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Moller operators and Lippmann–Schwinger equations for steplike potentials

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Abstract

The Moller operators and the associated Lippmann–Schwinger equations obtained from different partitionings of the Hamiltonian for a step-like potential barrier are worked out, compared and related.

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1. Introduction

One-dimensional (1D) quantum scattering theory is usually formulated for potentials that vanish asymptotically for both large positive and negative values of the coordinate x . It is well known that the degeneracy of the energy makes the full-line scattering problem somewhat more involved than partial-wave scattering on the half-line. Additional complications arise for step-like potentials, namely, when the potential tends to different constant values on both sides,

$$\lim_{x \rightarrow -\infty} V(x) = 0 \quad \lim_{x \rightarrow \infty} V(x) = V_0 > 0.$$

These conditions apply for example to electron collisions between different metals, in models of time-of-arrival measurement [1, 2], or in experiments with evanescent waves. In some cases it is enough to solve the Schrödinger equation numerically, subject to scattering boundary conditions, in order to obtain the transmission and reflection amplitudes. There are however applications where a formal theory of scattering is needed. By ‘formal theory’ we mean the network of operators (Moller, \hat{S} , \hat{T} and resolvents), which, together with their generic properties and relations, are used to describe the collision. These applications include obtaining approximate analytical formulae, perturbative analysis, inverse scattering methods based on ‘two-potential formulae’, kinetic theory or the study of characteristic times [3]. The work on the scattering theory of step-like potentials has concentrated on the inverse problem [4–6], characterizations of scattering data for classes of potentials [5], zero-energy

limits [7], Levinson's theorem [7] and compact formulae for the evolution of states with initial support on one half-line [8, 9]. This paper complements those mentioned by focusing on the formal setting of the theory. In particular, we stress the fact that several partitionings of the Hamiltonian are possible, and work out, compare and relate the Moller operators and the corresponding Lippmann–Schwinger (LS) equations derived from them. Compact expressions of the asymptotic transmission and reflection amplitudes are given in terms of different potential-dependent matrix elements. The formalism is presented with ‘physicist’s rigour’. Its validity is in any case easily checked for cut-off potentials that deviate from the two asymptotic values 0 and V_0 only in a finite domain, $[a, b]$, which is the case explicitly considered throughout. It is expected though that it will apply for other potentials as well, having smooth but sufficiently rapid decay.

For completeness, and in order to introduce the relevant concepts and notation, in section 2 we present a lightning review of Moller operators and LS equations for potentials that vanish on both sides (the ‘ordinary case’ hereafter), while some properties of scattering states of the Hamiltonian \hat{H} for step-like potentials are to be found in section 3. We discuss several partitionings of the Hamiltonian, together with the corresponding Moller operators and LS equations, in the subsequent sections, 4–6. So as best to illustrate the differences among the formalisms we address the issue of the existence of Born’s approximation in section 7.

2. Moller operators for potentials that vanish on both sides

In ordinary one-dimensional scattering the Moller operators $\hat{\Omega}_{\pm}$, defined by the strong limits

$$\hat{\Omega}_{\pm} = \lim_{t \rightarrow \mp\infty} e^{i\hat{H}t/\hbar} e^{-i\hat{H}_0 t/\hbar} \quad (1)$$

link the actual state ψ with its asymptotic free-motion reference states, ϕ_{in} and ϕ_{out} ,

$$\lim_{t \rightarrow -/+ \infty} \|\psi(t) - \phi_{\text{in/out}}(t)\| = 0.$$

The operator $\hat{\Omega}_{+}$ ($\hat{\Omega}_{-}$) provides the scattering state by acting on the incoming (outgoing) asymptote, ϕ_{in} (ϕ_{out}),

$$\hat{\Omega}_{+/-} |\phi_{\text{in/out}}(t)\rangle = |\psi(t)\rangle \quad (2)$$

for all t .

The total Hamiltonian, $\hat{H} = \hat{H}_0 + \hat{V}$, is composed by a free motion Hamiltonian, $\hat{H}_0 = \hat{p}^2/2m$, that governs the motion of the asymptotes, and a potential operator, \hat{V} , with a local coordinate representation $\langle x | \hat{V} | x' \rangle = \delta(x - x')V(x)$. The potential function $V(x)$ vanishes as $|x| \rightarrow \infty$, in such a way that the Moller operators in (1) exist. For concreteness, we shall in fact assume that $V(x)$ vanishes outside the finite interval $[a, b]$, with $a \leq 0$ and $b \geq 0$.

The infinite-time limits in the definition of $\hat{\Omega}_{\pm}$, (1), may also be expressed with the alternative forms

$$\hat{\Omega}_{\pm} = \lim_{\varepsilon \rightarrow 0_{\pm}} \mp \varepsilon \int_0^{\mp\infty} dt' e^{\pm\varepsilon t'} e^{i\hat{H}t'/\hbar} e^{-i\hat{H}_0 t'/\hbar}.$$

Inserting a resolution of the identity in momenta between $\hat{\Omega}_{\pm}$ and $|\phi_{\text{in}}(t)\rangle$ or $|\phi_{\text{out}}(t)\rangle$, and integrating over t' , results in

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} dp e^{-iE_p t/\hbar} |p^{+/-}\rangle \langle p | \phi_{\text{in/out}}(0)\rangle \quad (3)$$

where we have introduced the (improper) eigenstates of \hat{H} , with eigenvalue E_p ,

$$|p^\pm\rangle = \hat{\Omega}(E_p \pm i0)|p\rangle \equiv |p\rangle + \frac{1}{E_p \pm i0 - \hat{H}} \hat{V}|p\rangle \quad E_p = p^2/2m. \quad (4)$$

The states $|p\rangle$ (or $|q\rangle$), to be used in the following) are the usual plane wave states, $\langle x|p\rangle = \exp(ipx/\hbar)/\sqrt{2\pi\hbar}$ ($\langle x|q\rangle = \exp(iqx/\hbar)/\sqrt{2\pi\hbar}$). $\hat{\Omega}(z)$ is a parametrized Moller operator (to be distinguished from the abstract ones in (1)), which, unlike $\hat{\Omega}_\pm$, can be applied to plane waves, and can be defined through

$$\hat{\Omega}(z) = 1 + \hat{G}_0(z)\hat{T}(z).$$

In this equation,

$$\hat{T}(z) = \hat{V} + \hat{V}\hat{G}(z)\hat{V} \quad (5)$$

is the parametrized ‘ T -operator’, or transition T operator, and the operators

$$\hat{G}(z) \equiv (z - \hat{H})^{-1} \quad \text{and} \quad \hat{G}_0(z) \equiv (z - \hat{H}_0)^{-1}$$

are the resolvents for the Hamiltonians \hat{H} and \hat{H}_0 respectively. Equation (5) is called the operator LS equation. Expressions equivalent to (4) are obtained by using the operator LS equation (5) and the operator identity

$$\hat{G}_0(z)\hat{T}(z) = \hat{G}(z)\hat{V}$$

which lead to

$$|p^\pm\rangle = |p\rangle + \frac{1}{E_p \pm i0 - \hat{H}_0} \hat{T}(E_p \pm i0)|p\rangle = |p\rangle + \frac{1}{E_p \pm i0 - \hat{H}_0} \hat{V}|p^\pm\rangle. \quad (6)$$

Equations (4) and (6) are different alternative forms of the LS integral equation for the states $|p^\pm\rangle$. Note the structure of these states, composed by a free plane wave (incoming for $|p^+\rangle$, outgoing for $|p^-\rangle$) and a scattering part. The forms (6) are useful to determine the asymptotic behaviour of the states at large distances (for cut-off potentials this means $x < a, x > b$) since the matrix elements of $G_0(E_p \pm i0)$ (the Green function) are known,

$$\langle x|\frac{1}{z - \hat{H}_0}|x'\rangle = -\frac{im}{\hbar(2mz)^{1/2}} e^{i(2mz)^{1/2}|x-x'|/\hbar}.$$

In this expression the square root is defined with a branch cut along the positive axis. Using delta-function normalization (i.e. $\langle p^\pm|p'^\pm\rangle = \delta(p - p')$), the states behave outside $[a, b]$ as

$$\langle x|p^{\text{sign}(p)}\rangle = \frac{1}{h^{1/2}} \times \begin{cases} \exp(ipx/\hbar) + R^l(p) \exp(-ipx/\hbar) & x < a \\ T^l(p) \exp(ipx/\hbar) & x > b \end{cases} \quad (7)$$

$$\langle x|p^{-\text{sign}(p)}\rangle = \frac{1}{h^{1/2}} \times \begin{cases} T^r(-p) \exp(ipx/\hbar) & x < a \\ \exp(ipx/\hbar) + R^r(-p) \exp(-ipx/\hbar) & x > b. \end{cases} \quad (8)$$

In both (7) and (8) p is a label for the energy. Let us first interpret the states in (7): for $p > 0$, there is an incident plane wave from the left, with wavenumber p/\hbar , and $R^l(p)$ and $T^l(p)$ are the corresponding reflection and transmission amplitudes for left incidence; on the other hand, if $p < 0$, there is an outgoing plane wave towards the left, with wavenumber $|p|/\hbar$, and the corresponding amplitudes are not properly related to ‘transmission’ and ‘reflection’. However, since they are analytical continuations of the amplitudes for $p > 0$, the same notation is maintained. Similar considerations apply to the set of states described by (8).

The particular form of the amplitudes $T^{l,r}(p)$ and $R^{l,r}(p)$ for potentials composed by square barriers is easily obtained by matching the wavefunction and its derivative at the edges. However, this procedure is useless in more general cases. Expressions of the amplitudes for the

general case are obtained by comparing (7) and (8) with the coordinate representation of (6). In this way they can be related to on-the-energy-shell elements of the transition operators $\hat{T}(E_p \pm i0)$. We shall work out one case in detail, as a reference for later results. Assume $p > 0$ and $x > b$. In

$$\langle x|p^+\rangle = \langle x|p\rangle + \int_{-\infty}^{\infty} dx' \langle x|\hat{G}_0(E_p + i0)|x'\rangle \langle x'|\hat{T}(E_p + i0)|p\rangle$$

we can substitute $|x - x'|$ in the Green function by $x - x'$, since the support of $\langle x'|\hat{T}(E_p + i0)|p\rangle$ is necessarily restricted to be between a and b because of the dependence of \hat{T} on \hat{V} (see (5)) and the finite support of $V(x)$. Therefore,

$$\begin{aligned} \langle x|p^+\rangle &= \langle x|p\rangle - \frac{2\pi m i}{h} \frac{e^{ipx/\hbar}}{p} \int_{-\infty}^{\infty} dx' e^{-ipx'/\hbar} \langle x'|\hat{T}(E_p + i0)|p\rangle \\ &= \langle x|p\rangle - \frac{2\pi m i}{p} \langle x|p\rangle T_{p,p}^+ \end{aligned}$$

where

$$T_{p,p'}^{\pm} \equiv \langle p|\hat{T}(E_p \pm i0)|p'\rangle \quad |p| = |p'|.$$

Straightforward comparison with (7) leads to an explicit expression for $T^l(p)$. The rest of the amplitudes can be worked out similarly to obtain the following:

$$\begin{aligned} T(p) &= 1 - \frac{2i\pi m}{p} T_{p,p}^{\text{sign}(p)} \\ R^l(p) &= -\frac{2mi\pi}{p} T_{-p,p}^{\text{sign}(p)} \\ R^r(p) &= -\frac{2mi\pi}{p} T_{p,-p}^{\text{sign}(p)}. \end{aligned} \quad (9)$$

Note that time reversal invariance implies $T_{p,p}^{\pm} = T_{-p,-p}^{\pm}$, and therefore $T^r(p) = T^l(p) = T(p)$.

3. Scattering eigenstates of the Hamiltonian for step-like potentials

In the case of step-like potentials, the potential function $V(x)$ does not go to zero for either positive or negative x , when $|x| \rightarrow \infty$. We shall assume in what follows that $V(x)$ does indeed tend to zero as $x \rightarrow -\infty$, and to V_0 when $x \rightarrow +\infty$. In other words, we shall assume that $V(x)$ equals $V_0\theta(x) = V_0\theta(x)$ plus some localized additional potential of finite support or that tends to zero sufficiently fast when $|x| \rightarrow \infty$. In such a case, the scattering part of the energy spectrum is doubly degenerate above V_0 , corresponding physically to incidence from one side or the other. Below V_0 , however, there is only one linearly independent solution with an evanescent wave at $x > 0$. There may be bound states too, with energy $E_j < 0$. The resolution of the identity may be written in different ways, in particular as [8]

$$\hat{1} = \sum_j |E_j\rangle\langle E_j| + \int_{-\infty}^{-p_0} dp |p^{\pm}\rangle\langle p^{\pm}| + \int_{p_0}^{\infty} dp |p^{\pm}\rangle\langle p^{\pm}| \pm \int_0^{\pm p_0} dp |p^{\pm}\rangle\langle p^{\pm}|$$

where $p_0 = (2mV_0)^{1/2}$ and the states $|p^{\pm}\rangle$, to be defined below, have as in the ordinary case an energy $E_p = p^2/(2m)$. As pointed out above, p is a label of the energy. It can be positive or negative because of the degeneracy in energy.

The states $|p^+\rangle$, with $p > 0$, have an *incident* plane wave of wavenumber p/\hbar , and the states $|p^-\rangle$, $p < 0$, a corresponding outgoing one,

$$\langle x|p^{\text{sign}(p)}\rangle = \frac{1}{h^{1/2}} \times \begin{cases} \exp(ipx/\hbar) + R^l(p) \exp(-ipx/\hbar) & x < a \\ T^l(p) \exp(iqx/\hbar) & x > b \end{cases} \quad (10)$$

where $q = (p^2 - 2mV_0)^{1/2}$, with a branch cut that joins the branch points $p = \pm p_0$, going slightly below $\text{Im}(p) = 0$. In this way the sign of q is the same as the sign of p for $p^2 > p_0^2$, whereas it becomes positive imaginary for $-p_0 < p < p_0$.

The states $|p^+\rangle$ for $p < -p_0$ are defined by an *incident* plane wave from the right with wavelength $-\hbar/q (> 0)$, and states $|p^-\rangle$ with $p > p_0$ by an outgoing plane wave with wavelength \hbar/q ,

$$\langle x|p^{-\text{sign}(p)}\rangle = \frac{1}{h^{1/2}} \left(\frac{p}{q}\right)^{1/2} \times \begin{cases} T^r(-p) \exp(ipx/\hbar) & x < a \\ \exp(iqx/\hbar) + R^r(-p) \exp(-iqx/\hbar) & x > b \end{cases} \quad (11)$$

(always for $|p| > |p_0|$). The factor $(p/q)^{1/2}$ is necessary for the proper delta normalization, that is, $\langle p^+|p'^+\rangle = \delta(p - p')$, and the corresponding expression for the $|p^-\rangle$ scattering states. As in the ordinary case, the arguments of transmission or reflection amplitudes are always positive for states $|p^+\rangle$, and negative for states $|p^-\rangle$ independently of the sign of p .

The S matrix elements are defined as the coefficients multiplying the outgoing plane waves when the incident plane wave is normalized to unit flux. When both channels are open ($p > p_0$), the S matrix reads

$$S(p) = \begin{pmatrix} \left(\frac{q}{p}\right)^{1/2} T^l(p) & R^l(p) \\ R^r(p) & \left(\frac{p}{q}\right)^{1/2} T^r(p) \end{pmatrix}.$$

One may also obtain these matrix elements from $\langle p'^-|p^+\rangle$ by factoring out a delta function in the scattering energy. The unitarity of the S matrix, $SS^\dagger = 1$, implies relations among the amplitudes,

$$\begin{aligned} \frac{p}{q} |T^r(p)|^2 + |R^r(p)|^2 &= 1 \\ |R^l(p)|^2 + \frac{q}{p} |T^l(p)|^2 &= 1 \\ \frac{p}{q} T^r(p) R^l(p)^* + R^r(p) T^l(p)^* &= 0. \end{aligned} \quad (12)$$

For $0 < p < p_0$ only one channel is open, the S matrix reduces to a number, $R^l(p)$, and unitarity implies

$$R^l(p) R^l(p)^* = 1. \quad (13)$$

All these equations, the set (12) and (13), are also valid for negative label p , thus providing relations for the amplitudes associated with $|p^-\rangle$ states.

4. Steplike potentials. Multichannel formalism

The straightforward application of the Moller operators of section 2, based on the partitioning $\hat{H} = \hat{H}_0 + \hat{V}$, to step-like potentials is justified physically only for certain states. The key point is that \hat{H}_0 by itself only governs the asymptotic states that enter from the left (with incident positive momentum), or escape to the left (with negative outgoing momentum). So the LS equations presented in the previous section (that is, equations (4) and (6)) will only be applicable for $\{|p^{\text{sign}(p)}\rangle\}$. It will prove useful to rename \hat{H}_0 as $\hat{H}_l \equiv \hat{H}_0$, since it is the

Hamiltonian associated with the ‘left’ asymptotic channel. Correspondingly we define $\hat{V}_l \equiv \hat{V}$, so that the total Hamiltonian is partitioned as $\hat{H} = \hat{H}_l + \hat{V}_l$, and $\hat{\Omega}_\pm^l \equiv \hat{\Omega}_\pm$. Similarly, the states $|p^{-\text{sign}(p)}\rangle$, $|p| > |p_0|$, ‘start’ (for $p < -p_0$) or ‘end up’ ($p > p_0$) on the right, where the asymptotic Hamiltonian is $\hat{H}_r \equiv \hat{H}_0 + V_0$. We thus define $\hat{V}_r \equiv \hat{V} - V_0$, so that $\hat{H} = \hat{H}_r + \hat{V}_r$, and the corresponding Moller operators

$$\hat{\Omega}_\pm^r \equiv \lim_{t \rightarrow \mp\infty} e^{i\hat{H}_r t/\hbar} e^{-i\hat{H} t/\hbar}.$$

The asymptotic Hamiltonians have their own resolvents,

$$\hat{G}_\alpha(z) \equiv \frac{1}{z - \hat{H}_\alpha}$$

where $\alpha = r, l$ is the subscript to indicate the channel. Notice that $\hat{G}_l(z) = \hat{G}_0(z)$, using the notation of section 2, whereas $\hat{G}_r(z) = \hat{G}_0(z - V_0)$. Using the abstract Moller operators one may define parametrized ones, the corresponding LS equations thus taking the form

$$\begin{aligned} |p^{\text{sign}(p)}\rangle &= |p\rangle + \hat{G}_l[E_p + \text{sign}(p)i0]\hat{V}_l|p^{\text{sign}(p)}\rangle \\ &= |p\rangle + \hat{G}[E_p + \text{sign}(p)i0]\hat{V}_l|p\rangle \end{aligned} \quad (14)$$

$$\begin{aligned} |p^{-\text{sign}(p)}\rangle &= |q_N\rangle + \hat{G}_r[E_p - \text{sign}(p)i0]\hat{V}_r|p^{-\text{sign}(p)}\rangle \\ &= |q_N\rangle + \hat{G}[E_p - \text{sign}(p)i0]\hat{V}_r|q_N\rangle \quad |p| > |p_0| \end{aligned} \quad (15)$$

where $\langle x|q_N\rangle = (p/hq)^{1/2} \exp(ixq/\hbar)$. A noticeable difference from the ordinary case is that now the potential functions $V_\alpha(x)$ are not localized ($V_l(x)$ and $V_r(x)$ do not vanish for $x > b$ and $x < a$ respectively), so that the simple manipulations leading, for example, to (9), are no longer valid to obtain expressions for T^l and T^r . We cannot separate the exponential $e^{ip|x-x'|/\hbar}$ into x - and x' -dependent exponentials, and extract right away the x dependence. The separation can be done however to obtain R^l and R^r , which take the form

$$R^l(p) = \frac{-2\pi im}{p} \langle -p|\hat{V}_l|p^{\text{sign}(p)}\rangle \quad (16)$$

$$R^r(p) = \frac{-2\pi im}{p} \langle q_N|\hat{V}_r|p^{\text{sign}(p)}\rangle. \quad (17)$$

To obtain expressions for the transition amplitudes we rewrite the LS equations in terms of the potential of the other channel (see appendix A)

$$|p^{\text{sign}(p)}\rangle = \hat{G}_r[E_p + i \text{sign}(p)0]\hat{V}_r|p^{\text{sign}(p)}\rangle \quad (18)$$

$$|p^{-\text{sign}(p)}\rangle = \hat{G}_l[E_p - i \text{sign}(p)0]\hat{V}_l|p^{-\text{sign}(p)}\rangle \quad |p| > |p_0|. \quad (19)$$

Since the potentials in (18) and (19) vanish in regions of space different from the ones in (14) and (15), we may now find the missing expressions for the transmission amplitudes,

$$T^l(p) = \frac{-2\pi im}{q} \langle q|\hat{V}_r|p^{\text{sign}(p)}\rangle \quad (20)$$

$$T^r(p) = \frac{-2\pi im}{p} \langle -p|\hat{V}_l|p^{\text{sign}(p)}\rangle. \quad (21)$$

5. Jaworski–Wardlaw Moller operators

In their study of the time spent by a quantum particle in a given spatial region [3], Jaworski and Wardlaw introduced two different asymptotic Hamiltonians for incoming and outgoing

asymptotes,

$$\begin{aligned}\hat{H}_{\text{in}} &= \frac{\hat{p}^2}{2m} + V_0 \hat{F}_- \\ \hat{H}_{\text{out}} &= \frac{\hat{p}^2}{2m} + V_0 \hat{F}_+\end{aligned}$$

where \hat{F}_- and \hat{F}_+ are complementary projectors, $\hat{F}_- + \hat{F}_+ = \hat{1}$, over negative and positive momenta respectively,

$$\hat{F}_{\pm} = \pm \int_0^{\pm\infty} dp |p\rangle\langle p|.$$

Correspondingly, they defined Moller operators

$$\hat{\Omega}_{+/-}^{JW} = \lim_{t \rightarrow -/+ \infty} e^{i\hat{H}t/\hbar} e^{-i\hat{H}_{\text{in/out}}t/\hbar}. \quad (22)$$

Note that, as in the previous section, two different partitionings of the Hamiltonians are required, one for each Moller operator. They are however not based on right/left channels, but on a distinction between incoming and outgoing states. The physical reason for these definitions is clear: the positive-momentum part of the incoming asymptotes travels on the lower level at long negative times, whereas the negative-momentum part travels on the upper level. The outgoing asymptotes behave in the opposite way, with positive momenta on the upper level and negative momenta on the lower level at large positive times.

We shall now extend this formalism to produce the associated LS equations. First it is convenient to introduce a delta-normalized eigenbasis for \hat{H}_{in} and \hat{H}_{out} (explicitly, $\langle \text{in}(p) | \text{in}(p') \rangle = \delta(p - p')$, and similarly for $|\text{out}(p)\rangle$)

$$\begin{aligned}\langle x | \text{in}(p) \rangle &= h^{-1/2} \times \begin{cases} e^{ipx/\hbar} & p > 0 \\ |p/q|^{1/2} e^{iqx/\hbar} & p < -p_0 \end{cases} \\ \langle x | \text{out}(p) \rangle &= h^{-1/2} \times \begin{cases} |p/q|^{1/2} e^{iqx/\hbar} & p > p_0 \\ e^{ipx/\hbar} & p < 0 \end{cases}\end{aligned}$$

so that

$$\hat{H}_{\text{in/out}} |\text{in/out}(p)\rangle = E_p |\text{in/out}(p)\rangle.$$

Aside from the ordinary (momentum) resolution of the identity, $\hat{1} = \int_{-\infty}^{\infty} dp |p\rangle\langle p|$,

$$\begin{aligned}\hat{1} &= \int_{-\infty}^{-p_0} dp |\text{in}(p)\rangle\langle \text{in}(p)| + \int_0^{\infty} dp |\text{in}(p)\rangle\langle \text{in}(p)| \\ &= \int_{-\infty}^0 dp |\text{out}(p)\rangle\langle \text{out}(p)| + \int_{p_0}^{\infty} dp |\text{out}(p)\rangle\langle \text{out}(p)|.\end{aligned}$$

The connection between the abstract Moller operators (22) and LS equations for eigenstates of \hat{H} follows now closely the steps from (2) to (6), but making use of the above resolutions of the identity. We thus find

$$\begin{aligned}|\psi(t)\rangle &= \int_{-\infty}^{-p_0} dp |p^+\rangle \langle \text{in}(p) | \phi_{\text{in}}(t) \rangle + \int_0^{\infty} dp |p^+\rangle \langle \text{in}(p) | \phi_{\text{in}}(t) \rangle \\ |\psi(t)\rangle &= \int_{-\infty}^0 dp |p^-\rangle \langle \text{out}(p) | \phi_{\text{out}}(t) \rangle + \int_{p_0}^{\infty} dp |p^-\rangle \langle \text{out}(p) | \phi_{\text{out}}(t) \rangle\end{aligned}$$

with

$$|p^+\rangle = |\text{in}(p)\rangle + \hat{G}_{\text{in}}(E_p + i0) \hat{T}_{\text{in}}(E_p + i0) |\text{in}(p)\rangle \quad (23)$$

$$|p^-\rangle = |\text{out}(p)\rangle + \hat{G}_{\text{out}}(E_p - i0) \hat{T}_{\text{out}}(E_p - i0) |\text{out}(p)\rangle \quad (24)$$

and

$$\hat{G}_{\text{in/out}}(z) = (z - \hat{H}_{\text{in/out}})^{-1} \quad (25)$$

$$\hat{T}_{\text{in/out}}(z) = \hat{V}_{\text{in/out}} + \hat{V}_{\text{in/out}} \hat{G}(z) \hat{V}_{\text{in/out}} \quad (26)$$

corresponding to the two partitionings of the Hamiltonian, $\hat{H} = \hat{H}_{\text{in}} + \hat{V}_{\text{in}} = \hat{H}_{\text{out}} + \hat{V}_{\text{out}}$, where

$$\hat{V}_{\text{in}} = \hat{V} - V_0 \hat{F}_- \quad \text{and} \quad \hat{V}_{\text{out}} = \hat{V} - V_0 \hat{F}_+.$$

However, the potentials \hat{V}_{in} and \hat{V}_{out} are not localized. They do not vanish as $x \rightarrow \infty$ and this leads to problems similar to those encountered before when searching for expressions for the transmission amplitudes. They are actually more severe now because these potentials do not have a semibounded support; in addition, the zeroth-order Green functions, which can be explicitly obtained by integration in the complex momentum plane, are cumbersome to work with,

$$\langle x | \hat{G}_{\text{in}}(z) | x' \rangle = \langle x | \frac{\hat{F}_+}{z - \hat{H}_0} | x' \rangle + \langle x | \frac{\hat{F}_-}{z - V_0 - \hat{H}_0} | x' \rangle \quad (27)$$

$$\langle x | \hat{G}_{\text{out}}(z) | x' \rangle = \langle x | \frac{\hat{F}_+}{z - V_0 - \hat{H}_0} | x' \rangle + \langle x | \frac{\hat{F}_-}{z - \hat{H}_0} | x' \rangle. \quad (28)$$

The summands are particular cases of

$$\langle x | \frac{\hat{F}_\xi}{\zeta - \hat{H}_0} | x' \rangle = A \xi \text{sign}(x - x') + \theta[\xi(x - x')] \langle x | \hat{G}_0(\zeta) | x' \rangle$$

with $\xi = \pm$ and

$$A = \frac{2mi}{h(2m\xi)^{1/2}} [\text{ci}(y) \sin(y) - \text{si}(y) \cos(y)] \quad (29)$$

$$y = (2m\xi)^{1/2} |x - x'|/\hbar$$

where the square root with positive imaginary part is taken.

The scattering states defined through (23) and (24) are the same as those defined previously by the LS equations of the multichannel method (MM) presented in the previous section. In order to check the veracity of this statement, it is convenient to use the identity $\hat{G}_{\text{in/out}}(z) \hat{T}_{\text{in/out}}(z) = \hat{G}(z) \hat{V}_{\text{in/out}}$, together with the forms of the resolvents \hat{G} given in (14) and (15), and the defining expressions of the different potential operators involved.

6. Pure-step Hamiltonian as zeroth order

In this section we shall study one more possible partitioning of the Hamiltonian, by considering the Hamiltonian $\hat{H}_s = \hat{H}_0 + \hat{V}_\theta$ for the pure step potential $\hat{V}_\theta \equiv V_0 \theta(\hat{x})$, as the zeroth-order term for the complete Hamiltonian,

$$\hat{H} = \hat{H}_s + \hat{V}_s.$$

In other words, the total potential energy is decomposed into the pure step potential part and a localized part, as $\hat{V} = \hat{V}_\theta + \hat{V}_s$. It is easy to compute two different eigenbases of \hat{H}_s , whose elements are $|p_s^\pm\rangle$ respectively (labelled by p as before). Their explicit expression lends itself to identification of transmission and reflection amplitudes by comparison with expressions (10) and (11):

$$\begin{aligned} T_s^l(p) &= \frac{2p}{q+p} & R_s^l(p) &= \frac{p-q}{q+p} \\ T_s^r(p) &= \frac{2q}{p+q} & R_s^r(p) &= \frac{q-p}{p+q}. \end{aligned} \quad (30)$$

The Green function for \hat{H}_s is also known exactly [10],

$$\langle x | \hat{G}_s(E_p \pm i0) | x' \rangle = \pm \frac{m}{i\hbar} \begin{cases} \frac{1}{|p|} [e^{\pm i|p||x-x'|/\hbar} + r_{\pm} e^{\mp i|p|(x+x')/\hbar}] & x' < 0 \quad x < 0 \\ \frac{1}{|p|} t_{\pm} e^{\pm i(\mu_{\pm}x - |p|x')/\hbar} & x' < 0 \quad x > 0 \\ \frac{1}{|p|} t_{\pm} e^{\pm i(\mu_{\pm}x' - |p|x)/\hbar} & x' > 0 \quad x < 0 \\ \frac{1}{\mu_{\pm}} [e^{\pm i\mu_{\pm}|x-x'|/\hbar} - r_{\pm} e^{\pm i\mu_{\pm}(x+x')/\hbar}] & x' > 0 \quad x > 0 \end{cases} \quad (31)$$

where $E_p = |p|^2/2m$,

$$t_{\pm} = \frac{2|p|}{|p| + \mu_{\pm}}$$

$$r_{\pm} = \frac{|p| - \mu_{\pm}}{|p| + \mu_{\pm}}$$

and

$$\mu_{\pm} = \begin{cases} [2m(E_p - V_0)]^{1/2} & E_p > V_0 \\ \pm i[2m(V_0 - E_p)]^{1/2} & E_p < V_0. \end{cases}$$

A first advantage of this decomposition is that the state is governed asymptotically by \hat{H}_s both before and after the collision, to the right and to the left, so that the physically meaningful Moller operators can be defined, as in the ordinary case, by the two limits of a unique operator expression,

$$\hat{\Omega}_{\pm}^s = \lim_{t \rightarrow \mp\infty} e^{i\hat{H}t/\hbar} e^{-i\hat{H}_s t/\hbar}$$

which amounts to a formal simplification with respect to the partitionings of the two previous sections, and absence of extra indices. Steps analogous to those leading to (3), with the decomposition of unity in the basis of \hat{H}_s , provide us with

$$|\psi(t)\rangle = \int_{-\infty}^{-p_0} dp |p^+\rangle \langle p_s^+ | \phi_{in}(t) \rangle + \int_0^{\infty} dp |p^+\rangle \langle p_s^+ | \phi_{in}(t) \rangle$$

$$|\psi(t)\rangle = \int_{-\infty}^0 dp |p^-\rangle \langle p_s^- | \phi_{out}(t) \rangle + \int_{p_0}^{\infty} dp |p^-\rangle \langle p_s^- | \phi_{out}(t) \rangle$$

where

$$|p^{\pm}\rangle = |p_s^{\pm}\rangle + \hat{G}_s(E_p \pm i0) \hat{T}_s(E_p \pm i0) |p_s^{\pm}\rangle \quad (32)$$

and

$$\hat{T}_s(z) = \hat{V}_s + \hat{V}_s \hat{G}(z) \hat{V}_s.$$

A second advantage of this decomposition is that the potential function $V_s(x) = V(x) - V_0\theta(x)$ is now localized. One may thus obtain easily the explicit x -dependence of the coordinate representation of (32) and identify expressions for the transmission and reflection amplitudes

in terms of the localized potential (LP),

$$\begin{aligned}
 T^l(p) &= T_s^l(p) - \frac{2\pi m i}{q} \left(\frac{q}{p}\right)^{1/2} \langle p_s^{-\text{sign}(p)} | \hat{T}_s [E_p + \text{sign}(p)i0] | p_s^{\text{sign}(p)} \rangle \\
 T^r(p) &= T_s^r(p) - \frac{2\pi m i}{p} \left(\frac{q}{p}\right)^{1/2} \langle -p_s^{-\text{sign}(p)} | \hat{T}_s [E_p + \text{sign}(p)i0] | -p_s^{\text{sign}(p)} \rangle \\
 R^l(p) &= R_s^l(p) - \frac{2\pi m i}{p} \langle -p_s^{-\text{sign}(p)} | \hat{T}_s [E_p + \text{sign}(p)i0] | p_s^{\text{sign}(p)} \rangle \\
 R^r(p) &= R_s^r(p) - \frac{2\pi m i}{p} \langle p_s^{-\text{sign}(p)} | \hat{T}_s [E_p + \text{sign}(p)i0] | -p_s^{\text{sign}(p)} \rangle.
 \end{aligned} \tag{33}$$

The time-reversal antiunitary operator Θ changes the sign of $\hat{\Omega}_\pm^s$, $\Theta \hat{\Omega}_\pm^s = \hat{\Omega}_\mp^s \Theta$, as in the ordinary case. From the time reversal invariance of the Hamiltonian it follows that $\langle p | \hat{T}_s [E_p + \text{sign}(p)i0] | p' \rangle = \langle -p | \hat{T}_s [E_p + \text{sign}(p)i0] | -p' \rangle$ (on the energy shell), so the transmission amplitudes are related by $T^r(p) = (q/p)T^l(p)$.

The agreement with the previous compact expressions (16), (17), and (20), (21) is found by using (16), (17) and (20), (21) themselves for the step potential \hat{V}_θ , and the following non-trivial generalizations of the standard ‘two-potential’ formula to the two partitionings of the multichannel formalism (see appendix B):

$$\begin{aligned}
 \langle p | \hat{V} | \pm p^{-\text{sign}(p)} \rangle &= \langle p | \hat{V}_\theta | \pm p_s^{-\text{sign}(p)} \rangle + \langle p_s^{\text{sign}(p)} | \hat{V}_s | \pm p^{-\text{sign}(p)} \rangle \\
 \langle q_N | (\hat{V} - V_0) | \pm p^{\text{sign}(p)} \rangle &= \langle q_N | (\hat{V}_\theta - V_0) | \pm p_s^{\text{sign}(p)} \rangle + \langle p_s^{-\text{sign}(p)} | \hat{V}_s | \pm p^{\text{sign}(p)} \rangle.
 \end{aligned}$$

The use of the bra–ket notation, while standard and very convenient most of the time, requires rather greater attention than usual to describe adequately the evanescent case, when $q = i\gamma$, $\gamma > 0$. Irrespective of the value of p , $\langle q | x \rangle$ should always be interpreted as $h^{-1/2} \exp(-iqx)$. Similarly, $\langle p_s^\pm | x \rangle$ should *first* be written for real q and *then* continued analytically.

7. Born approximations

As an example to illustrate the differences of the three described formalisms we shall obtain the Born approximation of the reflectance $|R^l(p)|^2$ for the potential,

$$\hat{V} = \hat{V}_\theta + V_1 \delta(\hat{x}). \tag{34}$$

The exact result,

$$R^l(p) = \frac{p - q - (2imV_1/\hbar)}{p + q + (2imV_1/\hbar)}$$

may be obtained using (30), (33), $\delta(\hat{x}) = |0\rangle\langle 0|$ and

$$\hat{T}_s(z) = \frac{V_1 |0\rangle\langle 0|}{1 - V_1 \langle 0 | \hat{G}_s(z) | 0 \rangle}$$

or alternatively by straightforward computation.

We will now calculate the *different* Born approximations by retaining only the terms linear in the potential corresponding to each partitioning of the Hamiltonian. To be more precise, we will look at the LS equation for $|p^+\rangle$ in each approach, and retain terms of first order in the potential, that is, to first order in the difference between the total Hamiltonian and the incoming asymptotic Hamiltonian of reference. The resulting wavevector will be examined in the position representation for $x < 0$, and the result compared to (10) to extract $R^l(p)$. In fact this last step is not necessary for the MM (section 4) and the LP (section 6) approaches, since

we have already carried out this comparison in an exact manner (see (16) and (33)). Notice that we have indeed checked that in all three approaches we obtain the same scattering state $|p^+\rangle$.

In the MM, see (16), the first-order term in \hat{V}_l (which in this case is $\hat{V}_l = \hat{V}_\theta + V_1\delta(\hat{x})$) is

$$R_{\text{Born-MM}}^l(p) = \frac{-2\pi mi}{p} \langle -p | \hat{V}_\theta + V_1\delta(\hat{x}) | p \rangle = \frac{m(V_0 - 2ipV_1/\hbar)}{2p^2}. \quad (35)$$

The analysis to second order is more delicate, involving limits (as in $\hat{G}(E_p + i0)$), but it reveals that the singularity in $p = 0$ for the MM formalism actually worsens (it becomes of the form p^{-4}). This was only to be expected, given the non-locality of the perturbing potential in that case, which produces infrared singularities to all perturbation orders, which can only be resolved by a complete resummation of all terms.

We could also examine $R^r(p)$, to first order in $\hat{V}_r = \hat{V}_\theta + V_1\delta(\hat{x}) - V_0$, which in this case can be obtained from $R^l(p)$ by substituting p for q , and vice versa. This recipe actually holds for the Born approximation in the MM formalism, which leads to the result that the reflectance diverges for $|p| \rightarrow p_0$.

A Born approximation in the ‘in/out’ formalism of section 5 is much more problematic: for $x < 0$ and $p > 0$, the first order in \hat{V}_{in} of (23) is

$$\langle x | p^+ \rangle^{(1)} = \langle x | \text{in}(p) \rangle + \int_{-\infty}^{\infty} dx' \langle x | \hat{G}_{\text{in}}(E_p + i0) | x' \rangle \langle x' | \hat{V}_{\text{in}} | \text{in}(p) \rangle.$$

By substituting $\langle x | \hat{G}_{\text{in}}(E_p + i0) | x' \rangle$ (see (27) and (29)) and taking the limit $x \rightarrow -\infty$ to eliminate transient terms,

$$\langle x | p^+ \rangle^{(1)} = \frac{1}{\sqrt{\hbar}} \left[e^{ipx/\hbar} + \left(\frac{p-q}{2q} + \frac{mV_1}{i\hbar q} \right) e^{-iqx/\hbar} \right].$$

To this order, this approach provides a physically meaningless reflected wave with a momentum smaller than the incident one. This indicates that we do not recover in this manner a sensible approximation to the reflectance. Finally, the LP approach of the previous section gives, to first order in \hat{V}_s ,

$$R_{\text{Born-LP}}^l(p) = \frac{p-q}{p+q} - \frac{2\pi miV_1}{p} \langle -p_s^- | 0 \rangle \langle 0 | p_s^+ \rangle = \frac{p^2 - q^2 - 4miV_1p/\hbar}{(p+q)^2}. \quad (36)$$

The results of (35) and (36) are compared in figure 1, which clearly demonstrate the computational advantage of the LP approach, which starts from much better adapted initial functions. In particular it is relevant to note that the LP approach detects the change of regime in the reflectance due to the energy falling below the asymptotic level, which the multichannel formalism cannot even hint at in a perturbative scheme. In other words, the fact that only one channel is open, and (13) must hold, is overlooked by the perturbative expansion in the MM scheme, while there is a sharp change in behaviour of the perturbative expansion in the LP scheme from the one-channel to the two-channel case (even though (13) does not generically hold if we restrict ourselves to a finite number of terms).

8. Discussion

Given the simplicity of one-dimensional step-like potentials, we could not fail to provide a complete formal scattering theory for them. However, in pursuing this objective, we have met several interesting novel aspects with respect to ordinary scattering. Among them, the existence of different, all somehow ‘natural’, partitionings of the Hamiltonian is an important one, since it leads to different formal frameworks. Working out the details is at the very least

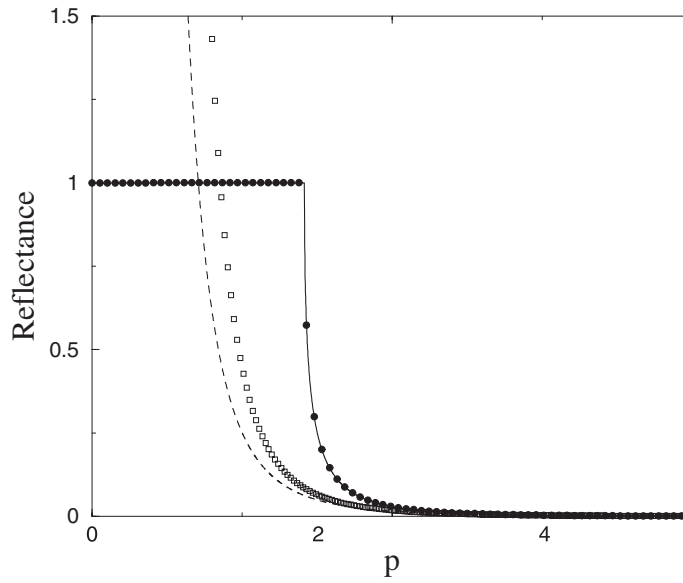


Figure 1. Exact reflectance (solid curve), first-order Born approximations for the LP approach (dots) and MM (dashed curve), and second-order approximation for the MM (squares) versus p . The potential is given in (34). $V_0 = 1$ au, $V_1 = 0.01$ au, $m = 1$ au.

laborious, frequently tedious, and we hope that our compact presentation and focus on the final results may save some time and help the practitioners to avoid pitfalls. With respect to the three possible methods described, the in/out formalism has some elegance, and this was historically our first choice. However, the zeroth-order Hamiltonians, non-LPs, or Green functions are not easy to deal with. This led us to look for other possibilities. Certain manipulations may benefit from the condensed forms of transmission and reflection amplitudes obtained following the MM, but in a practical calculation the LP approach will be generally preferable. It is also the most economical presentation since it reduces by half the number of equations needed, and is also the closest to ordinary scattering.

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Appendix A. Alternative forms of Lippmann–Schwinger equations

We give an example of obtaining the alternative LS equations in (18) and (19). Using

$$\hat{G}_l(z) = \hat{G}_r(z)[1 - V_0 \hat{G}_l(z)]$$

and $\hat{V}_r = \hat{V}_l - V_0$, (14) for $p > 0$ may be written as

$$|p^+\rangle = |p\rangle + \hat{G}_r(E_p + i0) \hat{V}_r |p^+\rangle + V_0 \hat{G}_l(E_p + i0) [1 - \hat{G}_r(E_p + i0) \hat{V}_r] |p^+\rangle.$$

Acting with the operator in parenthesis on $|p^+\rangle$, using $\hat{G}(z) = \hat{G}_l(z) + \hat{G}_l(z)\hat{V}_l\hat{G}(z)$, and (14), one finds (when operating $+i0$ must be kept as a small imaginary number)

$$|p^+\rangle = |p\rangle + \hat{G}_r(E_p + i0)\hat{V}_r|p^+\rangle + V_0\hat{G}_r(E_p + i0)|p\rangle$$

but the third term cancels the first one by acting with \hat{G}_r on $|p\rangle$, so that (18) (for $p > 0$) is obtained. One may proceed similarly for the other cases.

Appendix B. Two potential formulae

In this appendix we shall obtain one of the two potential formulae used in section 6. The other cases may be obtained similarly. Assume that $p < 0$. Then,

$$\begin{aligned} \langle p|\hat{V}|\pm p^+\rangle &= \langle p|\hat{V}_\theta + \hat{V}_s|\pm p^+\rangle \\ &= \langle p|(\hat{V}_\theta + \hat{V}_s)[|\pm p_s^+\rangle + \hat{G}_s(E_p + i0)\hat{T}_s(E_p + i0)|\pm p_s^+\rangle] \\ &= \langle p|\hat{V}_\theta|\pm p_s^+\rangle + \langle p|\hat{V}_\theta\hat{G}_s(E_p + i0)\hat{T}_s(E_p + i0)|\pm p_s^+\rangle + \langle p|\hat{V}_s|\pm p^+\rangle \\ &= \langle p|\hat{V}_\theta|\pm p_s^+\rangle + \langle p_s^-|\hat{V}_s|\pm p^+\rangle \end{aligned}$$

where we have used (32) and (14), the last one particularized for the pure step potential.

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