GREEN'S FUNCTION FOR ONE DIMENSIONAL SCHRÖDINGER EQUATION

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 11.16.

Griffiths derives the first Born approximation by writing the Schrödinger equation in integral form as

$$\psi(\mathbf{r})=\int G(\mathbf{r}-\mathbf{r}_0)\,Q(\mathbf{r}_0)\,d^3\mathbf{r}_0 \tag{1}$$

where

$$\begin{aligned}\left(\nabla^2+k^2\right)\psi &= Q &(2)\\ k &\equiv \frac{\sqrt{2mE}}{\hbar} &(3)\\ Q &\equiv \frac{2m}{\hbar^2}V\psi &(4)\end{aligned}$$

and G is the Green's function satisfying

$$\left(\nabla^2+k^2\right)G(\mathbf{r})=\delta^3(\mathbf{r}) \tag{5}$$

We can follow through Griffiths's derivation and adapt it for the one dimensional Schrödinger equation:

$$\left(\frac{d^2}{dx^2}+k^2\right)\psi=Q \tag{6}$$

where k and Q have the same definitions as above. In this case, the Green's function satisfies

$$\left(\frac{d^2}{dx^2}+k^2\right)G(x)=\delta(x) \tag{7}$$

and the integral form of the Schrödinger equation is

$$\psi(x)=\frac{2m}{\hbar^2}\int G(x-x_0)\,V(x_0)\,\psi(x_0)\,dx_0 \tag{8}$$

We can work with the Fourier transform of G:

$$G(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{ixs}g(s)\,ds \tag{9}$$

where s has the dimensions of 1/length. Plugging in 7 we get

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{d^2}{dx^2}+k^2\right)e^{ixs}g(s)\,ds=\delta(x) \tag{10}$$

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(-s^2+k^2\right)e^{ixs}g(s)\,ds=\delta(x) \tag{11}$$

We can now use the Fourier transform of the delta function (yes, it's *that* formula) to rewrite the RHS:

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(-s^2+k^2\right)e^{ixs}g(s)\,ds=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ixs}ds \tag{12}$$

$$g(s)=\frac{1}{\sqrt{2\pi}}\frac{1}{k^2-s^2} \tag{13}$$

Therefore

$$G(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{ixs}}{k^2-s^2}ds \tag{14}$$

This integral can be done using contour integration in the complex plane, if we choose a contour that runs along the (horizontal) s axis in the $+s$ direction from $s=-R$ to $s=+R$, then arcs back as a semicircle from $+R$ to $-R$. The problem is that the horizontal leg of this contour runs through the two singularities at $s=\pm k$, so we need to change the contour so that it loops around these singularities with small semicircles of radius ρ (see Fig. 11.10 in Griffiths). Cauchy's theorem states that the integral of an analytic function (that is, a function that doesn't have any singularities on the contour) around a closed contour is

$$\oint\frac{f(z)}{z-z_0}dz=2\pi i f(z_0) \tag{15}$$

if $z=z_0$ is the only singularity within the contour. (More generally, if the function to be integrated has more than one singularity at locations z_i, then the integral is $2\pi i\sum_i \mathrm{res}(z_i)$ where $\mathrm{res}(z_i)$ is the *residue* of the function at z_i.)

In fact, the derivation in Griffith isn't really correct, although his Green's function is valid. He chooses a contour that runs along the s axis and loops over the singularity at $s=-k$ and under the singularity at $s=+k$. He then states that by Cauchy's theorem, the integral is just $2\pi i f(+k)$. That is true for the contour shown in his book, but what we need is actually the limit of this integral as the radius of the little semicircles $\rho \to 0$. [To see that Griffiths's argument as it stands doesn't work, suppose we excluded *both* singularities by looping over them. In that case, the contour contains *no* singularities and the integral 14 is zero, which can't be true.]

To do it properly, we'll use Griffiths's contour but write out the integrals involved and take the limit as $\rho \to 0$. We start by taking $x > 0$ and integrating along the s axis from $-R$ to $-k-\rho$, then over the semicircle at $s = -k$ to $-k+\rho$, then from $-k+\rho$ to $k-\rho$, then under the semicircle at $s = +k$ to $k+\rho$, then from ρ to $+R$ and finally around the big semicircle from $+R$ back to $-R$. Since the contour contains only the singularity at $s = +k$, we have

$$\frac{1}{2\pi}\oint\frac{e^{ixz}}{k^2-z^2}dz = \frac{1}{2\pi}\oint\frac{e^{ixz}}{(k+z)(k-z)}dz \tag{16}$$

$$= -\frac{1}{2\pi}\oint\frac{e^{ixz}}{(z+k)(z-k)}dz \tag{17}$$

$$= -\frac{2\pi i}{2\pi}\frac{e^{ikx}}{2k} = -i\frac{e^{ikx}}{2k} \tag{18}$$

At this point, Griffiths assumes that this result is the same as $\int_{-\infty}^{\infty}\frac{e^{ixs}}{k^2-s^2}ds$, so the Green's function is

$$G(x) = -i\frac{e^{ikx}}{2k} \tag{19}$$

and the integral form is, from 8

$$\psi(x) = \psi_0(x) - \frac{im}{\hbar^2 k}\int e^{ik(x-x_0)}V(x_0)\,\psi(x_0)\,dx_0 \tag{20}$$

[Note that this answer cannot be correct, because

$$\int_{-\infty}^{\infty}\frac{e^{ixs}}{k^2-s^2}ds = \int_{-\infty}^{\infty}\frac{\cos xs}{k^2-s^2}ds + i\int_{-\infty}^{\infty}\frac{\sin xs}{k^2-s^2}ds \tag{21}$$

The first integrand on the RHS is an even function of s, and the second integrand is an odd function. Since we're integrating over an interval that is symmetric about $s = 0$, the second integral is zero, meaning that the overall integral must be *real*, which Griffiths's answer isn't.]

A similar analysis for $x < 0$ gives $G(x) = -i\frac{e^{-ikx}}{2k}$ so the overall integral form is

$$\psi(x)=\psi_0(x)-\frac{im}{\hbar^2 k}\int e^{ik|x-x_0|}V(x_0)\,\psi(x_0)\,dx_0 \tag{22}$$

However, this isn't really the correct way to do this. Let's look at it in more detail.

Since $x>0$, we can let the big semicircle go to infinity since xz has a positive imaginary part for all points on this semicircle, so $e^{ixz}\to 0$ as the semicircle goes to infinity, and the integral over that part of the contour also goes to zero. So we're left with

$$\left[\int_{-\infty}^{-k-\rho}+\int_{-k+\rho}^{k-\rho}+\int_{k+\rho}^{\infty}\right]\frac{e^{ixz}}{k^2-z^2}dz+\int_{-k}\frac{e^{ixz}}{k^2-z^2}dz+\int_{+k}\frac{e^{ixz}}{k^2-z^2}dz=-2\pi\left(i\frac{e^{ikx}}{2k}\right) \tag{23}$$

where the two integrals on the right are integrals around the little semicircles at $s=\pm k$. Note that the semicircle at $-k$ is traversed in a clockwise direction, while that at $+k$ is counterclockwise.

The integral around the semicircle at $s=-k$ is over z as it takes on the values $z=-k+\rho e^{i\theta}$ for $\pi\geq\theta\geq 0$ (that is, we start the integration at $\theta=\pi$and proceed to $\theta=0$), and for $s=+k$, $z=k+\rho e^{i\theta}$ for $-\pi\leq\theta\leq 0$. The only quantity that is being integrated over in these two integrals is θ, so we can transform to θ using $dz=i\rho e^{i\theta}d\theta$. We have

$$\int_{-k}\frac{e^{ixz}}{k^2-z^2}dz=\int_{\pi}^{0}\frac{e^{ix\left[-k+\rho e^{i\theta}\right]}}{2k\rho e^{i\theta}+\rho^2 e^{2i\theta}}i\rho e^{i\theta}d\theta \tag{24}$$

$$=ie^{-ikx}\int_{\pi}^{0}\frac{e^{ix\rho e^{i\theta}}}{2k+\rho e^{i\theta}}d\theta \tag{25}$$

Taking the limit, and reversing the limits of integration and hence the sign, we get

$$\lim_{\rho\to 0}\int_{-k}\frac{e^{ixz}}{k^2-z^2}dz = -ie^{-ikx}\int_0^{\pi}\frac{d\theta}{2k} \tag{26}$$

$$= -\frac{\pi i e^{-ikx}}{2k} \tag{27}$$

We can do the same calculation at the other singularity at $s=+k$ and we get

$$\lim_{\rho\to 0}\int_{+k}\frac{e^{ixz}}{k^2-z^2}dz=-\frac{\pi i e^{ikx}}{2k} \tag{28}$$

Putting these results into 23 and taking the limit there, we get

$$\int_{-\infty}^{\infty}\frac{e^{ixs}}{k^2-s^2}ds = -\frac{\pi i}{k}\frac{e^{ikx}-e^{-ikx}}{2} \tag{29}$$

$$= \frac{\pi}{k}\sin(kx) \tag{30}$$

(note that this answer is real, as required) so from 14 we get the Green's function

$$G(x)=\frac{1}{2k}\sin(kx) \tag{31}$$

and the integral form is, from 8

$$\psi(x)=\psi_0(x)+\frac{m}{2\hbar^2 k}\int\sin(k(x-x_0))V(x_0)\psi(x_0)dx_0 \tag{32}$$

where ψ_0 is a free particle solution of $\left(\frac{d^2}{dx^2}+k^2\right)\psi=0$.

If $x<0$, we need to use a large semicircle that is below the s axis, so that $xz>0$. The contour now includes the singularity at $s=-k$ and excludes the one at $s=+k$, and the contour is traversed clockwise, so we pick up a minus sign when using Cauchy's theorem:

$$\frac{1}{2\pi}\oint\frac{e^{ixz}}{k^2-z^2}dz=\frac{1}{2\pi}\oint\frac{e^{ixz}}{(k+z)(k-z)}dz \tag{33}$$

$$=-\frac{1}{2\pi}\oint\frac{e^{ixz}}{(z+k)(z-k)}dz \tag{34}$$

$$=+\frac{2\pi i}{2\pi}\frac{e^{-ikx}}{(-2k)}=-i\frac{e^{-ikx}}{2k} \tag{35}$$

Equation 23 now becomes

$$\left[\int_{-\infty}^{-k-\rho}+\int_{-k+\rho}^{k-\rho}+\int_{k+\rho}^{\infty}\right]\frac{e^{ixz}}{k^2-z^2}dz+\int_{-k}\frac{e^{ixz}}{k^2-z^2}dz+\int_{+k}\frac{e^{ixz}}{k^2-z^2}dz=-2\pi\left(i\frac{e^{-ikx}}{2k}\right) \tag{36}$$

The integrals around the two little semicircles are the same as before, so we get, for $x<0$:

$$\int_{-\infty}^{\infty}\frac{e^{ixs}}{k^{2}-s^{2}}ds = \frac{\pi i}{k}\frac{e^{ikx}-e^{-ikx}}{2} \tag{37}$$

$$= -\frac{\pi}{k}\sin\left(kx\right) \tag{38}$$

$$= \frac{\pi}{k}\sin\left(k\left|x\right|\right) \tag{39}$$

where the last line follows because $x<0$.

The above method gives the same answer for any choice of the little semicircles around the singularities, even if we choose the contour so that there are no singularities inside the contour.

Thus the integral form 32 becomes in general

$$\psi\left(x\right)=\psi_{0}\left(x\right)+\frac{m}{2\hbar^{2}k}\int\sin\left(k\left|x-x_{0}\right|\right)V\left(x_{0}\right)\psi\left(x_{0}\right)dx_{0} \tag{40}$$

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