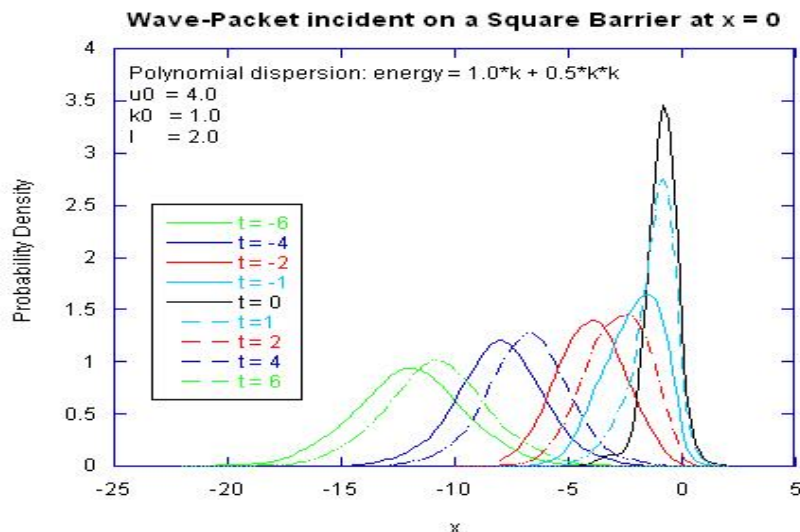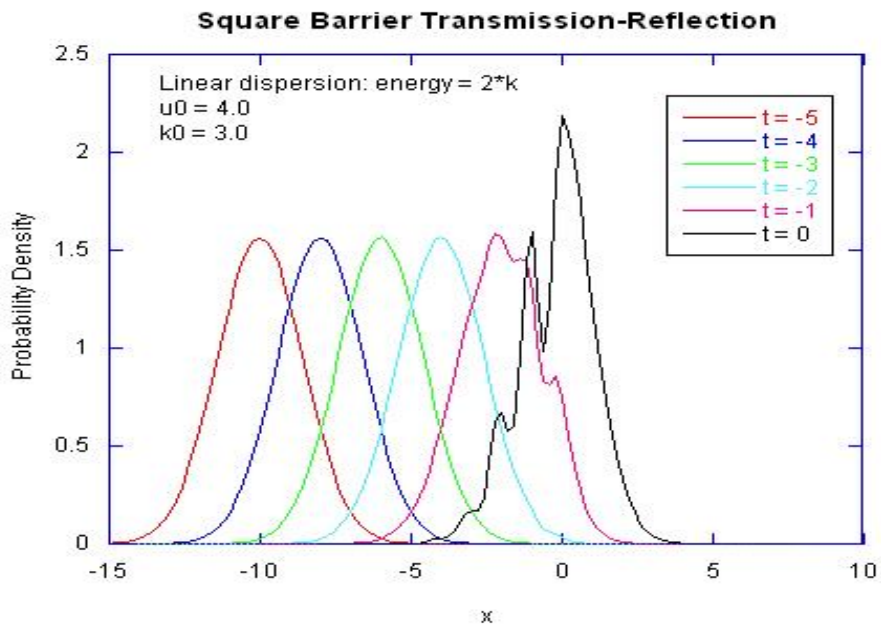
We mention one final detail here. There is no observable weight in the above figures in the classically forbidden region $x > 0$, at least for positions beyond the region of exponential decay of the wave-functions. However, if one looks carefully at the calculations, there is a tiny piece of wave-packet that is transmitted into the forbidden region. This corresponds to components of the wave-packet in (4.1) that have $k > \kappa_0$ - that is, energies above the barrier. These occur because we are relying on the Gaussian amplitude function in (4.1) to cut off the k-integral. Cohen-Tannoudji et al [3] actually force the upper limit of this integral to be κ_0 because any k-components greater than this would corrupt their argument based on the stationary phase method. Similarly, when looking at the partial reflection/transmission case discussed below, Cohen-Tannoudji et al force the lower limit of the integral to be κ_0. However, since we are analysing these cases by a full numerical evaluation not reliant on stationary phase arguments, we don't need to make these restrictions, which seem unnecessary from a general point of view.

4.2.2   Partial reflection-transmission

Now we consider the case where $k_0^2 > \kappa_0^2 = u_0$. Here we do expect transmission into the region $x > 0$, along with the specifically quantum effect of some reflection back into the region $x < 0$. The figure below shows results for a wave-packet with a linear dispersion law.
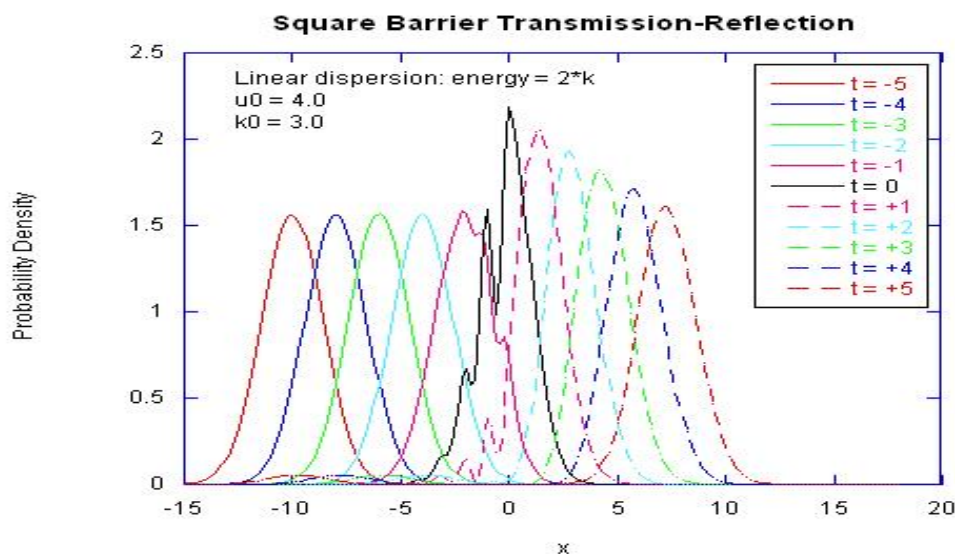

In this quite complicated picture, we see all of these phenomena. It's a little clearer if we take the figure apart and discuss it piece by piece. Below we show the motion of the wave-packet for $t \leq 0$.

Square Barrier Transmission-Reflection

Linear dispersion: energy = 2*k
u0 = 4.0
k0 = 3.0

t = -5
t = -4
t = -3
t = -2
t = -1
t = 0

This shows the expected movement towards the barrier, in whose vicinity the shape of the wave-packet becomes complicated by interference between the incident and reflected components.

The following figure shows the motion for $t > 0$.

Square Barrier Transmission-Reflection

Linear dispersion: energy = 2*k
u0 = 4.0
k0 = 3.0

t = +5
t = +4
t = +3
t = +2
t = +1
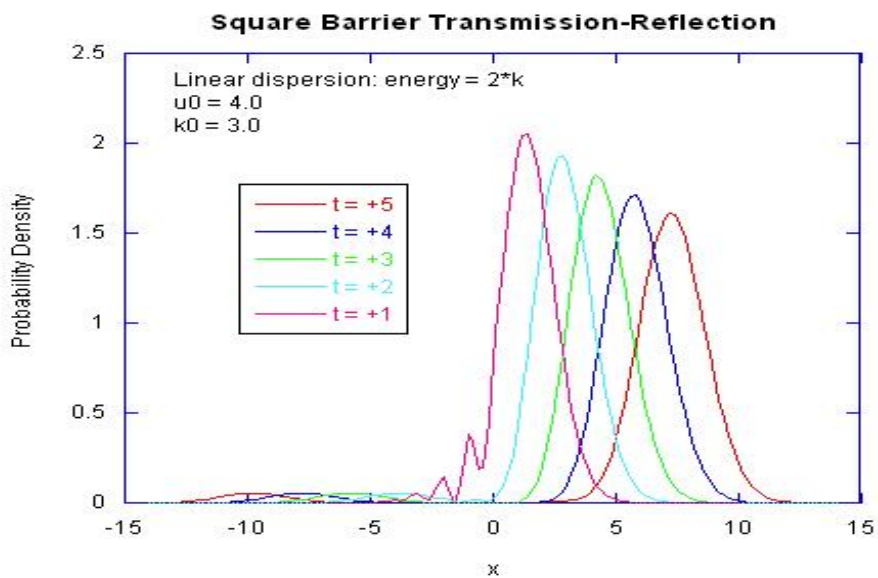
Here we see the transmitted wave-packet – it looks like it's spreading, even for this linear dispersion case, but this is really only a "relaxation" of the compression that occurs near the barrier. The transmitted wave travels more slowly than the incident wave, because its wave-vector is $\bar{k}$, not k. In fact, if one goes through the stationary phase calculation for the transmitted wave-packet, one

finds that the position of its peak is given by $x = \dfrac{\overline{k}}{k} v_0 t$. For the parameters of the calculation depicted above, $\dfrac{\overline{k}}{k} v_0 = \dfrac{\sqrt{5}}{3} 2 \sim 1.5$. The picture above shows that the transmitted wave-packet is indeed moving at this speed.

Notice also that there is some weight in the region $x < 0$. This is made more clearly visible below, where the scale is blown up.
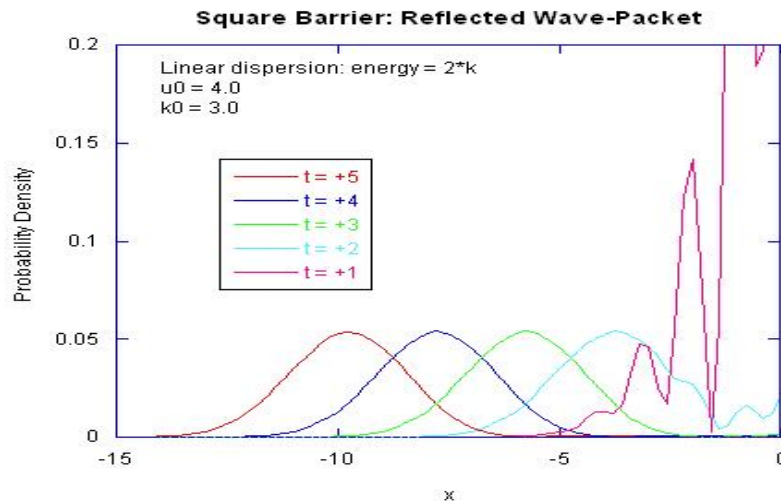
We can see the reflected wave-packet moving beautifully from right to left with just the right speed and with no phase-shift (compare the discussion in section 4.2.1). This is because the reflection amplitude $A(k)$ is purely real for $k > \kappa_0$ (see the figures in section 4.1).
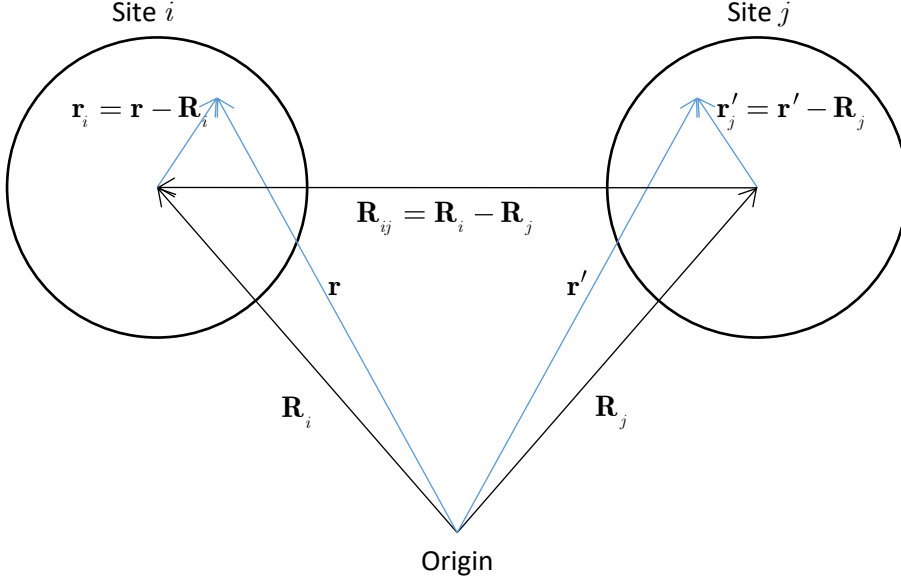
Finally, we note that in the limit $u_0 \to 0$ the numerical results of this section should agree exactly with those of section 3 on free-space propagation, and they do (once all the complications of staying on the right Riemann sheet are sorted out).

5   A general theory of wave-packet scattering

Consider a plane wave incident on a cluster, by which we mean anything from a single atom to a crystal. By the method of section 4 we can give a full time-dependent description of the scattering process in a cluster if we know its energy eigenstates. Since we're dealing with continuum states, as in section 4, the thing to do is to use the Lipmann-Schwinger equation for these energy eigenstates. In the language of multiple scattering theory [7], this reads

$$\psi_{\mathbf{k}}\left(\mathbf{r},\varepsilon^{+}\right)=e^{i\mathbf{k}\cdot\mathbf{r}}+\int d\mathbf{r}'\int d\mathbf{r}''G_{0}\left(\mathbf{r},\mathbf{r}';\varepsilon^{+}\right)T\left(\mathbf{r}',\mathbf{r}''\right)e^{i\mathbf{k}\cdot\mathbf{r}''}$$
$$=e^{i\mathbf{k}\cdot\mathbf{r}}+\sum_{ij}\int d\mathbf{r}'\int d\mathbf{r}''G_{0}\left(\mathbf{r},\mathbf{r}';\varepsilon^{+}\right)\tau^{ij}\left(\mathbf{r}',\mathbf{r}''\right)e^{i\mathbf{k}\cdot\mathbf{r}''} \tag{5.1}$$

A complete calculation requires these solutions (or, equivalently, the Green's function) in all regions of space, and multiple scattering theory provides this. Here we simply note that in regions far outside the cluster things are easier because the solutions are determined by the scattering amplitude alone.

Site i Site j

$\mathbf{r}_{i}=\mathbf{r}-\mathbf{R}_{i}$

$\mathbf{r}_{j}'=\mathbf{r}'-\mathbf{R}_{j}$

$\mathbf{R}_{ij}=\mathbf{R}_{i}-\mathbf{R}_{j}$

$\mathbf{r}$ $\mathbf{r}'$

$\mathbf{R}_{i}$ $\mathbf{R}_{j}$

Origin

The scattering amplitude of any object is defined by the asymptotic form of the wave function at distances large compared with the size of the cluster and therefore far away from any scattering potential. In general this asymptotic form is

$$\lim_{r\to\infty}\psi_{\mathbf{k}}\left(\mathbf{r},\varepsilon^{+}\right)=e^{i\mathbf{k}\cdot\mathbf{r}}+\psi_{\mathbf{k}}^{scat}\left(\mathbf{r},\varepsilon^{+}\right)=e^{i\mathbf{k}\cdot\mathbf{r}}+f\left(\mathbf{k}\right)\frac{e^{ikr}}{r} \tag{5.2}$$

Here $\varepsilon^{+}=\varepsilon+i0^{+}=k^{2}+i0^{+}$

To determine the scattering amplitude $f\left(\mathbf{k}\right)$ we will use the geometry depicted above and write the total wave function = incident wave plus scattered wave by means of the Lipmann-Schwinger equation (5.1). Expressing this in terms of the on-shell matrix elements of τ^{ij} allows us to write

$$f\left(\mathbf{k}\right)=-4\pi\sum_{ij}\sum_{LL'}i^{(l'-l)}Y_{L}^{*}\left(\hat{\mathbf{r}}\right)Y_{L'}\left(\hat{\mathbf{k}}\right)\sum_{L_{1}L_{2}}d_{LL_{1}}\left(-\mathbf{R}_{i}\right)\tau_{L_{1}L_{2}}^{ij}\left(d_{L'L_{2}}\left(-\mathbf{R}_{j}\right)\right)^{*}$$
$$=-4\pi\sum_{ij}\sum_{LL'}i^{(l'-l)}Y_{L}^{*}\left(\hat{\mathbf{r}}\right)Y_{L'}\left(\hat{\mathbf{k}}\right)\sum_{L_{1}L_{2}}d_{LL_{1}}\left(-\mathbf{R}_{i}\right)\tau_{L_{1}L_{2}}^{ij}d_{L_{2}L'}\left(\mathbf{R}_{j}\right) \tag{5.3}$$

where the real space structure constants $d_{LL'}\left(\mathbf{R}\right)$ occur. The single scatterer result $f^{SS}\left(\mathbf{k}\right)$ is obtained by letting $\tau_{L_{1}L_{2}}^{ij}=t_{L_{1}}\delta_{L_{1}L_{2}}\delta_{ij}$, $\mathbf{R}_{i}=0$ and noting that $\lim_{R\to 0}d_{LL'}\left(\mathbf{R}\right)=\delta_{LL'}$. Thus we easily find the familiar result (see, for example, Schiff [8]).

$$f^{ss}(\mathbf{k}) = -\sum_{l}(2l+1)t_l(k)P_l(\hat{\mathbf{r}}.\hat{\mathbf{k}})$$

$$= \frac{1}{k}\sum_{l}(2l+1)\sin\eta_l(k)e^{i\eta_l(k)}P_l(\hat{\mathbf{r}}.\hat{\mathbf{k}})$$

(5.4)

Following the argument of section 4.2.1, we can easily see from (5.4) that the Wigner delay time associated with the scattering of a partial wave of angular momentum l by a single atom is proportional to $\dfrac{d\eta_l(k)}{dk}$.

References

[1] "Waves", C A Coulson (Oliver and Boyd, 1949)

[2] "Quantum Mechanics (2nd edition)", L D Landau and E M Lifshitz (Pergamon, 1965)

[3] "Quantum Mechanics Vol I", C Cohen-Tannoudji, B Diu and F Laloë (Wiley 2005)

[4] "Modern Quantum Mechanics", J J Sakurai (Addison-Wesley, 1994)

[5] Plane-Wave-Packets Code Notes.doc, PJD (DL 2007)

[6] SB_WPD Code Notes.doc, PJD (DL 2007)

[7]   Multiple Scattering Theory Notes v3.0.docx, PJD (DL 2009)

[8] L I Schiff, "Quantum Mechanics", McGraw-Hill (3rd edition, 1968)

Appendix A   Gaussian wave-packets

Here are some useful results for Gaussians, for reference. Note that the following are special cases of the general formula [1]

$$\int_{-\infty}^{\infty} dx\, e^{ax}\, e^{-bx^2} = \left(\frac{\pi}{b}\right)^{1/2} e^{\frac{a^2}{4b}}$$

(A1)

A.1.   Normalisation Integral

The key result is

$$\left(2\pi\right)^{-1/2} \int_{-\infty}^{\infty} dx\, e^{-x^2/2l^2} = l$$

(A2)

From this we can easily show that if

$$g(x,l) = \left(\frac{1}{l\sqrt{\pi}}\right)^{1/2} e^{-x^2/2l^2}$$

(A3)

then

$$\int_{-\infty}^{\infty} dx\, \left(g(x,l)\right)^2 = 1$$

Thus $g(x,l)$ is the normalised Gaussian of width l.

A.2.   Fourier Transforms

The key result is

$$\left(2\pi\right)^{-1/2} \int_{-\infty}^{\infty} dx\, e^{-x^2/2l^2}\, e^{ikx} = l\, e^{-k^2 l^2/2}$$

(A4)

From this all required Fourier transforms (and the results above) can be derived.