1 Propagator and Resolvent

1.1 Introduction

The first chapter of this book is somewhat eclectic. It introduces concepts and tools that will be important later, and it also develops subjects that are not emphasized in many standard or more elementary courses of quantum mechanics.

We start by presenting the unitary time evolution operator and its integral kernel in the space representation, also known as the quantum-mechanical propagator. This important gadget reappears as the Moyal operator in the phase space formulation of Chapter 3, and it will be the central object in the path integral formulation of Chapter 4. The resolvent operator and Green's functions are also closely related to the quantum-mechanical propagator, and they play an important role in formal developments and in scattering theory. Although we do not present the general theory of scattering in this book, we dedicate a section to scattering in one-dimension, which illustrates the theory of the resolvent with explicit constructions. Some of the examples discussed in the section on one-dimensional scattering also provide our first examples of resonances, which we will study in much more detail in Chapter 5.

1.2 The Quantum-Mechanical Propagator

In quantum mechanics, time evolution between an initial time t_0 and a final time t_f is implemented by the unitary operator

$$\mathsf{U}(t_f, t_0), \tag{1.2.1}$$

which connects the quantum state of the system at time $t = t_0$ with the state at $t = t_f$:

$$\mathsf{U}(t_f, t_0)|\psi(t_0)\rangle = |\psi(t_f)\rangle. \tag{1.2.2}$$

It obviously satisfies the convolution law,

$$\mathsf{U}(t_f, t_0) = \mathsf{U}(t_f, t_1)\mathsf{U}(t_1, t_0). \tag{1.2.3}$$

Let H be the Hamiltonian operator of the quantum system. By using Schrödinger's equation,

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \mathsf{H}|\psi(t)\rangle, \tag{1.2.4}$$

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we deduce the evolution equation for the operator $\mathsf{U}(t,t_0)$:

$$i\hbar\frac{\partial \mathsf{U}(t,t_0)}{\partial t} = \mathsf{H}\mathsf{U}(t,t_0), \tag{1.2.5}$$

with initial condition

$$\mathsf{U}(t_0,t_0) = \mathbf{1}. \tag{1.2.6}$$

When the Hamiltonian H is time-independent (as we will assume most of the time in this book), we can solve the evolution equation to give

$$\mathsf{U}(t_f,t_0) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathsf{H}(t_f-t_0)}. \tag{1.2.7}$$

In this case, the evolution operator is invariant under time translation and only depends on the difference

$$T = t_f - t_0. \tag{1.2.8}$$

It is convenient to work in the position representation for the position operator. The corresponding eigenstates will be denoted by $|\boldsymbol{q}\rangle$, where $\boldsymbol{q} \in \mathbb{R}^d$. The integral kernel of the evolution operator in the position representation is called the *quantum-mechanical (QM) propagator*:

$$K(\boldsymbol{q}_f,\boldsymbol{q}_0;t_f,t_0) = \langle \boldsymbol{q}_f|\mathsf{U}(t_f,t_0)|\boldsymbol{q}_0\rangle. \tag{1.2.9}$$

The QM propagator can be regarded as a wavefunction at time $t = t_f$,

$$\psi(\boldsymbol{q},t_f) = K(\boldsymbol{q},\boldsymbol{q}_0;t_f,t_0), \tag{1.2.10}$$

which is obtained by evolving in time the state $|\boldsymbol{q}_0\rangle$ at $t = t_0$. This initial state is described by the wavefunction

$$\psi(\boldsymbol{q},t_0) = \delta(\boldsymbol{q} - \boldsymbol{q}_0), \tag{1.2.11}$$

and it is an eigenfunction of the position operator with eigenvalue $\boldsymbol{q}_0$. The QM propagator has a direct physical interpretation: it gives the probability amplitude that a particle located is at the point $\boldsymbol{q}_f$ at time t_f, given that it was at the point $\boldsymbol{q}_0$ at time t_0.

The evolution operator and the QM propagator contain detailed information about the spectrum and eigenfunctions of the Hamiltonian. Indeed, let us assume that H has a discrete and nondegenerate spectrum E_n, $n \geq 0$, with orthonormal eigenfunctions $|\phi_n\rangle$. Then, we have the spectral decompositions,

$$\mathsf{U}(t_f,t_0) = \sum_{n\geq 0} |\phi_n\rangle \mathrm{e}^{-\mathrm{i}E_n(t_f-t_0)/\hbar}\langle\phi_n|, \tag{1.2.12}$$

or, equivalently,

$$K(\boldsymbol{q}_f,\boldsymbol{q}_0;t_f,t_0) = \sum_{n\geq 0} \phi_n(\boldsymbol{q}_f)\mathrm{e}^{-\mathrm{i}E_n(t_f-t_0)/\hbar}\phi_n^*(\boldsymbol{q}_0). \tag{1.2.13}$$

Finally, let us note that the QM propagator is a solution of the time-dependent Schrödinger equation. If we denote the quantum counterparts of the canonical coordinates and momenta by the vectors of Heisenberg operators

$$\mathsf{q} = (\mathsf{q}_1,\ldots,\mathsf{q}_n), \qquad \mathsf{p} = (\mathsf{p}_1,\ldots,\mathsf{p}_n), \tag{1.2.14}$$

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then the QM propagator satisfies

$$\mathrm{i}\hbar \frac{\partial}{\partial t_f} K(\boldsymbol{q}_f, \boldsymbol{q}_0; t_f, t_0) = \mathsf{H}\left(\boldsymbol{q}_f, -\mathrm{i}\hbar \frac{\partial}{\partial \boldsymbol{q}_f}\right) K(\boldsymbol{q}_f, \boldsymbol{q}_0; t_f, t_0), \tag{1.2.15}$$

as well as

$$\mathrm{i}\hbar \frac{\partial}{\partial t_f} K(\boldsymbol{q}_f, \boldsymbol{q}_0; t_f, t_0) = \mathsf{H}\left(\boldsymbol{q}_0, \mathrm{i}\hbar \frac{\partial}{\partial \boldsymbol{q}_0}\right) K(\boldsymbol{q}_f, \boldsymbol{q}_0; t_f, t_0). \tag{1.2.16}$$

The evolution operator in quantum mechanics is closely related to other useful quantities. The first one is the (unnormalized) density operator for the canonical ensemble. This is defined by

$$\rho(\beta) = \mathrm{e}^{-\beta \mathsf{H}}, \tag{1.2.17}$$

and we recall that $k_B \beta$ is the inverse temperature of the system. The density operator can be obtained from the evolution operator by the so-called *Euclidean continuation* or *Wick rotation*:

$$T = -\mathrm{i}u, \qquad u = \beta\hbar. \tag{1.2.18}$$

Therefore, if we know the evolution operator, we know the density operator, and if we know the QM propagator, we know the integral kernel of the density operator, sometimes called the *density matrix*,

$$\langle \boldsymbol{q} | \rho(\beta) | \boldsymbol{q}' \rangle = \rho(\boldsymbol{q}, \boldsymbol{q}'; \beta). \tag{1.2.19}$$

More precisely, for a theory with a time-independent Hamiltonian, we have

$$\rho(\boldsymbol{q}, \boldsymbol{q}'; \beta) = K(\boldsymbol{q}, \boldsymbol{q}'; -\mathrm{i}\hbar\beta, 0). \tag{1.2.20}$$

Note that the unnormalized density matrix satisfies the differential equation

$$-\frac{\partial}{\partial \beta} \rho(\boldsymbol{q}, \boldsymbol{q}'; \beta) = \mathsf{H}\left(\boldsymbol{q}, -\mathrm{i}\hbar \frac{\partial}{\partial \boldsymbol{q}}\right) \rho(\boldsymbol{q}, \boldsymbol{q}'; \beta), \tag{1.2.21}$$

which is sometimes called the *Bloch equation*. This is the counterpart of (1.2.15). The initial condition is

$$\rho(\beta = 0) = \mathbf{1}. \tag{1.2.22}$$

This is of course the analogue of (1.2.5). The canonical partition function is easily obtained from the unnormalized density operator,

$$Z(\beta) = \mathrm{Tr}\, \rho(\beta) = \int_{\mathbb{R}^d} \mathrm{d}\boldsymbol{q}\, \rho(\boldsymbol{q}, \boldsymbol{q}; \beta). \tag{1.2.23}$$

The density matrix is even more useful than the QM propagator when extracting the spectral information, since it has the spectral decomposition

$$\rho(\boldsymbol{q}, \boldsymbol{q}'; \beta) = \sum_{n \geq 0} \phi_n(\boldsymbol{q}) \mathrm{e}^{-\beta E_n} \phi_n^*(\boldsymbol{q}'). \tag{1.2.24}$$

This means that we can extract the energies and eigenfunctions by performing a low temperature expansion (i.e. by considering the limit $\beta \to \infty$). The leading-order term gives the energy and wavefunction of the ground state, the next-to-leading term contains information about the first excited state, and so on.

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Let us now present three important examples where the quantum-mechanical propagator can be computed in closed form: the free particle, the harmonic oscillator, and a particle in a linear potential.

Example 1.2.1 *Propagator for the free particle*. The QM propagator can easily be computed for a free particle in one dimension, with Hamiltonian

$$\mathsf{H} = \frac{\mathsf{p}^2}{2m}. \tag{1.2.25}$$

Indeed, we have

$$\begin{aligned} K(q_f, q_0; t_f, t_0) &= \langle q_f | \exp\left[-\frac{\mathrm{i}(t_f - t_0)\mathsf{p}^2}{2m\hbar}\right] |q_0\rangle \\ &= \int_{\mathbb{R}} \langle q_f | p\rangle\langle p| \exp\left[-\frac{\mathrm{i}(t_f - t_0)\mathsf{p}^2}{2m\hbar}\right] |q_0\rangle \mathrm{d}p \\ &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}p(q_f - q_0)/\hbar}\mathrm{e}^{-\frac{\mathrm{i}(t_f - t_0)p^2}{2m\hbar}} \mathrm{d}p \\ &= \left(\frac{m}{2\pi \mathrm{i}\hbar(t_f - t_0)}\right)^{1/2} \exp\left[\frac{\mathrm{i}m}{2\hbar(t_f - t_0)}(q_f - q_0)^2\right], \end{aligned} \tag{1.2.26}$$

where we have used the Gaussian integral formula (C.1) and the result for the plane waves

$$\langle q|p\rangle = \psi_p(q) = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\mathrm{i}pq/\hbar}. \tag{1.2.27}$$

From (1.2.26), we can also deduce the canonical density matrix for a free particle:

$$\rho(q, q'; \beta) = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} \exp\left[-\frac{m}{2\beta\hbar^2}(q - q')^2\right]. \tag{1.2.28}$$

The generalization to D dimensions is straightforward. We have, for example,

$$K(\boldsymbol{q}_f, \boldsymbol{q}_0; t_f, t_0) = \left(\frac{m}{2\pi \mathrm{i}\hbar(t_f - t_0)}\right)^{D/2} \exp\left[\frac{\mathrm{i}m}{2\hbar(t_f - t_0)}(\boldsymbol{q}_f - \boldsymbol{q}_0)^2\right]. \tag{1.2.29}$$

In this way, one finds the well-known expression for the thermal partition function of a free particle in D dimensions:

$$Z(\beta) = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{D/2} V_D, \tag{1.2.30}$$

where V_D is the volume where the particle lives. □

Example 1.2.2 *Propagator for the harmonic oscillator*. Let us consider a quantum harmonic oscillator in one dimension, with Hamiltonian

$$\mathsf{H} = \frac{\mathsf{p}^2}{2m} + \frac{m\omega^2\mathsf{q}^2}{2}. \tag{1.2.31}$$

We will set $t_0 = 0$, which we can always do when H is time independent. Let us recall that the time-dependent Heisenberg operators associated to q, p are given by

$$\mathsf{q}_H(t) = \mathrm{e}^{\mathrm{i}\mathsf{H}t/\hbar}\,\mathsf{q}\,\mathrm{e}^{-\mathrm{i}\mathsf{H}t/\hbar}, \qquad \mathsf{p}_H(t) = \mathrm{e}^{\mathrm{i}\mathsf{H}t/\hbar}\,\mathsf{p}\,\mathrm{e}^{-\mathrm{i}\mathsf{H}t/\hbar}. \tag{1.2.32}$$

They satisfy the Heisenberg equation of motion (EOM), which reads in this case as

$$\dot{\mathsf{q}}_H(t) = \frac{1}{m}\mathsf{p}_H(t), \qquad \dot{\mathsf{p}}_H(t) = -m\omega^2 \mathsf{q}_H(t), \tag{1.2.33}$$

and can be integrated to give

$$\begin{aligned} \mathsf{q}_H(t) &= \cos(\omega t)\mathsf{q}_H(0) + \frac{1}{m\omega}\sin(\omega t)\mathsf{p}_H(0), \\ \mathsf{p}_H(t) &= -m\omega\sin(\omega t)\mathsf{q}_H(0) + \cos(\omega t)\mathsf{p}_H(0). \end{aligned} \tag{1.2.34}$$

We also recall that $\mathsf{q}_H(0) = \mathsf{q}$, $\mathsf{p}_H(0) = \mathsf{p}$ are the operators in the Schrödinger representation. Let us also denote

$$|q_0(t)\rangle = \mathrm{e}^{-\mathrm{i}\mathsf{H}t/\hbar}|q_0\rangle. \tag{1.2.35}$$

We want to calculate

$$K(q_f, q_0; t, 0) = \langle q_f | q_0(t)\rangle. \tag{1.2.36}$$

We first note that

$$\langle q_f|\mathsf{q}_H(-t)|q_0(t)\rangle = \langle q_f|\mathrm{e}^{-\mathrm{i}\mathsf{H}t/\hbar}\,\mathsf{q}\,\mathrm{e}^{\mathrm{i}\mathsf{H}t/\hbar}\mathrm{e}^{-\mathrm{i}\mathsf{H}t/\hbar}|q_0\rangle = q_0 K(q_f, q_0; t, 0). \tag{1.2.37}$$

On the other hand, by using the explicit solution of $\mathsf{q}_H(-t)$, we find

$$\begin{aligned} \langle q_f|\mathsf{q}_H(-t)|q_0(t)\rangle &= \cos(\omega t)\langle q_f|\mathsf{q}_H(0)|q_0(t)\rangle - \frac{1}{m\omega}\sin(\omega t)\langle q_f|\mathsf{p}_H(0)|q_0(t)\rangle \\ &= \cos(\omega t) q_f K(q_f, q_0; t, 0) + \frac{\mathrm{i}\hbar}{m\omega}\sin(\omega t)\frac{\partial}{\partial q_f}K(q_f, q_0; t, 0). \end{aligned} \tag{1.2.38}$$

Putting both results together, we obtain the following differential equation for the propagator:

$$\frac{\partial}{\partial q_f}K(q_f, q_0; t, 0) = \frac{m\omega}{\mathrm{i}\hbar\sin(\omega t)}\Big(q_0 - q_f\cos(\omega t)\Big)K(q_f, q_0; t, 0), \tag{1.2.39}$$

whose solution is

$$K(q_f, q_0; t, 0) = \mathcal{N}(t)\exp\left[\frac{\mathrm{i}m\omega}{\hbar\sin(\omega t)}\left(\frac{1}{2}q_f^2\cos(\omega t) - q_f q_0\right)\right]. \tag{1.2.40}$$

Here, $\mathcal{N}(t)$ is an undetermined function of t. To find this function, we use that

$$\mathrm{i}\hbar\frac{\partial}{\partial t}K(q_f, q_0; t, 0) = \langle q_f|\mathsf{H}|q_0(t)\rangle = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_f^2} + \frac{m\omega^2}{2}q_f^2\right)K(q_f, q_0; t, 0). \tag{1.2.41}$$

Plugging (1.2.40) into this equation, we obtain

$$\frac{\partial\mathcal{N}}{\partial t} = \left(-\frac{\omega}{2}\cot(\omega t) - \frac{\mathrm{i}m\omega^2}{2\hbar\sin^2(\omega t)}q_0^2\right)\mathcal{N}(t), \tag{1.2.42}$$

which is easily integrated to

$$\mathcal{N}(t) = \frac{C}{\sqrt{\sin(\omega t)}}\exp\left(\frac{\mathrm{i}m\omega}{2\hbar}\cot(\omega t)q_0^2\right). \tag{1.2.43}$$

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The quantum propagator can then be expressed as,

$$K(q_f, q_0; t, 0) = \frac{C}{\sqrt{\sin(\omega t)}} \exp\left[\frac{\mathrm{i} m\omega}{2\hbar \sin(\omega t)} \left(\left(q_f^2 + q_0^2\right)\cos(\omega t) - 2q_f q_0\right)\right]. \tag{1.2.44}$$

The constant C can be determined by considering the free particle limit $\omega \to 0$. In this limit, we should recover the result (1.2.26). This fixes

$$C = \sqrt{\frac{m\omega}{2\pi \mathrm{i}\hbar}}, \tag{1.2.45}$$

and we finally obtain

$$K(q_f, q_0; t_f, t_0) = \sqrt{\frac{m\omega}{2\pi \mathrm{i}\hbar \sin(\omega T)}} \exp\left[\frac{\mathrm{i} m\omega}{2\hbar \sin(\omega T)} \left(\left(q_f^2 + q_0^2\right)\cos(\omega T) - 2q_f q_0\right)\right], \tag{1.2.46}$$

where we used time translation invariance, and T is given in (1.2.8). □

Example 1.2.3 *Propagator for the linear potential*. Let us consider now the quantum Hamiltonian

$$\mathsf{H} = \frac{\mathsf{p}^2}{2m} - F\mathsf{q}, \tag{1.2.47}$$

which corresponds to a linear potential in one dimension. We can compute the QM propagator by using a method similar to that in the previous example. The Heisenberg EOM are

$$\dot{\mathsf{q}}(t) = \frac{\mathsf{p}(t)}{m}, \qquad \dot{\mathsf{p}}(t) = F, \tag{1.2.48}$$

which can be integrated immediately to

$$\begin{aligned} \mathsf{q}(t) &= \frac{Ft^2}{2m} + \frac{t}{m}\mathsf{p} + \mathsf{q}, \\ \mathsf{p}(t) &= Ft + \mathsf{p}, \end{aligned} \tag{1.2.49}$$

where $\mathsf{q} = \mathsf{q}(0)$, $\mathsf{p} = \mathsf{p}(0)$. Using this explicit solution we obtain

$$\langle q_f | \mathsf{q}(-t) | q_0(t)\rangle = \left(\frac{Ft^2}{2m} + \frac{\mathrm{i}\hbar t}{m}\frac{\partial}{\partial q_f} + q_f\right) K(q_f, q_0; t, 0), \tag{1.2.50}$$

and we find the equation

$$\frac{\partial}{\partial q_f} \log K(q_f, q_0; t, 0) = \frac{\mathrm{i} m}{t\hbar}\left(q_f - q_0 + \frac{Ft^2}{2m}\right). \tag{1.2.51}$$

This can be integrated as

$$K(q_f, q_0; t, 0) = \mathcal{N}(t) \exp\left[\frac{\mathrm{i} m}{t\hbar}\left(\frac{q_f^2}{2} - q_f q_0\right) + \frac{\mathrm{i} F q_f t}{2\hbar}\right]. \tag{1.2.52}$$

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To determine $\mathcal{N}(t)$, we again use the analogue of (1.2.41), which reads in this case as

$$\mathrm{i}\hbar\frac{\partial}{\partial t}K(q_f,q_0;t,0) = \langle q_f|\mathsf{H}|q_0(t)\rangle = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_f^2} - Fq_f\right)K(q_f,q_0;t,0). \quad (1.2.53)$$

Plugging (1.2.52) into this equation, we find

$$\frac{\partial}{\partial t}\log\mathcal{N}(t) = -\frac{1}{2t} + \frac{\mathrm{i}Fq_0}{2\hbar} - \frac{\mathrm{i}mq_0^2}{2\hbar t^2} - \frac{\mathrm{i}F^2t^2}{8m\hbar}, \quad (1.2.54)$$

so that

$$\mathcal{N}(t) = \frac{C}{\sqrt{t}}\exp\left(\frac{\mathrm{i}mq_0^2}{2\hbar t} + \frac{\mathrm{i}Fq_0t}{2\hbar} - \frac{\mathrm{i}F^2t^3}{24m\hbar}\right). \quad (1.2.55)$$

Again, the integration constant can be obtained by comparing the full result to the free particle limit, when $F \to 0$. Finally, one finds that,

$$K(q_f,q_0;t,0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\exp\left[\frac{\mathrm{i}m}{2t\hbar}\left(q_f-q_0\right)^2 + \frac{\mathrm{i}Ft}{2\hbar}(q_f+q_0) - \frac{\mathrm{i}F^2t^3}{24m\hbar}\right]. \quad (1.2.56)$$

□

An interesting aspect of the examples we have just considered is that both the exponent and the prefactor of the QM propagator are related to quantities in classical mechanics. Let us consider a classical path of trajectory, $q(t)$, satisfying the boundary conditions

$$\boldsymbol{q}(t_0) = \boldsymbol{q}_0, \qquad \boldsymbol{q}(t_f) = \boldsymbol{q}_f. \quad (1.2.57)$$

The classical action is a functional of the trajectory obtained by integrating the Lagrangian,

$$S(\boldsymbol{q}(t)) = \int_{t_0}^{t_f} L(\boldsymbol{q}(t),\dot{\boldsymbol{q}}(t))\mathrm{d}t. \quad (1.2.58)$$

As is well known from classical mechanics, this functional has an extremum when the trajectory $\boldsymbol{q}(t)$ solves the classical EOM. Indeed, if we perform a variation $\delta\boldsymbol{q}(t)$ preserving the boundary conditions (1.2.57), one has

$$\frac{\delta S}{\delta\boldsymbol{q}(t)} = -\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\right) + \frac{\partial L}{\partial\boldsymbol{q}}. \quad (1.2.59)$$

Let us denote by $\boldsymbol{q}_c(t)$ the solution to the Lagrange EOM with the boundary conditions (1.2.57) (which we assume to exist and to be unique, for simplicity). Then, we have

$$\left.\frac{\delta S}{\delta\boldsymbol{q}(t)}\right|_{\boldsymbol{q}(t)=\boldsymbol{q}_c(t)} = 0. \quad (1.2.60)$$

In the following, we will denote by S_c the value of the classical action on the classical trajectory:

$$S_c = S(\boldsymbol{q}_c(t)). \quad (1.2.61)$$

It is a function of the boundary data $\boldsymbol{q}_f$, $\boldsymbol{q}_0$, t_f, and t_0.

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In the case of the free particle in one dimension, the action reads

$$S(q(t)) = \frac{m}{2} \int_{t_0}^{t_f} (\dot{q}(t))^2 \, \mathrm{d}t. \tag{1.2.62}$$

The classical trajectory has constant velocity, equal to

$$\dot{q}_c(t) = \frac{q_f - q_0}{t_f - t_0}. \tag{1.2.63}$$

The classical action is in this case,

$$S_c = \frac{m}{2} \frac{(q_f - q_0)^2}{t_f - t_0}. \tag{1.2.64}$$

We can then write (1.2.26) as

$$K(q_f, q_0; t_f, t_0) = \frac{1}{\sqrt{2\pi i\hbar}} \left(-\frac{\partial^2 S_c}{\partial q_f \partial q_0} \right)^{1/2} \mathrm{e}^{\mathrm{i}S_c/\hbar}. \tag{1.2.65}$$

This result also holds for the harmonic oscillator and for the particle in a linear potential. Let us verify it for the harmonic oscillator. The solution to the classical EOM that satisfies the boundary conditions is

$$q_c(t) = q_0 \cos(\omega(t - t_0)) + \frac{q_f - q_0 \cos(\omega T)}{\sin(\omega T)} \sin(\omega(t - t_0)). \tag{1.2.66}$$

The classical action evaluated at this path is:

$$\begin{aligned} S_c &= \int_{t_0}^{t_f} \left(\frac{m\dot{q}_c^2}{2} - \frac{m\omega^2 q_c^2}{2} \right) \mathrm{d}t = \frac{m}{2} \dot{q}_c(t) q_c(t) \Big|_{t_0}^{t_f} - \frac{m}{2} \int_{t_0}^{t_f} q_c \left(\ddot{q}_c + \omega^2 q_c \right) \mathrm{d}t \\ &= \frac{m}{2} \left(\dot{q}_c(t_f) q_c(t_f) - \dot{q}_c(t_0) q_c(t_0) \right) = \frac{m\omega}{2\sin(\omega T)} \left(\left(q_f^2 + q_0^2 \right) \cos(\omega T) - 2 q_f q_0 \right). \end{aligned} \tag{1.2.67}$$

It is now easy to verify that the quantum propagator (1.2.46) also has the structure (1.2.65).

In the conventional formulation of quantum mechanics, the result (1.2.65) is somewhat surprising and far from obvious. Why does the calculation of a quantum-mechanical propagator involve the classical action of Lagrangian mechanics? We will find an *a priori* explanation of this structure in Chapter 4, in the context of the path integral formulation of quantum mechanics.

1.3 Resolvent and Green's Functions

The evolution operator $\mathsf{U}(t, t')$ is closely related to the Green's functions of the time-dependent Schrödinger operator

$$\mathrm{i}\hbar \frac{\partial}{\partial t} - \mathsf{H}. \tag{1.3.68}$$

Let us define

$$\mathsf{G}_{\pm}(t - t') = \pm\theta\left(\pm(t - t')\right) \mathsf{U}(t, t'). \tag{1.3.69}$$

The functions $\mathsf{G}_\pm(t)$ are called *retarded* (respectively, advanced) Green's functions. Obviously,

$$\mathsf{U}(t,t') = \mathsf{G}_+(t-t') - \mathsf{G}_-(t-t'). \tag{1.3.70}$$

From (1.2.5) it follows that $\mathsf{G}_\pm$ satisfy the Schrödinger equation with a delta function,

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \mathsf{H}\right)\mathsf{G}_\pm(t-t') = \mathrm{i}\hbar\delta(t-t'), \tag{1.3.71}$$

which is the defining equation for a Green's function.

After a Fourier transform w.r.t. t, this equation will become algebraic. We then introduce the Fourier transforms of the Green's functions:

$$\mathsf{G}_\pm(E) = \frac{1}{\mathrm{i}\hbar}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}Et/\hbar}\mathsf{G}_\pm(t)\mathrm{d}t, \tag{1.3.72}$$

with inverses,

$$\mathsf{G}_\pm(t) = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}Et/\hbar}\mathsf{G}_\pm(E)\mathrm{d}E. \tag{1.3.73}$$

Let us first consider $\mathsf{G}_+(E)$. Since $\mathsf{G}_+(t) = 0$ for $t < 0$, we find

$$\mathsf{G}_+(E) = \frac{1}{\mathrm{i}\hbar}\int_0^\infty \mathrm{e}^{\mathrm{i}Et/\hbar}\mathsf{G}_+(t)\mathrm{d}t. \tag{1.3.74}$$

In order to evaluate the integral over t, one introduces as a regularization the damping factor $\mathrm{e}^{-\epsilon t/\hbar}$, where $\epsilon > 0$ and small. This is equivalent to shifting the energy:

$$E \to E + \mathrm{i}\epsilon. \tag{1.3.75}$$

In this way, one finds

$$\mathsf{G}_+(E) = \lim_{\epsilon\to 0^+}\frac{1}{\mathrm{i}\hbar}\int_0^\infty \mathrm{e}^{\mathrm{i}(E+\mathrm{i}\epsilon)t/\hbar}\mathrm{e}^{-\mathrm{i}\mathsf{H}t/\hbar}\mathrm{d}t = \lim_{\epsilon\to 0^+}\frac{1}{E+\mathrm{i}\epsilon-\mathsf{H}}. \tag{1.3.76}$$

Note that, with the above regularization, the poles of $\mathsf{G}_+(E)$ are in the lower half-plane $\mathrm{Im}(E) < 0$. Therefore, when $t < 0$, the integral (1.3.73) can be computed by closing the contour in the upper half plane, and no contributions will appear, guaranteeing that $\mathsf{G}_+(t)$ vanishes. A similar calculation shows that

$$\mathsf{G}_-(E) = \lim_{\epsilon\to 0^+}\frac{1}{E-\mathrm{i}\epsilon-\mathsf{H}}. \tag{1.3.77}$$

These results suggest we introduce of the *resolvent operator*, defined by

$$\mathsf{G}(E) = \frac{1}{E-\mathsf{H}}. \tag{1.3.78}$$

Here, E is in general complex, so the resolvent is an operator-valued function on the complex plane. It follows from the above discussion that the operators $\mathsf{G}_\pm(E)$ are the limits of $\mathsf{G}(E)$ when E approaches the real axis from above or from below in the complex plane, respectively:

$$\mathsf{G}_\pm(E) = \lim_{\epsilon\to 0^+}\mathsf{G}(E\pm\mathrm{i}\epsilon). \tag{1.3.79}$$

This indicates that, as a function on the complex E plane, the resolvent has a branch cut on the real axis. We will see in a moment that this is the case already for the free

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particle in one dimension, and in Section 1.4 we will determine the analytic structure of the resolvent.

The resolvent is an operator, and in order to explore it in detail it is more useful to consider functions associated to it, such as its integral kernel or its trace. Its integral kernel is

$$G(\boldsymbol{x}, \boldsymbol{y}; E) = \langle \boldsymbol{x} | (E - \mathsf{H})^{-1} | \boldsymbol{y} \rangle, \tag{1.3.80}$$

and its trace will simply be denoted by

$$G(E) = \mathrm{Tr}\, \mathsf{G}(E). \tag{1.3.81}$$

It follows from (1.3.78) that the resolvent satisfies

$$(E - \mathsf{H})\mathsf{G}(E) = 1, \tag{1.3.82}$$

which is a time-independent Schrödinger equation with a delta source. If we consider a standard one-dimensional Hamiltonian of the form

$$\mathsf{H} = \frac{\mathsf{p}^2}{2m} + V(\mathsf{q}), \tag{1.3.83}$$

we find that the integral kernel of the resolvent satisfies

$$\left(\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} - V(x) + E \right) G(x, y; E) = \delta(x - y). \tag{1.3.84}$$

Example 1.3.1 *Resolvent for the free particle in one dimension*. For a free particle,

$$\mathsf{H} = \frac{\mathsf{p}^2}{2m}, \tag{1.3.85}$$

and the resolvent is given by

$$G(x, y; E) = \left\langle x \middle| \left(E - \frac{\mathsf{p}^2}{2m} \right)^{-1} \middle| y \right\rangle. \tag{1.3.86}$$

By introducing the resolution of identity,

$$\int_{\mathbb{R}} \mathrm{d}p |p\rangle\langle p| = \mathbf{1}, \tag{1.3.87}$$

we find

$$G(x, y; E) = \int_{\mathbb{R}} \langle x|p\rangle \frac{1}{E - p^2/(2m)} \langle p|y\rangle \mathrm{d}p = \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \frac{\mathrm{e}^{\mathrm{i}p(x-y)/\hbar}}{E - \frac{p^2}{2m}} \mathrm{d}p. \tag{1.3.88}$$

Since the answer only depends on the difference $x - y$ (which is expected, due to translation invariance), we will denote

$$G(x - y; E) \equiv G(x, y; E). \tag{1.3.89}$$

The integral in (1.3.88) depends on the value of E. If E is *not* on the positive real axis, the integral is well defined and can be computed by using the residue theorem. Let us suppose, for example, that $E < 0$. In this case, there are two poles on the imaginary axis at

$$\pm \mathrm{i} p_0 = \pm \mathrm{i} \sqrt{2m|E|} \tag{1.3.90}$$

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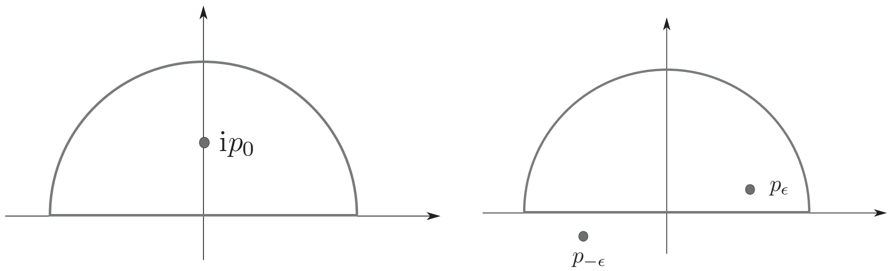

Figure 1.1 (Left) When $E < 0$, the poles are on the imaginary axis, and their position does not depend on the ϵ prescription. (Right) When $E > 0$, the poles for $G_+(x;E)$ are as shown in the figure.

(see Figure 1.1 [left]). Depending on whether $x > 0$ or $x < 0$, we can close the contour on the upper (respectively, lower) half plane and use Jordan's lemma. We obtain,

$$G(x;E) = -\frac{1}{\hbar}\sqrt{\frac{m}{-2E}}\,\mathrm{e}^{-\sqrt{-2mE}|x|/\hbar}, \qquad E < 0. \tag{1.3.91}$$

Let us now suppose that $E > 0$. In this case, there are singularities in the integration contour and it is crucial to shift $E \to E \pm \mathrm{i}\epsilon$, as expected from the previous discussion. We then consider,

$$G_\pm(x,y;E) = \lim_{\epsilon\to 0^+} \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \frac{\mathrm{e}^{\mathrm{i}p(x-y)/\hbar}}{E \pm \mathrm{i}\epsilon - \frac{p^2}{2m}}. \tag{1.3.92}$$

Let us first consider $G_+(x,y;E)$. The poles are no longer on the real axis, but at

$$p_{\pm\epsilon} = \pm\sqrt{2mE} \pm \mathrm{i}\epsilon \tag{1.3.93}$$

(see Figure 1.1 [right]). When $x > 0$, we close the contour integral in the upper half plane, and we pick up the residue of the pole with + sign. When $x < 0$, we close the contour on the lower half plane. We find,

$$G_+(x;E) = -\frac{\mathrm{i}}{\hbar}\sqrt{\frac{m}{2E}}\,\mathrm{e}^{\mathrm{i}\sqrt{2mE}|x|/\hbar}, \qquad E > 0. \tag{1.3.94}$$

If we compute $G_-(x;E)$, the poles will be at

$$\pm\sqrt{2mE} \mp \mathrm{i}\epsilon, \tag{1.3.95}$$

and

$$G_-(x;E) = \frac{\mathrm{i}}{\hbar}\sqrt{\frac{m}{2E}}\,\mathrm{e}^{-\mathrm{i}\sqrt{2mE}|x|/\hbar}, \qquad E > 0. \tag{1.3.96}$$

We conclude that the integral kernel of the resolvent is the following function on the complex plane E:

$$G(x;E) = -\frac{\mathrm{i}}{\hbar}\sqrt{\frac{m}{2E}}\,\mathrm{e}^{\mathrm{i}\sqrt{2mE}|x|/\hbar}, \tag{1.3.97}$$

where $\sqrt{E}$ has a branch cut along $[0,\infty)$. In particular, we have

$$\lim_{\epsilon\to 0^+} \sqrt{E \pm \mathrm{i}\epsilon} = \pm\sqrt{E}, \qquad E > 0, \tag{1.3.98}$$

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so that we recover the functions $G_\pm(x;E)$ as the limits of $G(x;E)$ as we approach the positive real axis. In addition,

$$\sqrt{E} = \mathrm{i}\sqrt{-E}, \qquad E < 0, \tag{1.3.99}$$

and we recover our previous result (1.3.91). A useful way to write down the resolvent is to introduce a complex variable k such that

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 |k|^2 \mathrm{e}^{2\mathrm{i}\alpha}}{2m}. \tag{1.3.100}$$

This parametrization is such that the complex plane of E is covered as $\alpha \in [0, \pi]$, i.e. as $\mathrm{Im}(k) > 0$. This is called the *physical sheet*. When the complex energy is of the form $E + \mathrm{i}\epsilon$, with $E > 0$, we take k real and positive:

$$k = \frac{\sqrt{2mE}}{\hbar}. \tag{1.3.101}$$

As we rotate in the E plane towards the negative axis, we have that $\alpha = \pi/2$, so that $E = -|E|$ is negative. In this case, k is chosen to be

$$k = |k|\mathrm{e}^{\mathrm{i}\pi/2} = \mathrm{i}|k| = \mathrm{i}\frac{\sqrt{2m|E|}}{\hbar}. \tag{1.3.102}$$

Finally, as $\alpha = \pi$, the complex energy is of the form $E - \mathrm{i}\epsilon$, with $E > 0$, and

$$k = -\frac{\sqrt{2mE}}{\hbar}. \tag{1.3.103}$$

With these conventions for k, the resolvent can be written as

$$G(x;E) = -\frac{\mathrm{i}m}{\hbar^2 k}\mathrm{e}^{\mathrm{i}k|x|}. \tag{1.3.104}$$

□

1.4 Analytic Properties of the Resolvent

In Section 1.3 we saw that the resolvent has a nontrivial analytic structure, as a function on the complex E plane. We will now obtain general information about this analytic structure, in terms of spectral information of the Hamiltonian H.

In general, the Hamiltonian H will have both a discrete spectrum, with eigenvalues E_n and eigenvectors $|\phi_n\rangle$, and a continuous spectrum with generalized eigenvectors $|\lambda\rangle$ and eigenvalues $E(\lambda)$. Here, λ is a label for these continuous states (it could be, for example, the momentum). The resolution of the identity for these states gives

$$\mathbf{1} = \sum_n |\phi_n\rangle\langle\phi_n| + \int \frac{\mathrm{d}\lambda}{N(\lambda)}|\lambda\rangle\langle\lambda|, \tag{1.4.105}$$

where

$$\langle\lambda|\lambda'\rangle = N(\lambda)\delta(\lambda - \lambda'). \tag{1.4.106}$$

Note that the factor of $1/N(\lambda)$ guarantees that

$$\left(\int \frac{\mathrm{d}\lambda}{N(\lambda)}|\lambda\rangle\langle\lambda|\right)|\lambda'\rangle = |\lambda'\rangle. \tag{1.4.107}$$

Let us now multiply the above identity by $(z - \mathsf{H})^{-1}$. We obtain,

$$\mathsf{G}(z) = \sum_n \frac{|\phi_n\rangle\langle\phi_n|}{z - E_n} + \int \frac{\mathrm{d}\lambda}{N(\lambda)} \frac{|\lambda\rangle\langle\lambda|}{z - E(\lambda)}. \tag{1.4.108}$$

Let us introduce the following projector of the continuous states onto those with energy E,

$$\mathsf{P}_E = \int \frac{\mathrm{d}\lambda}{N(\lambda)}|\lambda\rangle\delta(E - E(\lambda))\langle\lambda|. \tag{1.4.109}$$

In terms of this projector, we can write

$$\mathsf{G}(z) = \sum_n \frac{|\phi_n\rangle\langle\phi_n|}{z - E_n} + \int \mathrm{d}E \frac{\mathsf{P}_E}{z - E}. \tag{1.4.110}$$

In order to write an equation for complex functions of z (instead of operator-valued functions of z), we consider averages of the resolvent over an arbitrary unit norm state $|u\rangle$:

$$G_u(z) = \langle u|\mathsf{G}(z)|u\rangle. \tag{1.4.111}$$

We then obtain the spectral decomposition,

$$G_u(z) = \sum_n \frac{|\langle u|\phi_n\rangle|^2}{z - E_n} + \int \mathrm{d}E \frac{\langle u|\mathsf{P}_E|u\rangle}{z - E}. \tag{1.4.112}$$

Note that

$$\langle u|\mathsf{P}_E|u\rangle = \int \frac{\mathrm{d}\lambda}{N(\lambda)}\delta(E - E(\lambda))\, |\langle u|\lambda\rangle|^2 . \tag{1.4.113}$$

Let z be a point in the complex plane at a nonzero distance δ from the real axis. It is clear that

$$\left|\frac{1}{z - E}\right| \le \frac{1}{\delta}, \tag{1.4.114}$$

for any real E, and we find the upper bound

$$|G_u(z)| \le \frac{1}{\delta}\left\{\sum_n \left|\langle u|\phi_n\rangle\right|^2 + \int \mathrm{d}E\langle u|\mathsf{P}_E|u\rangle\right\} \le \frac{1}{\delta}, \tag{1.4.115}$$

since the term inside the brackets is just the norm of u, which is one by assumption. We conclude that $G_u(z)$ is bounded away from the real axis. Similarly, one finds that $G'_u(z)$ is bounded. Since $G_u(z)$ is given by a convergent infinite sum of analytic functions, it is an analytic function of z away from the real axis. A similar argument shows that $G_u(z)$ is analytic for any real value of z that is not an eigenvalue and does not belong to the continuous spectrum.

It is also clear that, for a generic u such that $\langle u|\phi_n\rangle \neq 0$, the point $z = E_n$ corresponding to the discrete spectrum is a *simple pole* of the resolvent. Let us now study what happens when z approaches a value of E in the continuous spectrum. We set $z = E \pm \mathrm{i}\epsilon$ and we calculate

$$\lim_{\epsilon\to 0} G_u(E \pm \mathrm{i}\epsilon) = \sum_n \frac{\left|\langle u|\phi_n\rangle\right|^2}{E \pm \mathrm{i}\epsilon - E_n} + \int \mathrm{d}E' \frac{\langle u|\mathsf{P}_{E'}|u\rangle}{E \pm \mathrm{i}\epsilon - E'}. \tag{1.4.116}$$

We now use the following equality of distributions,

$$\lim_{\epsilon\to 0} \frac{1}{x \pm \mathrm{i}\epsilon} = \mathrm{P}\frac{1}{x} \mp \pi\mathrm{i}\delta(x), \tag{1.4.117}$$

where P denotes the principal part. We find,

$$\lim_{\epsilon\to 0} G_u(E \pm \mathrm{i}\epsilon) = \sum_n \frac{\left|\langle u|\phi_n\rangle\right|^2}{E - E_n} + \mathrm{P}\int \mathrm{d}E' \frac{\langle u|\mathsf{P}_{E'}|u\rangle}{E - E'} \mp \pi\mathrm{i}\langle u|\mathsf{P}_E|u\rangle. \tag{1.4.118}$$

There is a discontinuity in the function when we approach a continuous eigenvalue from above or from below the real axis. We conclude that $G_u(E)$ has a *branch cut* along the continuous spectrum, and the discontinuity is given by

$$G_u(E + \mathrm{i}\epsilon) - G_u(E - \mathrm{i}\epsilon) = -2\pi\mathrm{i}\langle u|\mathsf{P}_E|u\rangle, \tag{1.4.119}$$

or, equivalently,

$$\mathrm{Im}\left(G_u(E + \mathrm{i}\epsilon)\right) = -\pi\langle u|\mathsf{P}_E|u\rangle. \tag{1.4.120}$$

Plugging this result back into (1.4.112), we obtain

$$G_u(z) = \sum_n \frac{\left|\langle u|\phi_n\rangle\right|^2}{z - E_n} - \frac{1}{\pi}\int_{\mathcal{C}} \frac{\mathrm{Im}\left(G_u(E + \mathrm{i}\epsilon)\right)}{z - E}\mathrm{d}E, \tag{1.4.121}$$

where the integral is along the branch cut $\mathcal{C}$ of the function.

This equality is simply a manifestation of Cauchy's theorem. Indeed, let us consider a counter-clockwise contour C in the complex plane, as shown in Figure 1.2,

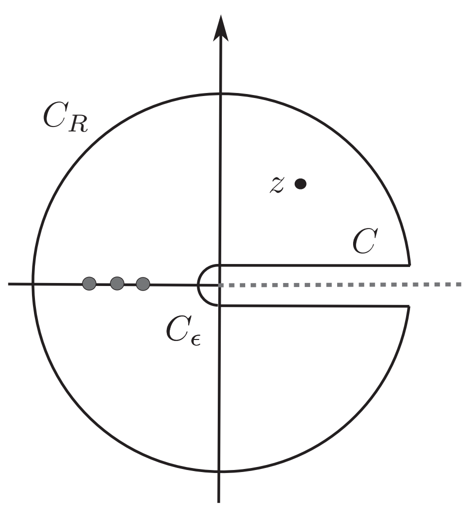

Figure 1.2 The contour C used in the integral (1.4.122).

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and enclosing a point $z \in \mathbb{C}\backslash\mathbb{R}$. For simplicity, we will assume that the branch cut of $G_u(E)$ starts at $E = 0$. Let us consider the integral

$$\oint_C f(z')\mathrm{d}z', \tag{1.4.122}$$

where the function

$$f(z') = \frac{G_u(z')}{z' - z}, \tag{1.4.123}$$

is analytic along the contour. The integral can be written as,

$$\oint_C f(z')\mathrm{d}z' = \int_{C_R} f(z')\mathrm{d}z' + \int_{C_\epsilon} f(z')\mathrm{d}z' + \int_\epsilon^\infty (f(x + \mathrm{i}\epsilon) - f(x - \mathrm{i}\epsilon))\mathrm{d}x, \tag{1.4.124}$$

where C_ϵ is small contour of radius ϵ around $z' = 0$, and C_R is a large contour of radius R. On the other hand, we can evaluate the integral by using Cauchy's residue theorem. There is a pole at $z' = z$, with residue $G_u(z)$. In addition, $G_u(z)$ has poles at $z = E_n$, $n \geq 0$, due to bound states, with residues R_n, and we have

$$\oint_C f(z')\mathrm{d}z' = 2\pi\mathrm{i}\left(G_u(z) + \sum_{n=0}^N \frac{R_n}{E_n - z}\right), \tag{1.4.125}$$

where $E_0, \ldots, E_N$ are the poles contained in the contour. Let us assume that the integrals around C_R and C_ϵ vanish as $R \to \infty$ and $\epsilon \to 0$ (this can be proved rigorously in some cases, such as in the one-dimensional situation considered below). We conclude that

$$G_u(z) = \sum_{n=0}^\infty \frac{R_n}{z - E_n} + \frac{1}{\pi}\int_0^\infty \frac{\mathrm{Im}(G_u(x + \mathrm{i}\epsilon))}{x - z}\mathrm{d}x. \tag{1.4.126}$$

This is precisely (1.4.121).

Although we have focused on the quantity $G_u(z)$, similar conclusions hold for other quantities, such as the integral kernel of the resolvent $G(\boldsymbol{x}, \boldsymbol{y}; E)$ or its trace $G(E)$. In the case of the integral kernel, we have the spectral decomposition

$$G(\boldsymbol{x}, \boldsymbol{y}; z) = \sum_n \frac{\phi_n(\boldsymbol{x})\phi_n^*(\boldsymbol{y})}{z - E_n} + \int \mathrm{d}E \frac{\langle \boldsymbol{x}|\mathsf{P}_E|\boldsymbol{y}\rangle}{z - E}. \tag{1.4.127}$$

Note that the simple poles of the integral kernel give information about the bound state spectrum, while their residues give information about the corresponding eigenfunctions. For the continuous spectrum, we have that

$$\langle \boldsymbol{x}|\mathsf{P}_E|\boldsymbol{y}\rangle = \int \frac{\mathrm{d}\lambda}{N(\lambda)}\langle \boldsymbol{x}|\lambda\rangle\langle\lambda|\boldsymbol{y}\rangle\delta(E - E(\lambda)). \tag{1.4.128}$$

Let us suppose that, for each value of E, there is a finite set of values of λ, λ_E, such that $E(\lambda_E) = E$. Then, this integral can be evaluated by using that

$$\delta(E - E(\lambda)) = \sum_{\lambda_E} \frac{1}{E'(\lambda_E)}\delta(\lambda - \lambda_E). \tag{1.4.129}$$

Let us denote by

$$\langle \boldsymbol{x}|\lambda\rangle = \psi_\lambda(\boldsymbol{x}), \tag{1.4.130}$$

the wavefunction corresponding to the state $|\lambda\rangle$. Then, we obtain

$$\langle \boldsymbol{x}|\mathsf{P}_E|\boldsymbol{y}\rangle = \sum_{\lambda_E} \frac{1}{N(\lambda_E)|E'(\lambda_E)|} \psi_{\lambda_E}(\boldsymbol{x})\psi^*_{\lambda_E}(\boldsymbol{y}). \tag{1.4.131}$$

As before, this function gives the discontinuity of the integral kernel of the resolvent across the cut:

$$G(\boldsymbol{x}, \boldsymbol{y}; E + \mathrm{i}\epsilon) - G(\boldsymbol{x}, \boldsymbol{y}; E - \mathrm{i}\epsilon) = -2\pi\mathrm{i}\langle \boldsymbol{x}|\mathsf{P}_E|\boldsymbol{y}\rangle. \tag{1.4.132}$$

In the following two examples, we verify this general result in two cases where the resolvent can be computed explicitly.

Example 1.4.1 *The one-dimensional free particle*. In Example 1.3.1 we computed the resolvents $G_\pm(x; E)$ explicitly in the case of a one-dimensional free particle. The discontinuity is given by

$$\begin{aligned} G_+(x; E) - G_-(x; E) &= -\frac{\mathrm{i}}{\hbar}\sqrt{\frac{m}{2E}}\mathrm{e}^{\mathrm{i}\sqrt{2mE}|x|/\hbar} - \frac{\mathrm{i}}{\hbar}\sqrt{\frac{m}{2E}}\mathrm{e}^{-\mathrm{i}\sqrt{2mE}|x|/\hbar} \\ &= -\frac{\mathrm{i}}{\hbar}\sqrt{\frac{2m}{E}}\cos\left(\frac{\sqrt{2mE}}{\hbar}x\right). \end{aligned} \tag{1.4.133}$$

Let us now evaluate the r.h.s. of (1.4.132), by using (1.4.131). We label the continuum spectrum by the momentum $\lambda = p$. Given an energy E, there are two momenta corresponding to it,

$$p_E = \pm\sqrt{2mE}. \tag{1.4.134}$$

The associated wavefunctions are given in (1.2.27), and they are normalized in such a way that $N(p) = 1$. Finally, we note that

$$E(p) = \frac{p^2}{2m}, \qquad E'(p) = \frac{p}{m}. \tag{1.4.135}$$

We then obtain from (1.4.131) (we set $y = 0$ by exploiting translation invariance)

$$-2\pi\mathrm{i}\langle x|\mathsf{P}_E|0\rangle = -2\pi\mathrm{i}\frac{m}{|p_E|}\frac{1}{2\pi\hbar}\left(\mathrm{e}^{\mathrm{i}|p_E|x/\hbar} + \mathrm{e}^{-\mathrm{i}|p_E|x/\hbar}\right), \tag{1.4.136}$$

which is precisely (1.4.133). □

Example 1.4.2 Let us consider the following one-dimensional Hamiltonian,

$$\mathsf{H} = 2\cosh\left(\frac{a\mathsf{p}}{\hbar}\right), \qquad a \in \mathbb{R}_{>0}, \tag{1.4.137}$$

which acts on wavefunctions as a difference operator

$$(\mathsf{H}\psi)(x) = \psi(x + \mathrm{i}a) + \psi(x - \mathrm{i}a). \tag{1.4.138}$$

The parameter a has dimensions of length. The Hamiltonian (1.4.137) is a deformation of the standard free particle Hamiltonian, in the sense that for $a\mathsf{p} \ll \hbar$ one finds

$$\mathsf{H} \approx 2 + \frac{a^2\mathsf{p}^2}{2\hbar^2}. \tag{1.4.139}$$

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This Hamiltonian appears in various contexts in mathematical physics. It is clear that the plane waves $\psi_p(x)$ in (1.2.27) are eigenfunctions of H, with eigenvalue

$$E = 2\cosh\left(\frac{ap}{\hbar}\right). \tag{1.4.140}$$

We will now calculate explicitly the resolvent of H. Clearly, H is diagonal in the momentum basis,

$$\langle p|(E-\mathsf{H})^{-1}|p'\rangle = \frac{1}{E - 2\cosh(ap/\hbar)}\delta(p-p'), \tag{1.4.141}$$

so we can write

$$G(x-y;E) = \langle x|(E-\mathsf{H})^{-1}|y\rangle = \int_{\mathbb{R}} \frac{\mathrm{d}p}{2\pi\hbar}\frac{\mathrm{e}^{\mathrm{i}p(x-y)/\hbar}}{E-2\cosh(ap/\hbar)}. \tag{1.4.142}$$

This integral can be computed using Cauchy's residue theorem. First, we change variables to $\xi = ap/\hbar$, so that

$$G(x;E) = \int_{\mathbb{R}} \frac{\mathrm{d}\xi}{2\pi a}\frac{\mathrm{e}^{\mathrm{i}\xi x/a}}{E-2\cosh\xi}. \tag{1.4.143}$$

In addition, we parametrize $E \in \mathbb{C}\backslash[2,\infty)$ as

$$E = 2\cosh k, \qquad 0 < \mathrm{Im}(k) \le \pi. \tag{1.4.144}$$

In this parametrization, the cut $[2,\infty)$ is covered twice as the variable k runs along the real line. We consider the contour C_R in the ξ plane shown in Figure 1.3. There are two poles inside the contour: $\xi = k$ and $\xi = 2\pi\mathrm{i} - k$. Then, we have

$$\begin{aligned}\lim_{R\to\infty}\oint_{C_R}\frac{\mathrm{d}z}{2\pi a}\frac{\mathrm{e}^{\mathrm{i}zx/a}}{E-2\cosh z} &= \left(1-\mathrm{e}^{-2\pi x/a}\right)G(x;E)\\ &= \frac{\mathrm{i}}{a}\left(\mathrm{Res}_{z=k}\frac{\mathrm{e}^{\mathrm{i}zx/a}}{E-2\cosh z} + \mathrm{Res}_{z=2\pi\mathrm{i}-k}\frac{\mathrm{e}^{\mathrm{i}zx/a}}{E-2\cosh z}\right)\\ &= -\frac{\mathrm{i}}{2a\sinh k}\left(\mathrm{e}^{\mathrm{i}kx/a} - \mathrm{e}^{-\mathrm{i}kx/a-2\pi x/a}\right),\end{aligned} \tag{1.4.145}$$

and we conclude that

$$G(x;E) = -\frac{\mathrm{i}}{2a\sinh k}\left(\frac{\mathrm{e}^{\mathrm{i}kx/a}}{1-\mathrm{e}^{-2\pi x/a}} + \frac{\mathrm{e}^{-\mathrm{i}kx/a}}{1-\mathrm{e}^{2\pi x/a}}\right). \tag{1.4.146}$$

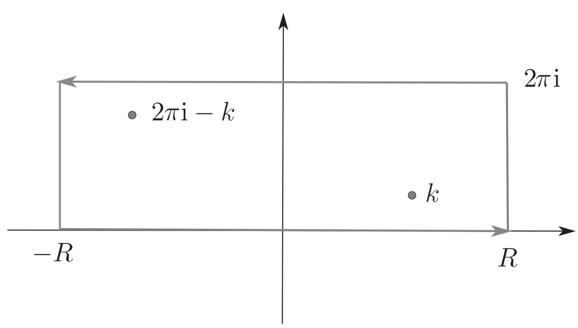

Figure 1.3 The contour C_R used in the integral (1.4.145).

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The discontinuity is easily calculated: since

$$E - 2 \approx k^2, \tag{1.4.147}$$

we see that $E \pm \mathrm{i}\epsilon$, $E > 2$, correspond to k positive and negative, as in Example 1.3.1 for the free particle. We then find

$$G(x; E + \mathrm{i}\epsilon) - G(x; E - \mathrm{i}\epsilon) = -\frac{\mathrm{i}}{a \sinh k} \cos(kx/a). \tag{1.4.148}$$

This is again in precise agreement with the general formulae (1.4.131), (1.4.132), since in this case

$$\langle x|\mathsf{P}_E|0\rangle = \frac{1}{2\pi a \sinh k} \cos(kx/a). \tag{1.4.149}$$

□

1.5 Scattering and Resolvent in One Dimension

In the case of standard Hamiltonians in one dimension, we can often construct the resolvent explicitly by considering special solutions to the Schrödinger equation. We will now present some fundamental results on this topic.

Let us consider a one-dimensional potential, $V(x)$, that has compact support or decreases rapidly at infinity, i.e.

$$V(x) \to 0, \qquad |x| \to \infty. \tag{1.5.150}$$

Then, we have a continuous spectrum of positive energies and we can consider scattering states. We will write the energy of a state in the continuum as

$$E = \frac{\hbar^2 k^2}{2m}, \tag{1.5.151}$$

where k defines the wave vector of the state. In this section we will set $m = 1/2$, $\hbar = 1$ to simplify our notation. Let us now introduce the two *Jost functions*, denoted by $f_1(x,k)$, $f_2(x,k)$. They are solutions to the Schrödinger equation

$$-\psi''(x) + V(x)\psi(x) = k^2\psi(x), \tag{1.5.152}$$

for real k, and they are uniquely characterized by their asymptotic behavior at infinity,

$$\begin{aligned} f_1(x,k) &= \mathrm{e}^{\mathrm{i}kx} + \cdots, \qquad x \to \infty, \\ f_2(x,k) &= \mathrm{e}^{-\mathrm{i}kx} + \cdots, \qquad x \to -\infty. \end{aligned} \tag{1.5.153}$$

They can, however, be extended analytically to complex k, provided that

$$\mathrm{Im}(k) > 0, \tag{1.5.154}$$

i.e. as long as k belongs to the physical sheet (we recall that the concept of physical sheet was introduced in Example 1.3.1).

Let us now assume that k is real and nonzero. Uniqueness of the solutions implies that

$$\overline{f_1(x,k)} = f_1(x,-k), \qquad \overline{f_2(x,k)} = f_2(x,-k), \tag{1.5.155}$$

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since both solve the Schrödinger equation with asymptotics $\exp(\mp \mathrm{i}kx)$ as $x \to \pm\infty$. The pairs $f_1(x,k)$ and $f_1(x,-k)$, as well as $f_2(x,k)$ and $f_2(x,-k)$, are bases of solutions to the Schrödinger equation. One way to check this is to consider their Wronskians. We recall that the Wronskian of two functions is given by

$$W(f,g) = f(x)g'(x) - g(x)f'(x). \tag{1.5.156}$$

The Wronskian of two solutions to the Schrödinger equation is a constant, and it vanishes if and only if the two solutions are linearly dependent. A simple computation indeed shows that

$$W(f_{1,2}(x,k), f_{1,2}(x,-k)) = \mp 2\mathrm{i}k, \tag{1.5.157}$$

therefore justifying our previous statement. Since $f_1(x,k)$ and $f_1(x,-k)$ are a basis, we can express $f_2(x,k)$ as a linear combination of them:

$$f_2(x,k) = a(k) f_1(x,-k) + b(k) f_1(x,k). \tag{1.5.158}$$

The coefficients $a(k)$ and $b(k)$ are sometimes called *transition coefficients*. They can be written in terms of Wronskians as follows:

$$a(k) = \frac{\mathrm{i}}{2k} W(f_1(x,k), f_2(x,k)), \qquad b(k) = \frac{\mathrm{i}}{2k} W(f_2(x,k), f_1(x,-k)). \tag{1.5.159}$$

In addition, when k is real they satisfy

$$\overline{a(k)} = a(-k), \qquad \overline{b(k)} = b(-k). \tag{1.5.160}$$

We can also write,

$$f_1(x,k) = a(k) f_2(x,-k) - b(-k) f_2(x,k), \tag{1.5.161}$$

which follows from the Wronskian relations. Plugging (1.5.158) in here, we find the normalization condition

$$|a(k)|^2 - |b(k)|^2 = 1. \tag{1.5.162}$$

From (1.5.158) and (1.5.161) we also deduce the asymptotic behavior of the Jost functions. For $f_1(x,k)$, we have

$$f_1(x,k) \approx \begin{cases} \mathrm{e}^{\mathrm{i}kx}, & x \to \infty, \\ a(k)\mathrm{e}^{\mathrm{i}kx} - b(-k)\mathrm{e}^{-\mathrm{i}kx}, & x \to -\infty, \end{cases} \tag{1.5.163}$$

while for $f_2(x,k)$ we find,

$$f_2(x,k) \approx \begin{cases} a(k)\mathrm{e}^{-\mathrm{i}kx} + b(k)\mathrm{e}^{\mathrm{i}kx}, & x \to \infty, \\ \mathrm{e}^{-\mathrm{i}kx}, & x \to -\infty. \end{cases} \tag{1.5.164}$$

We can also extend the coefficients $a(k)$, $b(k)$ to the complex k-plane. In order to do that, we consider Jost functions for complex values of k. In this more general setting, they satisfy

$$\overline{f_1(x,k)} = f_1(x,-\bar{k}), \qquad \overline{f_2(x,k)} = f_2(x,-\bar{k}). \tag{1.5.165}$$

Although $a(k)$ cannot vanish along the real line, due to the normalization condition (1.5.162), it can vanish if $\mathrm{Im}(k) \neq 0$. Let k_0 be a zero of $a(k)$ with a positive imaginary part:

$$a(k_0) = 0, \qquad \mathrm{Im}(k_0) > 0. \tag{1.5.166}$$

In this case, the Wronskian in (1.5.159) vanishes, therefore $f_1(x, k_0)$, $f_2(x, k_0)$ are linearly dependent:

$$f_1(x, k_0) = c_0 f_2(x, k_0). \tag{1.5.167}$$

On the other hand, if $\mathrm{Im}(k_0) > 0$, $f_1(x, k)$ decays exponentially as $x \to \infty$, and $f_2(x, k)$ decays exponentially as $x \to -\infty$. Since they are proportional to each other, $f_1(x, k)$ is a solution to the Schrödinger equation that decays exponentially as $|x| \to \infty$, and in particular it is square integrable. We conclude that, if k_0 is a zero of $a(k)$ with $\mathrm{Im}(k_0) > 0$, we have a bound state with energy $E = k_0^2$. However, since energies are real, we must have

$$k_0 = \mathrm{i}\kappa_0, \qquad \kappa_0 > 0. \tag{1.5.168}$$

It follows from (1.5.165) that the Jost functions are real.

The integral kernel of the resolvent can be written in terms of Jost functions, through the formula:

$$G(x, y; k) = \frac{1}{2\mathrm{i}ka(k)} \left(f_1(x, k) f_2(y, k) \theta(x - y) + f_1(y, k) f_2(x, k) \theta(y - x) \right). \tag{1.5.169}$$

In this equation, $\theta(x)$ is the Heaviside function. To prove this, we first note that

$$\begin{aligned} \partial_x^2 G(x, y; k) = {} & \frac{1}{2\mathrm{i}ka(k)} \left(f_1''(x, k) f_2(y, k) \theta(x - y) + f_1(y, k) f_2''(x, k) \theta(y - x) \right) \\ & + \frac{1}{2\mathrm{i}ka(k)} \left(f_1'(x, k) f_2(y, k) - f_1(y, k) f_2'(x, k) \right) \delta(x - y), \end{aligned} \tag{1.5.170}$$

where we have used that

$$f(x)\delta'(x) = -f'(0)\delta(x) + f(0)\delta'(x). \tag{1.5.171}$$

The last term in (1.5.170) can be written as

$$-\frac{1}{2\mathrm{i}ka(k)} W(f_1(x, k), f_2(x, k)) \delta(x - y) = \delta(x - y), \tag{1.5.172}$$

where we have used the first equation in (1.5.159). Since $f_1(x, k)$, $f_2(x, k)$ solve the Schrödinger equation with energy k^2, we conclude that

$$\left(k^2 + \frac{\partial^2}{\partial x^2} - V(x) \right) G(x, y; k) = \delta(x - y). \tag{1.5.173}$$

It is instructive to verify in the explicit expression (1.5.169) the general analytic properties of the resolvent discussed in Section 1.4. First of all, the discrete spectrum should lead to poles in the resolvent, and the residue at this pole should be given by

$$\mathrm{Res}_{\lambda = k_0^2} G(x, y; k) = \psi_{k_0}^*(x) \psi_{k_0}(y), \tag{1.5.174}$$

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where $\psi_{k_0}(x)$ is the normalized wavefunction with energy $E = k_0^2$. As required, the expression (1.5.169) has poles at the zeros of $a(k)$, which as we have just seen, correspond to bound states. We also have (we assume for simplicity that $x \geq y$)

$$\text{Res}_{\lambda=k_0^2} G(x, y; k) = \lim_{k \to k_0} (k^2 - k_0^2) G(x, y; k) = \frac{1}{\mathrm{i}a'(k_0)} f_1(x, k_0) f_2(y, k_0), \tag{1.5.175}$$

where we used (1.5.167) and we expanded $a(k)$ near $k = k_0$:

$$a(k) = a'(k_0)(k - k_0) + \cdots . \tag{1.5.176}$$

This assumes that k_0 is a simple zero of $a(k)$, as we will justify shortly. The normalized wavefunction $\psi_{k_0}(x)$ can be written as

$$\psi_{k_0}(x) = \frac{f_2(x, k_0)}{\| f_2(\cdot, k_0) \|}, \tag{1.5.177}$$

where $\| \cdot \|$ is the standard L^2 norm. Consistency between (1.5.174) and (1.5.175) requires that

$$a'(k_0) = -\mathrm{i} c_0 \| f_2(\cdot, k_0) \|^2, \tag{1.5.178}$$

where c_0 is the constant in (1.5.167). We will now show that the property (1.5.178) follows from a detailed analysis of the Jost solutions. Let y be a solution to the Schrödinger equation,

$$-y'' + V(x) y = k^2 y. \tag{1.5.179}$$

Taking a derivative w.r.t. k, which we denote by $\dot{}$, we find

$$-\dot{y}'' + V(x) \dot{y} = 2ky + k^2 \dot{y}. \tag{1.5.180}$$

Jost functions satisfy these two equations, so we can write

$$\begin{aligned} (-f_1'' + V(x) f_1 - k^2 f_1) \dot{f}_2 &= 0, \\ (-\dot{f}_2'' + V(x) \dot{f}_2 - 2k f_2 - k^2 \dot{f}_2) f_1 &= 0. \end{aligned} \tag{1.5.181}$$

Subtracting both equations, we find

$$f_1 \dot{f}_2'' - f_1'' \dot{f}_2 = -2k f_1 f_2, \tag{1.5.182}$$

or,

$$\frac{\mathrm{d}}{\mathrm{d}x} W(f_1, \dot{f}_2) = -2k f_1 f_2. \tag{1.5.183}$$

Exchanging the indices, we find

$$\frac{\mathrm{d}}{\mathrm{d}x} W(\dot{f}_1, f_2) = 2k f_1 f_2. \tag{1.5.184}$$

These relations can be integrated to obtain,

$$\begin{aligned} W(f_1, \dot{f}_2)\Big|_{-A}^{x} &= -2k \int_{-A}^{x} f_1(y, k) f_2(y, k) \mathrm{d}y, \\ W(\dot{f}_1, f_2)\Big|_{x}^{A} &= 2k \int_{x}^{A} f_1(y, k) f_2(y, k) \mathrm{d}y, \end{aligned} \tag{1.5.185}$$

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and after subtracting the second equation from the first, we obtain

$$W(\dot{f}_1, f_2)(x) + W(f_1, \dot{f}_2)(x) = -2k \int_{-A}^{A} f_1(y,k) f_2(y,k) \mathrm{d}k \\ + W(\dot{f}_1, f_2)(A) + W(f_1, \dot{f}_2)(-A). \tag{1.5.186}$$

The l.h.s. of this equation can be evaluated by taking a derivative w.r.t. k in the first equality of (1.5.159):

$$W(\dot{f}_1, f_2)(x) + W(f_1, \dot{f}_2)(x) = -2\mathrm{i}a(k) - 2\mathrm{i}ka'(k). \tag{1.5.187}$$

The r.h.s. of (1.5.186) must be independent of A, therefore we can evaluate it in the limit $A \to \infty$. To compute $W(\dot{f}_1, f_2)(A)$ in this limit, we note that, when $x \to \infty$,

$$\dot{f}_1(x,k) \approx \mathrm{i}x\, \mathrm{e}^{\mathrm{i}kx}, \tag{1.5.188}$$

while from (1.5.158) we have

$$f_2(x,k) \approx a(k)\mathrm{e}^{-\mathrm{i}kx} + b(k)\mathrm{e}^{\mathrm{i}kx}. \tag{1.5.189}$$

Finally we obtain

$$W(\dot{f}_1, f_2)(x) = \dot{f}_1 f_2' - \dot{f}_1' f_2 \approx 2kxa(k) - \mathrm{i}a(k) - \mathrm{i}b(k)\mathrm{e}^{2\mathrm{i}kx}, \qquad x \to \infty. \tag{1.5.190}$$

A similar calculation gives

$$W(f_1, \dot{f}_2)(x) = f_1 \dot{f}_2' - f_1' \dot{f}_2 \approx -2kxa(k) - \mathrm{i}a(k) + \mathrm{i}b(-k)\mathrm{e}^{-2\mathrm{i}kx}, \qquad x \to -\infty, \tag{1.5.191}$$

which can be used to evaluate $W(f_1, \dot{f}_2)(-A)$ for $A \to \infty$. If we now set $k = k_0$, $a(k_0) = 0$, and $k = \mathrm{i}\kappa_0$ with $\kappa_0 > 0$, so the exponentials appearing in (1.5.190), (1.5.191) vanish asymptotically. Therefore, the r.h.s. of (1.5.186), for $k = k_0$ and in the limit $A \to \infty$, simply gives

$$-2k_0 \int_{\mathbb{R}} f_1(y,k_0) f_2(y,k_0) \mathrm{d}y. \tag{1.5.192}$$

On the other hand, by evaluating (1.5.187) at $k = k_0$, we obtain

$$W(\dot{f}_1(x,k_0), f_2(x,k_0)) + W(f_1(x,k_0), \dot{f}_2(x,k_0)) = -2\mathrm{i}k_0 a'(k_0). \tag{1.5.193}$$

We conclude that

$$a'(k_0) = -\mathrm{i} \int_{\mathbb{R}} f_1(x,k_0) f_2(x,k_0) \mathrm{d}x, \tag{1.5.194}$$

which can be written as (1.5.178). As a consequence of this formula we verify that the zeros of $a(k)$ are simple, since the r.h.s. of (1.5.178) is nonzero.

We can also compute the discontinuity of the resolvent explicitly in the continuous part of the spectrum and verify the general result (1.4.132). The branch cut corresponds to the two determinations of $\sqrt{k^2} = \pm k$, as in the free particle case studied in Example 1.3.1. We find,

$$G(x,y;E+\mathrm{i}\epsilon) - G(x,y;E-\mathrm{i}\epsilon) = \frac{f_1(x,k)f_2(y,k)}{2\mathrm{i}ka(k)} + \frac{f_1(x,-k)f_2(y,-k)}{2\mathrm{i}ka(-k)}, \tag{1.5.195}$$

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where $k > 0$ and we have assumed for simplicity that $x \geq y$. We now use

$$f_1(x,-k) = \frac{1}{a(k)} f_2(x,k) - \frac{b(k)}{a(k)} f_1(x,k), \tag{1.5.196}$$

which follows from (1.5.158), as well as

$$f_2(y,k) = \frac{1}{a(-k)} f_1(y,-k) + \frac{b(k)}{a(-k)} f_2(y,-k), \tag{1.5.197}$$

which follows from (1.5.161). By applying this, the r.h.s. of (1.5.195) reads,

$$\begin{aligned} &\frac{f_1(x,k)}{2\mathrm{i}ka(k)} \left(\frac{1}{a(-k)} f_1(y,-k) + \frac{b(k)}{a(-k)} f_2(y,-k) \right) \\ &\quad + \frac{f_2(y,-k)}{2\mathrm{i}ka(-k)} \left(\frac{1}{a(k)} f_2(x,k) - \frac{b(k)}{a(k)} f_1(x,k) \right) \\ &= \frac{1}{2\mathrm{i}k|a(k)|^2} \left(f_1(x,k)\overline{f_1(y,k)} + f_2(x,k)\overline{f_2(y,k)} \right). \end{aligned} \tag{1.5.198}$$

We now introduce the functions

$$\psi_i(x,k) = \frac{1}{a(k)} f_i(x,k), \qquad i = 1,2, \qquad k > 0, \tag{1.5.199}$$

which correspond in this example to the wavefunctions appearing in (1.4.131). The labels $i = 1,2$ correspond to the two choices $\pm k$ associated to $E = k^2$. We can write (1.5.195) as

$$G(x,y;E+\mathrm{i}\epsilon) - G(x,y;E-\mathrm{i}\epsilon) = \frac{1}{2\mathrm{i}k} \sum_{i=1}^{2} \psi_i(x,k)\overline{\psi_i(y,k)}. \tag{1.5.200}$$

The functions $\psi_i(x,k)$ satisfy the orthogonality property

$$\int_{\mathbb{R}} \psi_i(x,k)\overline{\psi_j(x,p)}\mathrm{d}x = N(k)\delta_{ij}\delta(k-p), \qquad i = 1,2, \tag{1.5.201}$$

with

$$N(k) = 2\pi. \tag{1.5.202}$$

The property (1.5.201) can be proved by using that,

$$\frac{\mathrm{d}}{\mathrm{d}x} W\left(\psi_i(x,k), \overline{\psi_j(x,p)}\right) = (k^2 - p^2)\psi_i(x,k)\overline{\psi_j(x,p)}, \tag{1.5.203}$$

which follows from the fact that $\psi_i(x,k)$, $\overline{\psi_j(x,p)}$ satisfy the Schrödinger equation with energies k^2, p^2, respectively. Let us check (1.5.201) for $i = j = 1$. We find,

$$\begin{aligned} &\int_{-A}^{A} \psi_i(x,k)\overline{\psi_j(x,p)}\mathrm{d}x \\ &= \frac{1}{(k^2-p^2)a(k)\overline{a(p)}} \left\{ W\left(f_1(A,k), \overline{f_1(A,p)}\right) - W\left(f_1(-A,k), \overline{f_1(-A,p)}\right) \right\}. \end{aligned} \tag{1.5.204}$$

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To evaluate the Wronskian at $\pm A$, with A very large, we can use the asymptotic form of the Jost function in (1.5.163). One finds, after using (1.5.160),

$$\begin{aligned}&\frac{1}{(k^2-p^2)}\left\{W\left(f_1(A,k),\overline{f_1(A,p)}\right)-W\left(f_1(-A,k),\overline{f_1(-A,p)}\right)\right\}\\&\quad=\frac{\mathrm{i}}{k-p}\left\{-\mathrm{e}^{\mathrm{i}(k-p)A}+a(k)\overline{a(p)}\mathrm{e}^{-\mathrm{i}(k-p)A}-b(p)\overline{b(k)}\mathrm{e}^{\mathrm{i}(k-p)A}\right\}\\&\qquad+\frac{\mathrm{i}}{k+p}\left\{-a(k)b(p)\mathrm{e}^{-\mathrm{i}(k+p)A}+\overline{a(p)b(k)}\mathrm{e}^{\mathrm{i}(k+p)A}\right\}.\end{aligned} \tag{1.5.205}$$

As $A\to\infty$, this becomes a distribution. To determine it, we use the Riemann–Lebesgue theorem, which says that

$$\lim_{k\to\infty}\int_{\mathbb{R}} f(x)\mathrm{e}^{\mathrm{i}kx}\mathrm{d}x=0 \tag{1.5.206}$$

for any square-integrable function $f(x)$. Since $k,p>0$, the last line of (1.5.205) leads to a zero distribution as $A\to\infty$, while the second line leads to a distribution supported on the locus where $k=p$. We can therefore replace $a(p)$, $b(p)$ by $a(k)$, $b(k)$ and use (1.5.162) to conclude that

$$\begin{aligned}&\lim_{A\to\infty}\frac{1}{(k^2-p^2)a(k)\overline{a(p)}}\left\{W\left(f_1(A,k),\overline{f_1(A,p)}\right)-W\left(f_1(-A,k),\overline{f_1(-A,p)}\right)\right\}\\&=\lim_{A\to\infty}2\frac{\sin\left((k-p)A\right)}{k-p}=2\pi\delta(k-p).\end{aligned} \tag{1.5.207}$$

We conclude that (1.4.132) is satisfied, since in this case

$$-2\pi\mathrm{i}\langle x|\mathsf{P}_E|y\rangle=-\frac{\mathrm{i}}{2k}\sum_{i=1}^{2}\psi_i(x,k)\overline{\psi_i(y,k)}. \tag{1.5.208}$$

The functions $\psi_i(x,k)$ play an important role in scattering theory in one dimension, and they are sometimes called *scattering solutions*. Note that they are Jost functions but with a different normalization. It follows from (1.5.163) and (1.5.164) that these solutions have the following asymptotic behavior:

$$\psi_1(x,k)\approx\begin{cases}s_{11}\mathrm{e}^{\mathrm{i}kx}, & x\to\infty,\\ \mathrm{e}^{\mathrm{i}kx}+s_{21}\mathrm{e}^{-\mathrm{i}kx}, & x\to-\infty,\end{cases} \tag{1.5.209}$$

where

$$s_{11}=\frac{1}{a(k)},\qquad s_{21}=-\frac{b(-k)}{a(k)}, \tag{1.5.210}$$

while

$$\psi_2(x,k)\approx\begin{cases}\mathrm{e}^{-\mathrm{i}kx}+s_{12}\mathrm{e}^{\mathrm{i}kx}, & x\to\infty,\\ s_{22}\mathrm{e}^{-\mathrm{i}kx}, & x\to-\infty,\end{cases} \tag{1.5.211}$$

where

$$s_{12}=\frac{b(k)}{a(k)},\qquad s_{22}=\frac{1}{a(k)}. \tag{1.5.212}$$

The coefficients s_{ij}, $i, j = 1, 2$ have a very clear scattering interpretation. The solution $\psi_1(x, k)$ describes a particle coming from $-\infty$ (where it is free), moving to the right, and interacting with the potential. s_{11} and s_{21} are the amplitudes s of the transmitted and reflected waves, respectively. Similarly, $\psi_2(x, k)$ describes a particle coming from ∞ (where is free), moving to the left, and interacting with the potential. s_{12} and s_{22} are the amplitudes of the reflected and transmitted waves, respectively. The transmission and reflection coefficients are given by

$$T(k) = |s_{11}|^2 = |s_{22}|^2, \qquad R(k) = |s_{21}|^2 = |s_{12}|^2, \tag{1.5.213}$$

where we used the second relation in (1.5.160). Note that the relation (1.5.162) implies that

$$T(k) + R(k) = 1, \tag{1.5.214}$$

which expresses the conservation of probability for the Schrödinger equation. The coefficients s_{ij}, $i, j = 1, 2$ can be put inside a two by two matrix, called the *S-matrix*,

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}. \tag{1.5.215}$$

This matrix satisfies

$$SS^\dagger = \frac{1}{|a(k)|^2} \begin{pmatrix} 1 & b(k) \\ -\overline{b(k)} & 1 \end{pmatrix} \begin{pmatrix} 1 & -b(k) \\ \overline{b(k)} & 1 \end{pmatrix} = \mathbf{1}, \tag{1.5.216}$$

where we used (1.5.160) and (1.5.162), i.e. it is *unitary*. The unitarity property of the S-matrix expresses the conservation of probability (1.5.214). Note that zeros of $a(k)$ become poles of S.

Example 1.5.1 *The single delta potential.* Perhaps the simplest solvable scattering problem in one dimension is the delta function potential,

$$V(x) = g\delta(x). \tag{1.5.217}$$

The wavefunctions are continuous but their derivatives jump at the origin. The discontinuity in the derivative can be easily obtained by integrating the Schrödinger equation. Take $0 < \epsilon \ll 1$. Then,

$$\psi'(\epsilon) - \psi'(-\epsilon) = \int_{-\epsilon}^{\epsilon} \psi''(x)\mathrm{d}x = \int_{-\epsilon}^{\epsilon} \left(-k^2 + g\delta(x)\right) \psi(x)\mathrm{d}x = g\psi(0) + \mathcal{O}(\epsilon). \tag{1.5.218}$$

We will distinguish two regions in this problem, region I with $x < 0$, and region II with $x > 0$. Let us obtain the Jost function $f_1(x, k)$. The asymptotic formula (1.5.163) now describes the Jost function exactly, and we have

$$f_1(x, k) = \begin{cases} \mathrm{e}^{\mathrm{i}kx}, & x > 0, \\ a(k)\mathrm{e}^{\mathrm{i}kx} - b(-k)\mathrm{e}^{-\mathrm{i}kx}, & x < 0. \end{cases} \tag{1.5.219}$$

Imposing continuity of $f_1(x, k)$ one finds,

$$a(k) - b(-k) = 1, \tag{1.5.220}$$

while the discontinuity of the first derivative, (1.5.218), gives

$$a(k) + b(-k) = 1 - \frac{g}{ik}. \tag{1.5.221}$$

These two equations determine the transition coefficients,

$$a(k) = 1 - \frac{g}{2ik}, \qquad b(k) = \frac{g}{2ik}. \tag{1.5.222}$$

As a check, note that they verify the conjugation conditions (1.5.160) and the normalization condition (1.5.162). Similarly, the second Jost function agrees with its asymptotic expression (1.5.164):

$$f_2(x,k) = \begin{cases} a(k)e^{-ikx} + b(k)e^{ikx}, & x > 0, \\ e^{-ikx}, & x < 0. \end{cases} \tag{1.5.223}$$

As an application of this result, let us suppose that $g = -\lambda$, $\lambda > 0$, so the potential supports bound states. The coefficient $a(k)$ vanishes precisely for

$$k_0 = \frac{i\lambda}{2}, \tag{1.5.224}$$

which has $\mathrm{Im}(k_0) > 0$. This corresponds to a bound state with energy

$$E_0 = -\frac{\lambda^2}{4}, \tag{1.5.225}$$

and with a normalizable wavefunction

$$\psi_{k_0}(x) \propto e^{-\lambda|x|/2}. \tag{1.5.226}$$

□

Example 1.5.2 *The double delta potential.* Our second example is the double delta potential,

$$V(x) = B\left(\delta(x-a) + \delta(x+a)\right). \tag{1.5.227}$$

As in the previous example, the wavefunction is continuous, but its first derivative has discontinuities at $x = \pm a$. The Jost function $f_1(x,k)$ has the form,

$$f_1(x,k) = \begin{cases} e^{ikx}, & x \geq a, \\ A_1 e^{ikx} + A_2 e^{-ikx}, & -a \leq x \leq a, \\ a(k)e^{ikx} - b(-k)e^{-ikx}, & x \leq a. \end{cases} \tag{1.5.228}$$

Imposing the continuity of the function and the discontinuity of its first derivative at $x = \pm a$, we obtain the values of A_1, A_2, $a(k)$, and $b(k)$. To write down the result for $a(k)$, it is useful to introduce the following functions:

$$\phi_0(\mu) = \frac{1}{\mu}\left(\mu + i\beta e^{i\mu}\cos\mu\right), \qquad \phi_1(\mu) = \frac{1}{\mu}\left(\mu + \beta e^{i\mu}\sin\mu\right), \tag{1.5.229}$$

where

$$\mu = ka, \qquad \beta = Ba. \tag{1.5.230}$$

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In terms of these functions, one finds

$$a(k) = 2\frac{\phi_0(\mu)\phi_1(\mu)}{\phi_0(\mu)\phi_1(-\mu) + \phi_0(-\mu)\phi_1(\mu)}. \tag{1.5.231}$$

We can use this result to determine, for example, the bound states of this potential. The zeros of $a(k)$ are given by zeros of $\phi_0(\mu)$ or of $\phi_1(\mu)$ with $k = \mathrm{i}\kappa$, $\kappa > 0$. Zeros of $\phi_0(\mu)$ with $\mu = \mathrm{i}\gamma_0$ satisfy the equation

$$1 + \mathrm{e}^{-2\gamma_0} = -\frac{2\gamma_0}{\beta}. \tag{1.5.232}$$

A simple graphical analysis of this equation shows the result is that, when $\beta < 0$, there is one single root with $\gamma_0 > 0$. This is a first bound state in this potential. Let us now look for zeros of $\phi_1(\mu)$ with $\mu = \mathrm{i}\gamma_1$. They satisfy

$$1 - \mathrm{e}^{-2\gamma_1} = -\frac{2\gamma_1}{\beta}. \tag{1.5.233}$$

This again has one solution with $\gamma_1 > 0$ provided $\beta < -1$. We conclude that in the double delta potential there is a bound state for $-1 \leq \beta < 0$, and two bound states when $\beta < -1$. □

Example 1.5.3 *The Pöschl–Teller potential*. The Pöschl–Teller potential is given by

$$V(x) = -\frac{\hbar^2}{2m}\frac{\alpha^2\lambda(\lambda-1)}{\cosh^2(\alpha x)}. \tag{1.5.234}$$

We will consider three different situations:

1. When $\lambda > 1$ we have a potential well.
2. When $1/2 \leq \lambda < 1$, we have a low barrier.
3. When

$$\lambda = \frac{1}{2} + \mathrm{i}\ell, \qquad \ell > 0, \tag{1.5.235}$$

we have a high barrier.

As we will see, the low and high barriers have different physical properties. The Schrödinger equation in the presence of the potential (1.5.234) reads

$$\psi''(x) + \left(k^2 + \frac{\alpha^2\lambda(\lambda-1)}{\cosh^2(\alpha x)}\right)\psi(x) = 0, \tag{1.5.236}$$

where we have set $\hbar = 2m = 1$. Let us perform the change of variables

$$y = \tanh(\alpha x), \tag{1.5.237}$$

and let us write the wavefunction as

$$\psi(x) = (1+y)^{\mathrm{i}\bar{k}/2}(1-y)^{-\mathrm{i}\bar{k}/2}\phi(y), \qquad \bar{k} = \frac{k}{\alpha}. \tag{1.5.238}$$

Then, the Schrödinger equation reads

$$(1-y^2)\phi''(y) + 2(\mathrm{i}\bar{k} - y)\phi'(y) + \lambda(\lambda-1)\phi(y) = 0. \tag{1.5.239}$$

Performing the further change

$$z = \frac{1+y}{2}, \tag{1.5.240}$$

we find a hypergeometric equation

$$z(1-z)\phi''(z) + \left(\mathrm{i}\bar{k} - 2z + 1\right)\phi'(z) + \lambda(\lambda-1)\phi(z) = 0. \tag{1.5.241}$$

By using the general theory of these equations, we obtain two independent solutions. The first one

$$z^{-\mathrm{i}\bar{k}}{}_2F_1\left(\lambda - \mathrm{i}\bar{k}, 1-\lambda-\mathrm{i}\bar{k}; 1-\mathrm{i}\bar{k}; z\right), \tag{1.5.242}$$

is appropriate near $z = 0$, which corresponds to $x \to -\infty$. The second solution

$$z^{-\mathrm{i}\bar{k}}{}_2F_1\left(\lambda - \mathrm{i}\bar{k}, 1-\lambda-\mathrm{i}\bar{k}; 1-\mathrm{i}\bar{k}; 1-z\right), \tag{1.5.243}$$

is appropriate near $z = 1$, which corresponds to $x \to \infty$. Since

$$1 - \tanh^2(\alpha x) \approx 4\mathrm{e}^{-2\alpha|x|}, \qquad |x| \to \infty, \tag{1.5.244}$$

we conclude that the Jost functions of the problem are

$$\begin{aligned} f_1(x,k) &= 2^{\mathrm{i}\bar{k}}(1-\tanh^2(\alpha x))^{-\mathrm{i}\bar{k}/2}{}_2F_1\left(\lambda-\mathrm{i}\bar{k}, 1-\lambda-\mathrm{i}\bar{k}; 1-\mathrm{i}\bar{k}; \frac{1-\tanh(\alpha x)}{2}\right), \\ f_2(x,k) &= 2^{\mathrm{i}\bar{k}}(1-\tanh^2(\alpha x))^{-\mathrm{i}\bar{k}/2}{}_2F_1\left(\lambda-\mathrm{i}\bar{k}, 1-\lambda-\mathrm{i}\bar{k}; 1-\mathrm{i}\bar{k}; \frac{1+\tanh(\alpha x)}{2}\right). \end{aligned} \tag{1.5.245}$$

Let us now calculate the coefficients $a(k)$ and $b(k)$. To do this, we can for example determine the asymptotics of $f_1(x,k)$ as $x \to -\infty$. This can be done by using the transformation properties of the hypergeometric functions, which imply in particular that (see eq. (9.5.7) of Lebedev (1972)):

$$\begin{aligned} &{}_2F_1\left(\lambda-\mathrm{i}\bar{k}, 1-\lambda-\mathrm{i}\bar{k}; 1-\mathrm{i}\bar{k}; 1-z\right) \\ &\quad = \frac{\Gamma(1-\mathrm{i}\bar{k})\Gamma(\mathrm{i}\bar{k})}{\Gamma(1-\lambda)\Gamma(\lambda)}{}_2F_1\left(\lambda-\mathrm{i}\bar{k}, 1-\lambda-\mathrm{i}\bar{k}; 1-\mathrm{i}\bar{k}; z\right) \\ &\qquad + z^{\mathrm{i}\bar{k}}\frac{\Gamma(1-\mathrm{i}\bar{k})\Gamma(-\mathrm{i}\bar{k})}{\Gamma(\lambda-\mathrm{i}\bar{k})\Gamma(1-\lambda-\mathrm{i}\bar{k})}{}_2F_1\left(1-\lambda, \lambda; 1+\mathrm{i}\bar{k}; z\right). \end{aligned} \tag{1.5.246}$$

We then have that, when $x \to -\infty$,

$$f_1(x,k) \approx \frac{\Gamma(1-\mathrm{i}\bar{k})\Gamma(\mathrm{i}\bar{k})}{\Gamma(1-\lambda)\Gamma(\lambda)}\mathrm{e}^{-\mathrm{i}kx} + \frac{\Gamma(1-\mathrm{i}\bar{k})\Gamma(-\mathrm{i}\bar{k})}{\Gamma(\lambda-\mathrm{i}\bar{k})\Gamma(1-\lambda-\mathrm{i}\bar{k})}\mathrm{e}^{\mathrm{i}kx}, \tag{1.5.247}$$

and we conclude that

$$a(k) = \frac{\Gamma(1-\mathrm{i}\bar{k})\Gamma(-\mathrm{i}\bar{k})}{\Gamma(\lambda-\mathrm{i}\bar{k})\Gamma(1-\lambda-\mathrm{i}\bar{k})}, \qquad b(k) = -\frac{\Gamma(1+\mathrm{i}\bar{k})\Gamma(-\mathrm{i}\bar{k})}{\Gamma(1-\lambda)\Gamma(\lambda)}. \tag{1.5.248}$$

From here one calculates the transmission coefficient $T(k)$ as

$$T(k) = \frac{\sinh^2(\pi k/\alpha)}{\sinh^2(\pi k/\alpha) + \sin^2(\pi\lambda)}. \tag{1.5.249}$$

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The bound states for the potential well can also be found from the above explicit formula for $a(k)$. The zeros occur at the poles of the denominator. There are two types of poles, given by

$$\begin{aligned} k_1(n) &= -\mathrm{i}\alpha(n+\lambda), \qquad n \in \mathbb{Z}_{\geq 0}, \\ k_2(n) &= \mathrm{i}\alpha(\lambda - 1 - n), \qquad n \in \mathbb{Z}_{\geq 0}. \end{aligned} \tag{1.5.250}$$

Bound states require $\mathrm{Im}(k) > 0$. It is easy to see that this only happens when we have a well (i.e. $\lambda > 1$) and is due to the poles at $k = k_2(n)$. In addition, there is a maximal possible value of n:

$$n_{\max} = \begin{cases} [\lambda - 1], & \text{if } \lambda \notin \mathbb{Z}, \\ \lambda - 2, & \text{if } \lambda \in \mathbb{Z}, \end{cases} \tag{1.5.251}$$

where $[\cdot]$ denotes the integer part. Therefore, there are only a finite number of bound states. For example, if $\lambda = 2$, we have exactly one bound state with $n = 0$. Note that in both the well and the low barrier case we have poles in which k is purely imaginary and $\mathrm{Im}(k) < 0$. The corresponding states are called *antibound states*. They are eigenfunctions of the Schrödinger equation with a real eigenvalue, but they do not belong to $L^2(\mathbb{R})$ (on the contrary, they increase exponentially at infinity). Finally, in the case of a high barrier, the poles lead to eigenfunctions with complex eigenvalues. These states are called *resonances* and we will discuss them in detail in Chapter 5. □

Another interesting result that follows from the analysis of Jost functions is an explicit expression for the trace of the resolvent in terms of the function $a(k)$, when $E \in \mathbb{C}\backslash[0,\infty]$ in the physical sheet (i.e. $\mathrm{Im}(k) > 0$). The trace of the resolvent is itself divergent, but it can be regularized by subtracting the result for the free particle, i.e. the case in which the potential vanishes. Quantities for the free particle will be denoted by a 0 subindex. Since for the free particle one has

$$f_1(x,k) = \mathrm{e}^{\mathrm{i}kx}, \qquad f_2(x,k) = \mathrm{e}^{-\mathrm{i}kx} = f_1(x,-k), \tag{1.5.252}$$

we have that

$$a_0(k) = 1, \qquad b_0(k) = 0, \tag{1.5.253}$$

and

$$\mathrm{Tr}\left(\mathsf{G}(k) - \mathsf{G}_0(k)\right) = \frac{1}{2\mathrm{i}ka(k)} \int_{\mathbb{R}} \left(f_1(x,k) f_2(x,k) - a(k)\right) \mathrm{d}x. \tag{1.5.254}$$

The integral can be evaluated using the results (1.5.186), (1.5.187), (1.5.190), and (1.5.191). We obtain, for A large,

$$\int_{-A}^{A} f_1(x,k) f_2(x,k) \mathrm{d}x \approx 2Aa(k) + \mathrm{i}\dot{a}(k). \tag{1.5.255}$$

In this calculation, we have used the fact that, for $\mathrm{Im}(k) > 0$, the exponentials appearing in (1.5.190), (1.5.191) vanish as $A \to \infty$. We then obtain,

$$\mathrm{Tr}\left(\mathsf{G}(k) - \mathsf{G}_0(k)\right) = \frac{1}{2k} \frac{\mathrm{d}}{\mathrm{d}k} \log a(k). \tag{1.5.256}$$

1.6 Bibliographical Notes

In this book we assume some previous knowledge of quantum mechanics. There are many excellent textbooks that provide the appropriate background. My favourite, recent introduction is the book by Konishi and Paffuti (2009), which contains a fantastic collection of solved exercises and touches on many different (and modern) topics. In my view, the best references for an advanced treatment of the subject are the two-volume set by Galindo and Pascual (1990), and the book by Takhtajan (2008). They provide careful treatments of all the subjects they cover, and they are rigorous without being pedantic.

The quantum-mechanical propagator is introduced in most advanced textbooks of quantum mechanics, such as, for example, Galindo and Pascual (1990). The examples discussed in Section 1.2 of this chapter are based on Galitski et al. (2013). A useful introduction to resolvent operators is presented in Cohen-Tannoudji et al. (2012) and Konishi and Paffuti (2009). Example 1.4.2 is based on Faddeev and Takhtajan (2014). The presentation of scattering theory in one dimension closely follows Galindo and Pascual (1990) and, in particular, Takhtajan (2008). The double delta potential is analyzed in detail in Galindo and Pascual (1990), and useful references for the Pöschl–Teller potential are Galindo and Pascual (1990) and Çevik et al. (2016).