

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

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

where

$$(\nabla^2 + k^2)\psi = Q \quad (2)$$

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \quad (3)$$

$$Q \equiv \frac{2m}{\hbar^2} V\psi \quad (4)$$

and G is the Green's function satisfying

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

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

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

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

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

and the integral form of the Schrödinger equation is

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

We can work with the Fourier transform of G :

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

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

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

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

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

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

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

Therefore

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

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 $+$ 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

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

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 $2\pi i \sum_i \text{res}(z_i)$ where $\text{res}(z_i)$ 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 $\rho \rightarrow 0$. [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 $\rho \rightarrow 0$. 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

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

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

$$= -\frac{2\pi i}{2\pi} \frac{e^{ikx}}{2k} = -i \frac{e^{ikx}}{2k} \quad (18)$$

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

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

and the integral form is, from 8

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

[Note that this answer cannot be correct, because

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

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

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

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 $e^{ixz} \rightarrow 0$ as the semicircle goes to infinity, and the integral over that part of the contour also goes to zero. So we're left with

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

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

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

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

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

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

$$= -\frac{\pi i e^{-ikx}}{2k} \quad (27)$$

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

$$\lim_{\rho \rightarrow 0} \int_{+k} \frac{e^{ixz}}{k^2 - z^2} dz = -\frac{\pi i e^{ikx}}{2k} \quad (28)$$

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

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

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

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

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

and the integral form is, from 8

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

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:

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

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

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

Equation 23 now becomes

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

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

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

$$= -\frac{\pi}{k} \sin(kx) \quad (38)$$

$$= \frac{\pi}{k} \sin(k|x|) \quad (39)$$

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

The above method gives the same answer for any choice of the little semi-circles 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

$$\psi(x) = \psi_0(x) + \frac{m}{2\hbar^2 k} \int \sin(k|x - x_0|) V(x_0) \psi(x_0) dx_0 \quad (40)$$

PINGBACKS

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