Formal and Precise Derivation of the Green Functions for a Simple Potential

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Abstract

In formal scattering theory, Green functions are obtained as solutions of a distributional equation. In this paper, we use the Sturm-Liouville theory to compute Green functions within a rigorous mathematical theory. We shall show that both the Sturm-Liouville theory and the formal treatment yield the same Green functions. We shall also show how the analyticity of the Green functions as functions of the energy keeps track of the so-called "incoming" and "outgoing" boundary conditions.

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1 Introduction

Green functions are essential tools in mathematical physics [1, 2]. Most books on scattering theory [3, 4] only provide a computational procedure to obtain Green functions without any reference to a mathematical setting. Here we provide that mathematical framework for the example of a square barrier potential. In this example, the mathematical framework is given by the Sturm-Liouville theory [5].

We consider a square barrier potential of height V_0,

$$V(r) = \begin{cases} 0 & 0 < r < a \\ V_0 & a < r < b \\ 0 & b < r < \infty \, . \end{cases} \tag{1.1}$$

Due to the spherical symmetry of the potential, spherical coordinates come in handy. The expression for the Hamiltonian in spherical coordinates (for s-waves) is

$$h \equiv -\frac{d^2}{dr^2} + V(r) \, . \tag{1.2}$$

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In order to obtain a linear operator from the formal differential operator (1.2), we need to define a domain in the Hilbert space $L^2([0,\infty), dr)$ on which h acts. The domain we choose is

$$\mathcal{D}(H) = \{ f(r) \mid (hf)(r), f(r) \in L^2([0,\infty), dr),\ f(0) = 0,\ f(r) \in AC^2[0,\infty) \} \,. \tag{1.3}$$

On this domain, the formal differential operator (1.2) induces a self-adjoint operator H (cf. [5]). The spectrum of this operator is the positive real line $[0,\infty)$ (cf. [5]).

Both formal and Sturm-Liouville approaches use the solutions of the time-independent Schrödinger equation,

$$\left(-\frac{d^2}{dr^2} + V(r) \right) \sigma(r,E) = E\sigma(r,E) \,, \tag{1.4}$$

as their basic source of information. The difference is that physicists, fearful of using complex energies when working with self-adjoint Hamiltonians, solve (1.4) using real energies. The Sturm-Liouville approach uses complex energies. This is in no contradiction with the self-adjointness of the Hamiltonian, since the eigenfunctions that correspond to complex energies lie outside the domain (1.3) on which the Hamiltonian is self-adjoint.

In the next section, we show that the formal and the Sturm-Liouville approaches yield the same Green functions. In our calculations, we will use the following branch of the square root function:

$$\sqrt{\cdot} : \{ E \in \mathbb{C} \mid \ -\pi < \arg(E) \leq \pi \} \longmapsto \{ E \in \mathbb{C} \mid \ -\pi/2 < \arg(E) \leq \pi/2 \} \,. \tag{1.5}$$

2 Computation of the Green Functions

2.1 Formal Approach

To compute the (radial) Green functions, physicists solve the following distributional equation:

$$\left(-\frac{d^2}{dr^2} + V(r) - E \right) G(r,s;E) = -\delta(r-s) \,, \quad E \in [0,\infty) \,, \tag{2.1}$$

subject to certain boundary conditions. Equation (2.1) says that for $r \neq s$, $G(r,s;E)$ obeys the radial Schrödinger equation (1.4) and the following boundary conditions:

$$G(a-,s;E) = G(a+,s;E) \tag{2.2}$$

$$G(b-,s;E) = G(b+,s;E) \tag{2.3}$$

$$\frac{\partial}{\partial r} G(a-,s;E) = \frac{\partial}{\partial r} G(a+,s;E) \tag{2.4}$$

$$\frac{\partial}{\partial r} G(b-,s;E) = \frac{\partial}{\partial r} G(b+,s;E) \,. \tag{2.5}$$

At $r = s$ it is continuous, but its derivative has a discontinuity of 1,

$$\frac{\partial}{\partial r} G(s+0,s;E) - \frac{\partial}{\partial r} G(s-0,s;E) = 1 \,, \tag{2.6}$$

due to the delta function. At the origin, the Green function must be regular,

$$G(0,s;E)=0\,. \tag{2.7}$$

There are two linearly independent Green functions that we are mostly interested in: the *incoming* and the *outgoing* Green functions. The outgoing Green function G^+ satisfies Eq. (2.1), the boundary conditions (2.2)-(2.7), and an "outgoing boundary condition" at infinity,

$$G^+(r,s;E)\sim e^{i\sqrt{E}r}\,, \quad \text{for } r\to\infty\,. \tag{2.8}$$

The boundary condition (2.8) means that very far from the potential region the function G^+ behaves as an outgoing wave. The expression for this outgoing Green function is [3]

$$G^+(r,s;E)=\frac{\chi(r_<;E)\Omega_+(r_>;E)}{W(\chi,\Omega_+)}\,, \tag{2.9}$$

where $r_<$ and $r_>$ refer to the smaller and to the bigger of r and s, respectively, $\chi(r;E)$ is the solution of the Schrödinger equation that vanishes at the origin, $\Omega_+(r;E)$ is the solution of the Schrödinger equation that satisfies an "outgoing boundary condition" at infinity, and $W(\chi,\Omega_+)$ is the the Wronskian of χ and Ω_+. More precisely, $\chi(r;E)$ satisfies Eq. (1.4) and the boundary conditions

$$\begin{aligned}
\chi(0;E) &= 0 && (2.10)\\
\chi(a+;E) &= \chi(a-;E) && (2.11)\\
\chi'(a+;E) &= \chi'(a-;E) && (2.12)\\
\chi(b+;E) &= \chi(b-;E) && (2.13)\\
\chi'(b+;E) &= \chi'(b-;\ E)\,. && (2.14)
\end{aligned}$$

Its expression is given by

$$\chi(r;E)=\begin{cases}\sin(\sqrt{E}r) & 0<r<a\\ \mathcal{J}_1(E)e^{i\sqrt{(E-V_0)}r}+\mathcal{J}_2(E)e^{-i\sqrt{(E-V_0)}r} & a<r<b\\ \mathcal{J}_3(E)e^{i\sqrt{E}r}+\mathcal{J}_4(E)e^{-i\sqrt{E}r} & b<r<\infty\,.\end{cases} \tag{2.15}$$

The functions $\mathcal{J}_1$-$\mathcal{J}_4$ are such that $\chi(r;E)$ satisfies the boundary conditions (2.10)-(2.14) and are given in the Appendix. The function $\Omega_+(r;E)$ satisfies Eq. (1.4) and the boundary conditions

$$\begin{aligned}
\Omega_+(a+;E) &= \Omega_+(a-;E) && (2.16)\\
\Omega_+'(a+;E) &= \Omega_+'(a-;E) && (2.17)\\
\Omega_+(b+:E) &= \Omega_+(b-;E) && (2.18)\\
\Omega_+'(b+;E) &= \Omega_+'(b-:\ E) && (2.19)\\
\Omega_+(r;E) &\sim e^{i\sqrt{E}r}\,,\ r\to\infty\,. && (2.20)
\end{aligned}$$

The solution $\Omega_+(r;E)$ reads (see the Appendix for the explicit expressions of $\mathcal{A}_1^+$-$\mathcal{A}_4^+$)

$$\Omega_+(r;E) = \left\{ \begin{array}{ll} \mathcal{A}_1^+(E)e^{i\sqrt{E}r} + \mathcal{A}_2^+(E)e^{-i\sqrt{E}r} & 0<r<a \\ \mathcal{A}_3^+(E)e^{i\sqrt{(E-V_0)}r} + \mathcal{A}_4^+(E)e^{-i\sqrt{(E-V_0)}r} & a<r<b \\ e^{i\sqrt{E}r} & b<r<\infty \, . \end{array} \right. \tag{2.21}$$

The Wronskian of $\chi(r;E)$ and $\Omega_+(r;E)$ is

$$W(\chi,\Omega_+) = 2i\sqrt{E}\mathcal{J}_4(E) \, . \tag{2.22}$$

The outgoing Green function is therefore given by

$$G^+(r,s;E) = \frac{\chi(r_<;E)\Omega_+(r_>;E)}{2i\sqrt{E}\mathcal{J}_4(E)} \, . \tag{2.23}$$

The incoming Green function G^- satisfies Eq. (2.1), the boundary conditions (2.2)-(2.7), and an “incoming boundary condition” at infinity,

$$G^-(r,s;E) \sim e^{-i\sqrt{E}r} \, , \quad \text{for } r\to\infty \, . \tag{2.24}$$

Condition (2.24) says that far away from the potential region G^- behaves as an incoming wave. The expression for this incoming Green function is

$$G^-(r,s;E) = \frac{\chi(r_<;E)\Omega_-(r_>;E)}{W(\chi,\Omega_-)} \, , \tag{2.25}$$

where $\chi(r;E)$ is the solution of the Schrödinger equation that vanishes at the origin, $\Omega_-(r;E)$ is the solution of the Schrödinger equation that satisfies an “incoming boundary condition” at infinity, and $W(\chi,\Omega_-)$ is the the Wronskian of χ and Ω_-. The eigenfunction $\chi(r;E)$ is given by (2.15). The eigenfunction $\Omega_-(r;E)$ satisfies the Schrödinger equation subject to the following boundary conditions:

$$\begin{aligned} \Omega_-(a+;E) &= \Omega_-(a-;E) && (2.26) \\ \Omega'_-(a+;E) &= \Omega'_-(a-;E) && (2.27) \\ \Omega_-(b+:E) &= \Omega_-(b-;E) && (2.28) \\ \Omega'_-(b+;E) &= \Omega'_-(b-:\ E) && (2.29) \\ \Omega_-(r;E) &\sim e^{-i\sqrt{E}r} \, , \ r\to\infty \, , && (2.30) \end{aligned}$$

and its expression is given by

$$\Omega_-(r;E) = \left\{ \begin{array}{ll} \mathcal{A}_1^-(E)e^{i\sqrt{E}r} + \mathcal{A}_2^-(E)e^{-i\sqrt{E}r} & 0<r<a \\ \mathcal{A}_3^-(E)e^{i\sqrt{(E-V_0)}r} + \mathcal{A}_4^-(E)e^{-i\sqrt{(E-V_0)}r} & a<r<b \\ e^{-i\sqrt{E}r} & b<r<\infty \, . \end{array} \right. \tag{2.31}$$

The functions $\mathcal{A}_1^-$-$\mathcal{A}_4^-$ make $\Omega_-(r;E)$ satisfy the boundary conditions (2.26)-(2.30). The Wronskian of $\chi(r;E)$ and $\Omega_-(r;E)$ is

$$W(\chi, \Omega_-) = -2i\sqrt{E}\mathcal{J}_3(E)\,. \tag{2.32}$$

Therefore, the expression of the incoming Green function is

$$G^-(r,s;E) = -\frac{\chi(r_<;E)\Omega_-(r_>;E)}{2i\sqrt{E}\mathcal{J}_3(E)}\,. \tag{2.33}$$

2.2 Sturm-Liouville Approach

In this section, we compute the Green functions using the Sturm-Liouville theory. The Green function appears as a kernel of integration when we write the resolvent of the Hamiltonian H as an integral operator,

$$(E-H)^{-1} f(r) = \int_0^\infty G(r,s;E) f(s)\, ds\,, \quad E \notin [0,\infty)\,. \tag{2.34}$$

From Eq. (2.34) one can formally derive Eq. (2.1).

As mentioned in the Introduction, physicists avoid computing Green functions using complex energies, but rather impose the incoming and outgoing boundary conditions. The Sturm-Liouville theory deals directly with complex energies in a way that keep track of the "in" and "out" boundary conditions.

The procedure to compute the Green function for our Hamiltonian H is given by the following theorem (see Theorem XIII.3.16 in [5]):

Theorem 1 Let H be the self-adjoint operator derived from the real formal differential operator (1.2) by the imposition of the boundary condition $f(0)=0$. Let $\mathrm{Im}(E) \neq 0$. Then there is exactly one solution $\chi(r;E)$ of $(h-E)\sigma = 0$ square-integrable at 0 and satisfying the boundary condition $f(0)=0$, and exactly one solution $\Omega(r;E)$ of $(h-E)\sigma=0$ square-integrable at infinity. The resolvent $(E-H)^{-1}$ is an integral operator whose kernel $G(r,s;E)$ is given by

$$G(r,s;E) = \left\{ \begin{array}{ll} \frac{\chi(r;E)\,\Omega(s;E)}{W(\chi,\Omega)} & r<s \\ \frac{\chi(s;E)\,\Omega(r;E)}{W(\chi,\Omega)} & r>s\,. \end{array} \right. \tag{2.35}$$

The incoming and outgoing Green functions are defined by

$$G^\pm(r,s;E) = \lim_{\mu\to 0} G(r,s;E\pm i\mu)\,. \tag{2.36}$$

From Eq. (2.36) it follows that the Green functions $G^\pm$ are just the boundary values on the real axis of the kernel (2.35), which is a function of complex variable. Thus $G^\pm$ keep track of what is "incoming" and of what is "outgoing" by specifying which side of the cut of the resolvent we are on. In our example, the cut of the resolvent, i.e., the spectrum of the Hamiltonian, is the positive real axis.

First we compute the kernel (2.35) in the region $\mathrm{Im}(E) > 0$. In this region, the eigenfunction $\chi(r;E)$ in (2.35) satisfies the boundary conditions

$$\chi(0;E) = 0\,, \tag{2.37}$$

$$\chi(r;E) \in AC^2([0,\infty))\,, \tag{2.38}$$

$$\chi(r;E) \text{ is square integrable at } 0\,. \tag{2.39}$$

The boundary condition (2.38) implies the boundary conditions (2.11)-(2.14), and (2.39) is automatically fulfilled. This means that the eigenfunction $\chi(r;E)$ of Theorem 1, which is unique, is the same as the eigenfunction of Eq. (2.15), although now E is allowed to run over the upper half-plane of complex numbers.

The eigenfunction $\Omega(r;E)$ of Theorem 1, that we denote by $\Omega_+(r;E)$ for the case of $\mathrm{Im}(E) > 0$, satisfies the Schrödinger equation and the boundary conditions

$$\Omega_+(r;E) \in AC^2([0,\infty))\,, \tag{2.40}$$

$$\Omega_+(r;E) \text{ is square integrable at } \infty\,. \tag{2.41}$$

The boundary condition (2.40) implies the continuity conditions (2.16)-(2.19). Condition (2.41) is, for $\mathrm{Im}(E) > 0$, equivalent to (2.20). Thus the (unique) function $\Omega_+(r;E)$ of Theorem 1 coincides with (2.21), E being now any complex number with positive imaginary part. Thus, for $\mathrm{Im}(E) > 0$, the expression of $G(r,s;E)$ in (2.35) is given by (2.9), although now E is allowed to be any complex number in the upper half-plane.

For $\mathrm{Im}(E) < 0$, the situation is similar. The eigenfunction $\chi(r;E)$ of Theorem 1 is also given by (2.15). The other eigenfunction in (2.35), that we denote by $\Omega_-(r;E)$, coincides with the eigenfunction of Eq. (2.31). Needless to say, E can now be any complex number in the lower half-plane. Therefore, the kernel (2.35) is given by (2.33), E now being any complex number with negative imaginary part.

If we now compute the limits in (2.36), we obtain exactly the same outgoing and incoming Green functions as those obtained in the previous section.

3 Conclusions

We have seen that the Green functions obtained by applying the Sturm-Liouville theory are the same as those used in formal scattering theory. We have also seen that in order to find out what is "incoming" and what is "outgoing", the Sturm-Liouville theory substitutes the standard physicists boundary conditions by statements on the analyticity of the Green functions with respect to the energy variable—knowing which side of the cut we are on is tantamount to knowing what is "incoming" and what is "outgoing".

These conclusions are not restricted to the square barrier potential. Actually, they hold for potentials that decrease fast enough at the origin and at infinity, and that do not have too many discontinuities.

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Appendix

The functions that appear in the expressions of the eigenfunctions in Section 2.1 are given by

$$\mathcal{J}_1(E) = \frac{1}{2} e^{-i\sqrt{(E-V_0)}a} \left(\sin(\sqrt{E}a) + \frac{\sqrt{E}}{i\sqrt{(E-V_0)}} \cos(\sqrt{E}a) \right) \tag{3.1}$$

$$\mathcal{J}_2(E) = \frac{1}{2} e^{i\sqrt{(E-V_0)}a} \left(\sin(\sqrt{E}a) - \frac{\sqrt{E}}{i\sqrt{(E-V_0)}} \cos(\sqrt{E}a) \right) \tag{3.2}$$

$$\begin{aligned}\mathcal{J}_3(E) = \frac{1}{2} e^{-i\sqrt{E}b} \Bigg[&\left(1 + \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{i\sqrt{(E-V_0)}b} \mathcal{J}_1(E) \\ &+ \left(1 - \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{-i\sqrt{(E-V_0)}b} \mathcal{J}_2(E) \Bigg]\end{aligned} \tag{3.3}$$

$$\begin{aligned}\mathcal{J}_4(E) = \frac{1}{2} e^{i\sqrt{E}b} \Bigg[&\left(1 - \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{i\sqrt{(E-V_0)}b} \mathcal{J}_1(E) \\ &+ \left(1 + \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{-i\sqrt{(E-V_0)}b} \mathcal{J}_2(E) \Bigg] ,\end{aligned} \tag{3.4}$$

$$\mathcal{A}_3^+(E) = \frac{1}{2} e^{-i\sqrt{(E-V_0)}b} \left(1 + \frac{\sqrt{E}}{\sqrt{(E-V_0)}}\right) e^{i\sqrt{E}b} \tag{3.5}$$

$$\mathcal{A}_4^+(E) = \frac{1}{2} e^{i\sqrt{(E-V_0)}b} \left(1 - \frac{\sqrt{E}}{\sqrt{(E-V_0)}}\right) e^{i\sqrt{E}b} \tag{3.6}$$

$$\begin{aligned}\mathcal{A}_1^+(E) = \frac{1}{2} e^{-i\sqrt{E}a} \Bigg[&\left(1 + \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{i\sqrt{(E-V_0)}a} \mathcal{A}_3^+(E) \\ &+ \left(1 - \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{-i\sqrt{(E-V_0)}a} \mathcal{A}_4^+(E) \Bigg]\end{aligned} \tag{3.7}$$

$$\mathcal{A}_2^+(E) = \frac{1}{2} e^{i\sqrt{E}a} \Bigg[\left(1 - \frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right) e^{i\sqrt{(E-V_0)}a} \mathcal{A}_3^+(E)$$

$$+\left(1+\frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right)e^{-i\sqrt{(E-V_0)}b}\mathcal{A}_4^+(E)\Bigg]\,. \tag{3.8}$$

$$\mathcal{A}_3^-(E)=\frac{1}{2}e^{-i\sqrt{(E-V_0)}b}\left(1-\frac{\sqrt{E}}{\sqrt{(E-V_0)}}\right)e^{-i\sqrt{E}b} \tag{3.9}$$

$$\mathcal{A}_4^-(E)=\frac{1}{2}e^{i\sqrt{(E-V_0)}b}\left(1+\frac{\sqrt{E}}{\sqrt{(E-V_0)}}\right)e^{-i\sqrt{E}b} \tag{3.10}$$

$$\mathcal{A}_1^-(E)=\frac{1}{2}e^{-i\sqrt{E}a}\Bigg[\left(1+\frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right)e^{i\sqrt{(E-V_0)}a}\mathcal{A}_3^-(E)$$

$$+\left(1-\frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right)e^{-i\sqrt{(E-V_0)}a}\mathcal{A}_4^-(E)\Bigg] \tag{3.11}$$

$$\mathcal{A}_2^-(E)=\frac{1}{2}e^{i\sqrt{E}a}\Bigg[\left(1-\frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right)e^{i\sqrt{(E-V_0)}a}\mathcal{A}_3^-(E)$$

$$+\left(1+\frac{\sqrt{(E-V_0)}}{\sqrt{E}}\right)e^{-i\sqrt{(E-V_0)}a}\mathcal{A}_4^-(E)\Bigg]\,. \tag{3.12}$$

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