Scattering Calculations in One Dimension

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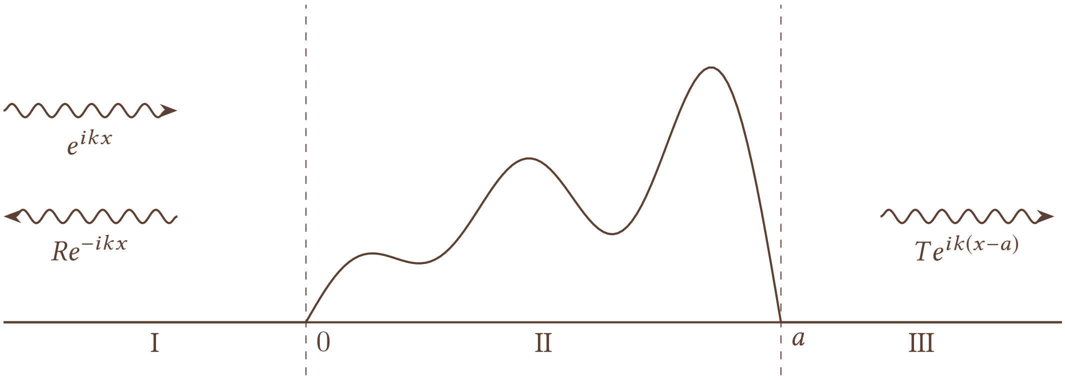

Suppose that V has compact support, i.e. $V = 0$ outside some interval, which we may call $[0, a]$ for definiteness. We would like to understand what happens when we send a particle in from the left: will it go through, or bounce back off the barrier? This being quantum mechanics, the answer is of course that both happen, with a certain probability; therefore we want to calculate the probabilities.

We could work with wavepackets, but it is far more algebraically tractable if we work with a steady incident beam:[1] the probability current suggests that we use e^{ikx} as an incident wave.

1 General Theory

Region I Outside $[0, a]$, the potential is zero, so the solution satisfies the free Schrödinger equation, $-\psi'' = k^2\psi$. On the left of the potential, which we generically call Region I, we expect to have an incident wave and a reflected wave. Since the equations are linear, we can choose the incident wave to have magnitude 1. The reflected wave we give the reflexion coefficient, R,[2] and the total solution in Region I is

$$\psi(x) = e^{ikx} + Re^{-ikx}. \tag{1}$$

Region II In Region II, the potential can be arbitrarily complicated, but the wavefunction must still satisfy a second-order ODE, namely $-\psi'' + V\psi = k^2\psi$. Provided the potential is nonsingular at $x = 0$, we can choose a pair of solutions $s(x)$ and $c(x)$ so that $s(0) = 0$ and $s'(0) = 1$, $c(0) = 1$ and $c'(0) = 0$.[3] Then the solution in Region II is

$$\psi(x) = Ac(x) + Bs(x). \tag{2}$$

Region III In Region III, we again have the free Schrödinger equation, and we expect only a transmitted wave, so we take the solution to be

$$\psi(x) = Te^{ik(x-a)}, \tag{3}$$

where we set the phase up to make the calculation simpler.[4]

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[1] The algebra will already be bad enough when we do it this way.

[2] The notation used for the reflection and transmission coefficients, and their absolute values, is not standardised. We shall at least be consistent in this work.

[3] Obviously these will be the sine and cosine, or the hyperbolic versions, if the potential is constant; hence the names.

[4] Obviously we can reinsert the phase later if we want.

1.1 Reflexion and Transmission

What can we say about R and T so far? One result we know is that the "probability density"[5] is constant, since there is no time-dependence in ψ. Therefore the continuity equation implies that the probability current is constant, and hence the same in Region I as Region III. Clearly in Region III, $j = (\hbar k/m)\,|T|^2$. In Region I,

$$j = \frac{\hbar}{m}\Im\left((e^{-ikx} + \bar{R}e^{ikx})(ike^{ikx} - ikRe^{-ikx})\right) = \frac{\hbar k}{m}(1 - |R|^2).$$

Then conservation of the probability current implies that

$$1 = |R|^2 + |T|^2 . \tag{4}$$

We therefore call $|R|^2$ the *reflexion probability* and $|T|^2$ the *transmission probability*.

1.2 General Matching

We enforce continuity of ψ and ψ' at 0 and a. This gives two sets of two equations:

$$1 + R = A \tag{5}$$

$$ik(1 - R) = B \tag{6}$$

$$Ac(a) + Bs(a) = T \tag{7}$$

$$Ac'(a) + Bs'(a) = ikT. \tag{8}$$

Of course, we don't care about A and B in the slightest, just the coefficients R and T. There are two directions we can go to eliminate A and B: starting with the I–II equations, or starting with the II–III ones.

I–II first The way we've set the equations up makes this approach begin nice and straightforwardly: we can substitute for A and B directly:

$$T = (1 + R)c(a) + ik(1 - R)s(a) = (c(a) + iks(a)) + (c(a) - iks(a))R \tag{9}$$

$$ikT = (1 + R)c'(a) + ik(1 - R)s'(a) = (c'(a) + iks'(a)) + (c'(a) - iks'(a))R. \tag{10}$$

$$\begin{aligned}(c'(a) + iks'(a)) + (c'(a) - iks'(a))R &= ik(c(a) + iks(a)) + ik(c(a) - iks(a))R \\ [c'(a) - iks'(a) - ikc(a) - k^2 s(a)]R &= ikc(a) - k^2 s(a) - c'(a) - iks'(a) \\ R &= \frac{-(c'(a) + k^2 s(a)) + ik(c(a) - s'(a))}{c'(a) - k^2 s(a) - ik(c(a) + s'(a))}\end{aligned}$$

For T, the algebra starts to look rather hairy.

$$\begin{aligned}[(c'(a) - iks'(a)) - ik(c(a) - iks(a))]T &= (c'(a) - iks'(a))(c(a) + iks(a)) - (c(a) - iks(a))(c'(a) + iks'(a)) \\ T &= \frac{(c'(a) - iks'(a))(c(a) + iks(a)) - (c(a) - iks(a))(c'(a) + iks'(a))}{c'(a) - k^2 s(a) - ik(c(a) + s'(a))} \\ &= \frac{2ik(s(a)c'(a) - c(a)s'(a))}{c'(a) - k^2 s(a) - ik(c(a) + s'(a))}\end{aligned}$$

But we recognise the numerator of this expression: it's just the Wronskian of s and c, evaluated at a. Since s and c solve the time-independent Schrödinger equation, their Wronskian is constant. Of course, we've set it up so that $s(0)c'(0) - c(0)s'(0) = -1$, which implies that $s(a)c'(a) - c(a)s'(a) = -1$ too, and hence we have our final expressions for R and T:

$$\begin{aligned}R &= \frac{c'(a) + k^2 s(a) + ik(-c(a) + s'(a))}{-c'(a) + k^2 s(a) + ik(c(a) + s'(a))} \\ T &= \frac{2ik}{-c'(a) + k^2 s(a) + ik(c(a) + s'(a))}.\end{aligned}$$

[5] Whatever that is for an unnormalisable beam.

II–III first To go the other way, we start with

$$Ac(a) + Bs(a) = T$$
$$Ac'(a) + Bs'(a) = ikT,$$

and solve for A and B. As we recall from IA, Linear Algebra, or some other corner of our brains, the inverse of the matrix corresponding to the left-hand side is

$$\begin{pmatrix} c(a) & s(a) \\ c'(a) & s'(a) \end{pmatrix}^{-1} = \frac{1}{c(a)s'(a) - s(a)c'(a)} \begin{pmatrix} s'(a) & -s(a) \\ -c'(a) & c(a), \end{pmatrix} = \begin{pmatrix} s'(a) & -s(a) \\ -c'(a) & c(a), \end{pmatrix},$$

because c and s are solutions to the time-independent Schrödinger equation, so their Wronskian is constant and equal to $c(0)s'(0) - s(0)c'(0) = 1$. Therefore

$$A = T(s'(a) - iks(a)) \tag{11}$$
$$B = T(-c'(a) + ikc(a)). \tag{12}$$

Substituting these into the I–II equation, we find

$$1 + R = T(s'(a) - iks(a)) \tag{13}$$
$$ik(1 - R) = T(-c'(a) + ikc(a)). \tag{14}$$

It is now easy to find R and T, by multiplying the first equation by ik and adding and subtracting. We find

$$T = \frac{2ik}{-c'(a) + k^2 s(a) + ik(c(a) + s'(a))} \tag{15}$$
$$R = \frac{iks'(a) + k^2 s(a) + c'(a) - ikc(a)}{2ik} T = \frac{c'(a) + k^2 s(a) + ik(-c(a) + s'(a))}{-c'(a) + k^2 s(a) + ik(c(a) + s'(a))}. \tag{16}$$

Alternative On the other hand, if we're in the business of making things easier, why not set up the Region II basis so that two of the equations are trivial? Define C, S as the solutions to the time-independent Schrödinger equation in region II with $C(a) = S'(a) = 1$ and $S(a) = C'(a) = 0$. Then the equations are

$$1 + R = AC(0) + BS(0) \tag{17}$$
$$ik(1 - R) = AC'(0) + BS'(0) \tag{18}$$
$$A = T \tag{19}$$
$$B = ikT. \tag{20}$$

We can now go straight in and substitute into the first two equations:

$$1 + R = T(C(0) + ikS(0)) \tag{21}$$
$$ik(1 - R) = T(C'(0) + ikS'(0)) \tag{22}$$

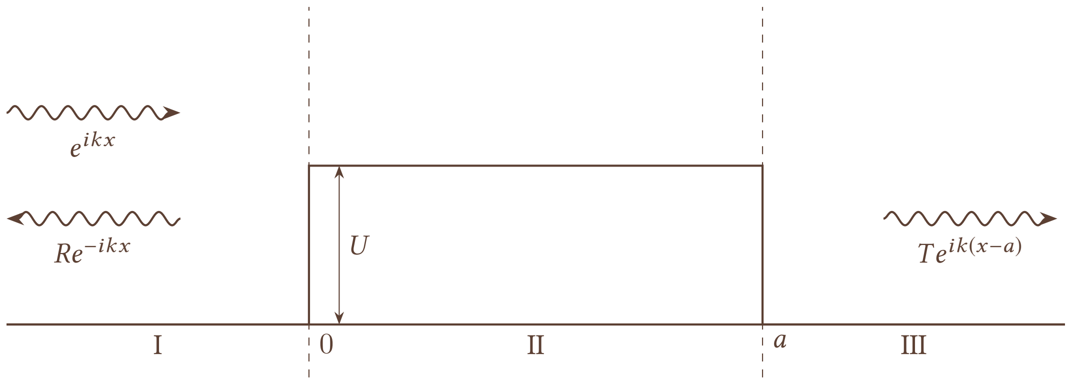
Multiplying the first by ik and adding and subtracting,

$$T = \frac{2ik}{C'(0) - k^2 S(0) + ik(C(0) + S'(0))} \tag{23}$$
$$R = \frac{C'(0) + k^2 S(0) + ik(C(0) - S'(0))}{2ik} T = \frac{C'(0) + k^2 S(0) + ik(C(0) - S'(0))}{C'(0) - k^2 S(0) + ik(C(0) + S'(0))}, \tag{24}$$

which was probably the easiest of all.

Therefore, the top tips are:

1. Choose a basis so that the calculation is as simple as possible. Sines and cosines, or $\sin \alpha(x - a)$ and $\cos \alpha(x - a)$, for example, rather than exponentials.
2. Start the calculation at the right end.
3. Remember the Wronskian may come in handy.



2 Rectangular Barrier

One of the most annoying calculations in this course is calculating R and T for the potential

$$V(x) = U\chi_{[0,a]}(x), \tag{25}$$

a rectangular box of height U and width a. Bearing in mind our experience in the general case, the sensible bases for ψ are

$$\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & x < 0 \\ A\cos\alpha(x-a) + B\frac{1}{\alpha}\sin\alpha(x-a) & 0 \leqslant x \leqslant a \\ Te^{ik(x-a)} & x > a \end{cases}, \tag{26}$$

with $k = \sqrt{2mE}/\hbar$ and $\alpha = \sqrt{2m(E-U)}/\hbar$.

We then have the equations

$$1 + R = A\cos\alpha a - \frac{B}{\alpha}\sin\alpha a \tag{27}$$
$$ik(1-R) = \alpha A\sin\alpha a + B\cos\alpha a \tag{28}$$
$$A = T \tag{29}$$
$$B = ikT. \tag{30}$$

Substituting the second two in the first two,

$$1 + R = T(\cos\alpha a - ik\alpha^{-1}\sin\alpha a) \tag{31}$$
$$ik(1-R) = T(\alpha\sin\alpha a + ik\cos\alpha a). \tag{32}$$

Multiplying the first equation by ik and adding and subtracting, we find

$$\begin{aligned} T &= \frac{2ik}{\alpha\sin\alpha a + ik\cos\alpha a + ik\cos\alpha a + k^2\alpha^{-1}\sin\alpha a} \\ &= \frac{2ik}{(\alpha^2+k^2)\alpha^{-1}\sin\alpha a + 2ik\cos\alpha a} \end{aligned} \tag{33}$$

$$\begin{aligned} R &= T\frac{ik(\cos\alpha a - ik\alpha^{-1}\sin\alpha a) - (\alpha\sin\alpha a + ik\cos\alpha a)}{2ik} = T\frac{(k^2-\alpha^2)\alpha^{-1}\sin\alpha a}{2ik} \\ &= \frac{(k^2-\alpha^2)\alpha^{-1}\sin\alpha a}{(\alpha^2+k^2)\alpha^{-1}\sin\alpha a + 2ik\cos\alpha a}. \end{aligned} \tag{34}$$

Especially useful is that written like this, the equation is indifferent as to whether $U - E$ is positive or negative: we have $\cos iz = \cosh z$ and $\sin iz/iz = \sinh z/z$, so the trigonometric functions simply transform into hyperbolic functions if $E < U$.

3 Limits

Writing $u^2 = 2mU/\hbar^2$, we have $\alpha^2 = k^2 - u^2$. Then before proceeding, it is useful to note that $k^2 + \alpha^2 = 2k^2 - u^2$, and $k^2 - \alpha^2 = u^2$. Then we have the expressions

$$T = \frac{2ik}{(2k^2 - u^2)\alpha^{-1} \sin \alpha a + 2ik \cos \alpha a}. \tag{35}$$

$$R = \frac{u^2\alpha^{-1} \sin \alpha a}{(2k^2 - u^2)\alpha^{-1} \sin \alpha a + 2ik \cos \alpha a} \tag{36}$$

Wide barrier There are two cases, depending on the sign of $U - E$. If U is smaller than E, we have the surprising result that for certain values of a, there are energies at which the wave is either completely reflected, or completely transmitted though the barrier. This is in contrast to most classical situations, where one cannot occur without the other: there is no energy lost in this situation.

On the other hand, if $E < U$, $\alpha = i\beta$ is imaginary, and we can write T and R as

$$T = \frac{2ik}{(k^2 - \beta^2)\beta^{-1} \sinh \beta a + 2ik \cosh \beta a} \tag{37}$$

$$R = \frac{(k^2 + \beta^2)\beta^{-1} \sinh \beta a}{(k^2 - \beta^2)\beta^{-1} \sinh \beta a + 2ik \cosh \beta a}. \tag{38}$$

As $a \to \infty$, both hyperbolic functions $\sim e^x/2$, so

$$T \sim \frac{2ik\beta}{(k^2 - \beta^2) + 2ik\beta} 2e^{-\beta a}$$

$$R \sim \frac{(k^2 + \beta^2)}{(k^2 - \beta^2) + 2ik\beta} = \frac{k - i\beta}{k + i\beta},$$

i.e. the transmission coefficient converges exponentially to zero, the reflexion coefficient to a complex number of unit modulus.

Tall barrier If instead we fix a and let $U \to \infty$, then $\beta \sim \sqrt{2mU}/\hbar$, and the dominant contribution comes from the $\sqrt{U} \sinh U$ terms, and we find

$$R \sim -1 - \frac{2ik}{u} \qquad T \sim -e^{-a\sqrt{u^2-k^2}} \frac{2ik}{u}, \tag{39}$$

and so unsurprisingly it is very likely that the particle is reflected; further, we see the reflection picks up a phase change of π, which is what we expect classically.

Small energy Here we take $E \to 0$. We find that again the probability of reflection increases to 1, but not in the same way as making the barrier infinitely high: the behaviour is in fact

$$R \sim -1 - \frac{2ik}{u} \coth ua, \qquad T \sim -\frac{2ik}{u} \operatorname{csch} ua. \tag{40}$$

Delta potential If we let $U \to \infty$, $a \to 0$ so that $Ua = \lambda$ is constant, we find that, setting $K = k\hbar^2/m\lambda$,

$$R \to \frac{1}{iK - 1}, \qquad T \to \frac{iK}{iK - 1}, \tag{41}$$

which is the same as the result one obtains by solving the problem directly with a δ potential.

4 Aside: The Scattering Matrix

So far, we have only discussed a wave incoming from the left. What about the same from the right? And for that matter, what about both at once? Generically, we would expect these to be different, at least if the potential is not symmetric.

Both at once is easy to answer: since the equations are linear, if we have a linear combination of incoming waves from the left and the right, the relation is described by a linear combination of the individual cases.

In other words, if the incoming waves have coefficients I_1 and I_2, the outgoing ones O_1 and O_2, where 1 and 2 denote the regions of the axis,[6] so that

$$\psi(x) = \begin{cases} I_1 e^{ikx} + O_1 e^{-ikx} & \text{Region I} \\ I_2 e^{-ikx} + O_2 e^{ikx} & \text{Region III} \end{cases},$$

then we have the relationship

$$\begin{pmatrix} O_1 \\ O_2 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix},$$

or in vectors and matrices, $O = SI$. This matrix is called the S-*matrix* S or $S(k)$, and it tells us everything we want to know about the scattering properties of V for waves of a given wave.

The case we have already considered can be written as $I_1 = 1, I_2 = 0, R = O_1 = S_{11}$ and $T = O_2 = S_{21}$.

Doing exactly the same calculation of the conserved probability current as before, we find

$$|I_1|^2 + |I_2|^2 = |O_1|^2 + |O_2|^2 ,$$

so in terms of S, we have

$$|I|^2 = |O|^2 = I^* S^\dagger S I,$$

and hence $S^\dagger S = 1$, so S is *unitary*.

Other nice things to know:

- If V is real, $\bar{\psi}$ is also a solution. Hence the same relationship applies with I, O replaced by O^*, I^* respectively:[7]

  $$I^* = SO^*,$$

  and hence

  $$I^* = SS^* I^*,$$

  so $SS^* = 1$. Similarly, $S^*S = 1$. Combined with unitarity, this gives $S = S^\mathsf{T}$, so in this case S is also symmetric, at least when k is real.

- In the previous case, if $S_{11} = R$ and $S_{21} = T$, then symmetry implies that $S_{12} = T$ as well, and then Hermiticity forces $S_{22} = -R^* T/T^*$.[8] Hence for a real potential, scattering from the right is quite similar to scattering from the left, in that the reflexion and transmission coefficients have the same modulus, but the phase of the reflexion coefficient is different.

- Replacing k by $-k$ also swaps the I and O vectors, so $S(k)S(-k) = 1$, and hence $S(-k) = S(k)^\dagger$.

- The S-matrix also has a use in finding bound states: suppose that we replace k by $i\kappa$ with $\Im\kappa > 0$. Then the O_1 and O_2 functions are decaying, but the I_1 and I_2 ones are not, and hence to have a normalisable solution, we must have $I = 0$, but $O \neq 0$. This suggests that

  $$0 \neq O = S(i\kappa)0,$$

  and therefore $S(i\kappa)$ must have a singularity if κ is the correct value for a ground state. Similarly, the time-reversal argument implies that $S(-i\kappa) = S(i\kappa)^\dagger$ has a zero, or at least becomes degenerate so that nonzero vectors are taken to zero. Hence a bound state must have $\det S(-i\kappa) = 0$. (This is necessary, but not sufficient, in fact.)

For more details about the S-matrix, see Applications of Quantum Mechanics in Part II.

[6] Apologies for this rather peculiar notation.

[7] Note that the $e^{\pm ikx}$ swap places: this symmetry is actually *time-reversal*.

[8] If $T = 0$, S_{22} can be any complex number of modulus 1. But computing directly shows that T is never zero, unless we cannot construct the basis of solutions we have worked with.