Green's Functions

A detailed analysis of Green's Functions, and their applications to multiple relevant physics problems

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1 Introduction

Assume you have a problem of the form

$$\mathcal{L}y(x) = f(x) \tag{1}$$

subject to certain homogenous boundary conditions where $\mathcal{L}$ is a linear differential operator, $y(x)$ is the unknown function and $f(x)$ is the inhomogeneous term. The Green's function method is a powerful method to solve such problems. A Green's Function for an operator $\mathcal{L}$ is a function $G(x, x')$ such that $\mathcal{L}G(x, x') = \delta(x - x')$, where $\delta(x - x')$ is the Dirac delta function and $\mathcal{L}$ is any linear differential operator. This means in simpler terms that the Green's function is the impulse response of the operator.

We will first show that the Green's function if found could help us solve the inhomogeneous differential equation $\mathcal{L}y(x) = f(x)$, where $\mathcal{L}$ is a linear differential operator.

$$\mathcal{L}y = f(x) \tag{2}$$

$$\mathcal{L}G(x, x') = \delta(x - x') \tag{3}$$

Using the 2 above equations, we can find the solution to the inhomogeneous differential equation by convolving the Green's function with the inhomogeneous term.

$$y(x) = \int_a^b G(x, x')f(x')dx' \tag{4}$$

We will first show that equation (4) holds by applying the operator $\mathcal{L}$ on both sides of equation (4).

$$\begin{aligned}
\mathcal{L}y(x) &= \mathcal{L}\int_a^b G(x, x')f(x')dx' \\
&= \int_a^b \mathcal{L}G(x, x')f(x')dx' \\
&= \int_a^b \delta(x - x')f(x')dx' \\
&= f(x)
\end{aligned}$$

We also note by inspecting equation 3 that if the Green's function satisfies the boundary conditions of the problem, then the solution $y(x)$ will also satisfy the boundary conditions. This shows that we can use the Green's function to get a solution to the inhomogeneous differential equation. A more general solution can then of course be obtained by adding a homogenous solution to $\mathcal{L}$, since $\mathcal{L}$ is linear and $\mathcal{L}y_{hom}(x) = 0$

$$y(x) = y_{hom}(x) + \int_a^b G(x, x')f(x')dx'$$

2 One Dimensional Green's Function

Before we look at the more relevant 3D Green's functions, let us first discuss the properties of the one dimensional Green's functions.

2.1 Properties of One Dimensional Green's Function

2.1.1 General Second order differential operators

We will now discuss second order differential operators, as they are the ones that pop up most commonly in physics.
Let us assume a general form of $\mathcal{L}$ that is as follows:

$$\mathcal{L} \equiv \alpha(t)\frac{d^2}{dt^2} + \beta(t)\frac{d}{dt} + \gamma(t) \tag{5}$$

We want to of course solve the equation:

$$\mathcal{L}x(t) = f(t) \tag{6}$$

Which is the equation usually used to model forced, damped harmonic oscillators (an especially important toy model in physics) if we set (α, β, γ) to be constants. We are interested in finding $G(t, t')$, such that $\mathcal{L}G(t, t') = \delta(t - t')$ as we can then, as previously shown, obtain $x(t) = \int_a^b G(t, t')f(t')dt'$. We are then left to solve the differential equation $\mathcal{L}G(t, t') = \delta(t - t')$.
We will follow a very simple procedure. Assume you have a given differential operator $\mathcal{L}$ subject to homogenous boundary conditions at points a and b respectively.

1. Split the interval into 2 segments one for $a \leq t < t'$ and the other for $t' < t \leq b$
2. The differential equation will reduce to $\mathcal{L}G(t, t') = 0$ for both intervals since t' isn't included in the intervals.
3. Solve each of the differential equations while satisfying its respective boundary conditions.
4. Enforce appropriate matching conditions at $t = t'$.

2.1.2 Continuity of the Green's Function at $t = t'$

To inspect the needed continuity conditions for this class of Green's functions we will integrate the equation $\mathcal{L}G(t, t') = \delta(t - t')$ explicitly with respect to t for a very small interval around t'.

$$\mathcal{L}G(t, t') \equiv \alpha(t)\frac{d^2}{dt^2}G(t, t') + \beta(t)\frac{d}{dt}G(t, t') + \gamma(t)G(t, t') = \delta(t - t') \tag{7}$$

$$\frac{d^2}{dt^2}G(t, t') + \frac{\beta(t)}{\alpha(t)}\frac{d}{dt}G(t, t') + \frac{\gamma(t)}{\alpha(t)}G(t, t') = \frac{\delta(t - t')}{\alpha(t)} \tag{8}$$

Where $\alpha(t)$ is not 0 except maybe at a couple of finite points (at which $G(t, t')$ and its derivative can be taken to be continuous as we will see below).
First, by inspection we see that if $G(t, t')$ was discontinuous, $\frac{d}{dt}G(t, t') \propto \delta(t)$, and $\frac{d^2}{dt^2}G(t, t') \propto \delta'(t)$ which doesn't fit with $\mathcal{L}G(t, t') = \delta(t - t')$. So, we can conclude that $G(t, t')$ must be continuous,

and its derivative is bounded.
We now integrate to identify the requirement on the continuity of $\frac{d}{dt}G(t,t')$.

$$\int_{t'-\epsilon}^{t'+\epsilon} \frac{d^2}{dt^2}G(t,t')dt + \int_{t'-\epsilon}^{t'+\epsilon} \frac{\beta(t)}{\alpha(t)}\frac{d}{dt}G(t,t')dt + \int_{t'-\epsilon}^{t'+\epsilon} \frac{\gamma(t)}{\alpha(t)}G(t,t')dt = \int_{t'-\epsilon}^{t'+\epsilon} \frac{\delta(t-t')}{\alpha(t)}dt$$
$$\frac{d}{dt}G(t,t')\Big|_{t=t'-\epsilon}^{t=t'+\epsilon} = \frac{1}{\alpha(t)}$$

If we closely inspect the equation above we see that it's impossible to satisfy if $\frac{d}{dt}G(t,t')$ is continuous since if we take the limit as $\epsilon \to 0$ and both of the terms are continuous they will both give 0. We can however relax the continuity condition by allowing the derivative of $G(t,t')$ to be discontinuous while still enforcing continuity on $G(t,t')$. Since $\frac{d}{dt}G(t,t')$ and $\frac{\beta(t)}{\alpha(t)}$ are bounded the second term goes to zero, and the same thing applies for the third term.

$$\lim_{\epsilon\to 0}\left[\frac{dG}{dt}\Big|_{t=t'+\epsilon} - \frac{dG}{dt}\Big|_{t=t'-\epsilon}\right] = \frac{1}{\alpha(t')} \tag{9}$$

The Green's Function will take the form:

$$G(t,t') = \begin{cases} A(t')y_1(t) & a \le t < t' \\ B(t')y_2(t) & t' < t \le b \end{cases} \tag{10}$$

Where $y_1(t)$ is the solution in the first interval less than t' and $y_2(t)$ is the solution in the second interval greater than t' with each of these solutions satisfying the boundary condition within its respective solution interval.

Where $y_1(t),\ y_2(t)$ are homogenous solutions of $\mathcal{L}$ and satisfy their respective boundary conditions $y_1(a) = y_2(b) = 0$. We are now left to match the two solutions using appropriate continuity conditions.

2.1.3 General solution

We can now use the conditions we found to obtain the general solution.
By enforcing continuity of $G(t,t')$ we get:

$$A(t')y_1(t') = B(t')y_2(t') \tag{11}$$

The jump discontinuity gives:

$$B(t')y_2'(t') - A(t')y_1'(t') = \frac{1}{\alpha(t')} \tag{12}$$

Solving these together we get:

$$B(t')\left(y_2'(t) - y_1'(t')\frac{y_2(t')}{y_1(t')}\right) = \frac{1}{\alpha(t)}$$
$$B(t') = \frac{y_1(t')}{\alpha(t)(y_1(t')y_2'(t') - y_1'(t')y_2(t'))}$$

Where $W(t') \equiv y_1(t')y_2'(t') - y_1'(t')y_2(t')$ is the Wronskian.
So, we have the general solution as:

$$G(t,t') = \begin{cases} \frac{y_1(t)y_2(t')}{\alpha(t)W(t')} & a \leq t < t' \\ \frac{y_1(t')y_2(t)}{\alpha(t)W(t')} & t' < t \leq b \end{cases} \tag{13}$$

For second order linear differential operators with homogenous boundary conditions.

2.2 Sturm-Liouville Operators

To show the properties of the one dimensional Green's function, we will be assuming $\mathcal{L}$ is a Sturm-Liouville operator.

$$\mathcal{L}y(x) = \frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) + q(x)y(x) = f(x) \tag{14}$$

$$\mathcal{L}G(x,x') = \delta(x-x') \tag{15}$$

2.2.1 Symmetry Property

An important property we seek to show is that if our operator is hermitian then its Green's function will be symmetric with respect to x and x'.

$$G(x,x') = G^*(x'x) \tag{16}$$

To proof this we go do the definition of a hermitian operator. An operator is hermitian if

$$\begin{gathered} < \mathcal{L}y_1|y_2 > = < y_1|\mathcal{L}y_2 > \\ < \mathcal{L}G(x,x_1')|G(x,x_2') > = < G(x,x_1')|\mathcal{L}G(x,x_2') > \\ < \delta(x-x_1')|G(x,x_2') > = < G(x,x_1')|\delta(x-x_2') > \\ \int G(x,x_2')\delta(x-x_1')dx = \int G^*(x,x_1')\delta(x-x_2')dx \\ G(x_1',x_2') = G^*(x_2',x_1') \end{gathered}$$

This gives us the general form for the symmetry condition of the Green's function. However we will only be dealing with real differential operators and so our Green's function will always be real so we can say that if $\mathcal{L}$ is hermitian

$$G(x,x') = G(x',x) \tag{17}$$

2.2.2 Eigenfunction Expansions

Given the self adjoint hermitian operator $\mathcal{L}$ has a set of eigenfunctions, denoted ϕ_n which form an orthonormal basis on the boundaries (a,b), such that

$$\mathcal{L}\phi_n(x) = \lambda_n\phi_n(x), \quad \langle\phi_n|\phi_m\rangle = \delta_{nm}$$

We may expand our functions of interest with respect to these eigenfunctions according to

$$f(x) = \sum_{n=1}^{\infty} a_n\phi_n(x)$$

Hence, we expand $G(x,x')$ on both the x and x' variables

$$G(x,x') = \sum_{nm} g_{nm}\phi_n(x)\phi_m^*(x'), \quad \delta(x-x') = \sum_m \phi_m(x)\phi_m^*(x')$$

where g_{nm} are the expansion constants. hence, our equation

$$\mathcal{L}G(x,x') = \delta(x-x')$$

becomes

$$\mathcal{L}\sum_{nm} g_{nm}\phi_n(x)\phi_m^*(x') = \sum_m \phi_m(x)\phi_m^*(x')$$

and after applying the $\mathcal{L}$

$$\sum_{nm} \lambda_n g_{nm}\phi_n(x)\phi_m^*(x') = \sum_m \phi_m(x)\phi_m^*(x')$$

and since the expansion necessitates orthogonality,

$$\lambda_n g_{nm} = \delta_{nm}$$

in turn, our Green's function is

$$G(x,x') = \sum_n \frac{\phi_n(x)\phi_n^*(x')}{\lambda_n}$$

which is valid for higher dimensions. This result is equivalent to the those obtained through other methods.

2.2.3 Obtaining the Green's Function for a Hermitian Operator

Before we move on to solving an example lets see how we could simplify equation (10) in case our operator is hermitian. We use the continuity condition as well as the symmetry condition to simplify the Green's function. We assume we have x_1 and x_2 such that $x_1 < x_2$.

$$\begin{aligned}
G(x_1,x_2) &= Ah_1(x_2)y_1(x_1) \\
G(x_2,x_1) &= Ah_2(x_1)y_2(x_2) \\
G(x_1,x_2) &= G(x_2,x_1) \\
h_1(x_2)y_1(x_1) &= h_2(x_1)y_2(x_2)
\end{aligned}$$

From the continuity condition we have that $h_1(x_2)y_1(x_2) = h_2(x_2)y_2(x_2)$ and so we can simplify the Green's function by dividing the equation above by the continuity condition.

$$\begin{aligned}
h_1(x_2)y_1(x_1) &= h_2(x_1)y_2(x_2) \\
h_1(x_2)y_1(x_2) &= h_2(x_2)y_2(x_2) \\
\frac{y_1(x_1)}{y_1(x_2)} &= \frac{h_2(x_1)}{h_2(x_2)}
\end{aligned}$$

This can only be satisfied if $h_2(x) = y_1(x)$. The same can be shown for h_1 and y_2 by taking $x_2 < x_1$ and following the same procedure. This shows that if the operator is hermitian then the Green's function will take the form:

$$G(x, x') = \begin{cases} Ay_2(x')y_1(x) & a \leq x < x' \\ Ay_1(x')y_2(x) & x' < x \leq b \end{cases} \tag{18}$$

The computation of the constant A will be obtained from the discontinuity condition since we already used the continuity condition along with the symmetry condition to reach the above form. We rewrite the discontinuity equation using the definition of G we have above.

$$A[y_2'(x')y_1(x') - y_1'(x)y_2(x)] = \frac{1}{p(x')}$$

Noting that the coeffecient next to A is the wronskian of the functions $y_1(x)$ and $y_2(x)$ we rewrite A as

$$A = \frac{1}{p(x')W(y_1, y_2)} \tag{19}$$

Where we can show that the Wronskian times the weight function will be a constant, we can do this by taking it's derivative with respect to x and using Abel's identity.
We have $\alpha(x) = p(x)$ and $\beta(x) = p'(x)$ (which is the requirement to be self-adjoint).

$$\frac{d}{dx}(pW) = p'W + pW' = p'W - p\frac{p'}{p}W = p'W - p'W = 0$$

So, $p(x')W(y_1, y_2)$ is a constant, which is consistent with the eigenfunction expansion.

2.3 Green's Function for Bessel Differential Operator

Let us now solve an example to find the Green's function for the First Order Parametric Bessel differential operator. We first note that the Bessel differential operator is hermitian and so we can use the simplified form of the Green's function. The Bessel differential operator is given by:

$$\mathcal{L} \equiv x^2\frac{d^2}{dx^2} + x\frac{d}{dx} + (k^2x^2 - 1) \tag{20}$$

We assume the operator is subject to homogenous boundary conditions at $x = 0$ and $x = 1$. We first split the interval into 2 segments $0 \leq x < x'$ and $x' < x \leq b$. We then solve the differential equation in each of the intervals.
The solution to the differential equation in the first interval $0 \leq x < x'$ is given by:

$$\begin{aligned} \mathcal{L}G(x, x') &= 0 \\ G(x, x') &= A(x')J_1(kx) + B(x')Y_1(kx) \\ G(0, x') &= 0 \Rightarrow B(x') = 0 \\ G(x, x') &= A(x')J_1(kx) = A(x')y_1(x) \end{aligned}$$

Similarly the solution in the second interval $x' < x \leq 1$ is given by:

$$\begin{aligned}
G(x,x') &= C(x')J_1(kx) + D(x')Y_1(kx) \\
G(1,x') &= 0 \\
C(x') &= -D(x')\frac{Y_1(K)}{J_1(K)} \\
G(x,x') &= D(x')\left(Y_1(kx) - \frac{Y_1(K)}{J_1(K)}J_1(kx)\right) = D(x')y_2(x)
\end{aligned}$$

We can now write our Green's function using the symmetry property to note that $D(x') = y_1(x')$ and $C(x') = y_2(x')$.

$$G(x,x') = \begin{cases} AJ_1(kx)\left(Y_1(kx') - \frac{Y_1(k)}{J_1(k)}J_1(kx')\right) & 0 \leq x < x' \\ AJ_1(kx')\left(Y_1(kx) - \frac{Y_1(k)}{J_1(k)}J_1(kx)\right) & x' < x \leq 1 \end{cases} \tag{21}$$

Now all what's left is to determine the value of the constant A which can be easily done through equation 12 since the operator is hermitian. We will first evaluate the Wronskian of y_1 and y_2.

$$\begin{aligned}
y_1 &= J_1(kx) \\
y_2 &= Y_1(kx) - \frac{Y_1(K)}{J_1(K)}J_1(kx)
\end{aligned}$$

$$W(y_1,y_2) = J_1(kx)\left(\frac{d}{dx}\left(Y_1(kx)\right) - \frac{Y_1(K)}{J_1(K)}\frac{d}{dx}\left(J_1(kx)\right)\right) - \frac{d}{dx}\left(J_1(kx)\right)\left(Y_1(kx) - \frac{Y_1(K)}{J_1(K)}J_1(kx)\right)$$

Simplifying the above expression we get:

$$W(y_1,y_2) = J_1(kx)\frac{d}{dx}\left(Y_1(kx)\right) - \frac{d}{dx}\left(J_1(kx)\right)Y_1(kx) \tag{22}$$

The above equation is the Wronskian of a first kind and second kind Bessel which is a well known Wronskian that is equal to $\frac{2}{\pi x'}$. Substituting that into our equation for A we get $A = \frac{\pi}{2}$. Thus we have the Green's Function for the First Order Parametric Bessel Differential Operator as

$$G(x,x') = \begin{cases} \frac{\pi}{2}J_1(kx)\left(Y_1(kx') - \frac{Y_1(k)}{J_1(k)}J_1(kx')\right) & 0 \leq x < x' \\ \frac{\pi}{2}J_1(kx')\left(Y_1(kx) - \frac{Y_1(k)}{J_1(k)}J_1(kx)\right) & x' < x \leq 1 \end{cases} \tag{23}$$

We can now solve the differential equation below

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (k^2x^2 - 1)y = f(x) \tag{24}$$

by evaluating

$$y(x) = \int_a^b G(x,x')f(x')dx' \tag{25}$$

2.4 Obtaining Green's Function for a Non Hermitian Operator

Next we will solve a simple example simply to demonstrate how to deal with Non Hermitian operators.

$$\mathcal{L}y = \frac{d^2y}{dx^2} + y = f(x)$$
$$y(0) = y'(0) = 0$$

We note that the solution to the homogenous version of the differential equation above takes the form $y = A\sin(x) + B\cos(x)$. However in the first interval there is no way to satisfy both boundary conditions forcing our Green's function for the first interval to be 0. In the second interval we note that there are no boundary conditions meaning that our Greens function will be the entire homogenous solution. This allows us to write:

$$G(x, x') = \begin{cases} 0 & 0 \le x < x' \\ A(x')\sin(x) + B(x')\cos(x) & x' < x \le 1 \end{cases} \tag{26}$$

Since our operator isn't hermitian we cannot use the simplified formulas but instead must enforce the continuity conditions and calculate the values of A and B.

$$\begin{aligned} G(x^+, x') =& G(x^-, x') \\ A(x')\sin(x') +& B(x')\cos(x') = 0 \\ A(x')\sin(x') =& -B(x')\cos(x') \end{aligned}$$

Next enforcing the discontinuity conditions:

$$\frac{dG(x^+, x')}{dx} - \frac{dG(x^-, x')}{dx} = \frac{1}{p(x')} = 1$$
$$A(x')\cos(x) - B(x')\sin(x) = 1$$

We us the 2 equations obtained above to solve for A and B

$$A(x')\sin(x') = -B(x')\cos(x')$$
$$A(x')\cos(x) - B(x')\sin(x) = 1$$
$$A(x') = \cos(x')$$
$$B(x') = -\sin(x')$$

Noting that the conditions for symmetry failed since the operator is not hermitian we can write our Green's function after simplifying using basic trignometric identities as:

$$G(x, x') = \begin{cases} 0 & 0 \le x < x' \\ \sin(x - x') & x' < x \le 1 \end{cases} \tag{27}$$

Which makes sense since this equation models a forced simple harmonic oscillator, if we take y to be the displacement and x to be the time. For the oscillator to be causal, there must be no displacement caused to $t < t'$ which is before anything perturbed the oscillator. And also since $\mathcal{L}$ is translationally invariant, we get $G(x, x')$ as $G(x - x')$.

3 Green's Function for Laplacian Operator

In this section we will obtain the green's function for the Laplacian operator which will allow us to solve any equation of the form

$$\nabla^2\psi(\mathbf{r}) = f(\mathbf{r}) \tag{28}$$

We will first solve it in a direct way that allows us to easily obtain the Green's function however it won't be applicable in all cases. Then we will obtain it in a general method through Fourier transform.

3.1 Direct Approach

We aim to obatin a function $G(\mathbf{r}, \mathbf{r'})$ such that

$$\nabla^2 G(\mathbf{r}, \mathbf{r'}) = \delta^3(\mathbf{r} - \mathbf{r'}) \tag{29}$$

where $\mathbf{r}$ and $\mathbf{r'}$ are both 3 dimensional position vectors. As an attempt at finding our green's function we will use that the laplacian is translationally invariant and will only be a function of the distance between $\mathbf{r}$ and $\mathbf{r'}$. Such a green's function is invariant under translation. This simplifies our equation to

$$\nabla^2 G(\Delta r) = \delta^3(\Delta r) \tag{30}$$

We next will integrate both sides of the above equation over a sphere centered at r' and has a radius of Δr. We also note that the laplacian can be written as a divergence and a gradient. Then we apply the divergence theroem.

$$\begin{aligned}
\iiint \nabla^2 G(\Delta r) dv &= \iiint \delta^3(\Delta r) dv \\
&= \iiint \nabla \cdot \nabla G(\Delta r) dv \\
&= \oiint \nabla \mathbf{G}(\Delta r) \cdot d\mathbf{A} = 1
\end{aligned}$$

We also note that since G is only a function of r then its gradient will only have 1 term given by $\nabla \mathbf{G}(\Delta r) = \frac{dG}{d\Delta r}\mathbf{e}_r$. Since we are integrating over a spherical shell of constant radius Δr the derivative will be a constant and can be extracted from the integral. The integral simply becomes the area of the sphere yielding

$$4\pi(\Delta r)^2 \frac{dG}{d\Delta r} = 1 \tag{31}$$

We can easily solve the differential equation above yielding

$$G(\Delta r) = -\frac{1}{4\pi\Delta r} + c$$

For physical reasons we note that the Green's function could for example represent electric potential and thus we would require c to be 0. We finally obtain our Green's function as

$$G(\mathbf{r}, \mathbf{r'}) = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r'}|} \tag{32}$$

3.2 Fourier Transform Method

We start with the equation for our Green's function

$$\nabla^2 G(\Delta r) = \delta^3(\Delta r) \tag{33}$$

We then we write both sides of the above equation in terms of their 3 dimensional inverse Fourier transform integrals.
The 3D fourier transform could be thought of as obtaining a fourier transform for each of the 3 dimensions of our r vector.

$$\frac{1}{(2\pi)^3}\iiint -k^2 G_n e^{i\mathbf{k}\cdot\mathbf{r}} d^3k = \frac{1}{(2\pi)^3}\iiint e^{i\mathbf{k}\cdot\mathbf{r}} d^3k$$

Before we move on let us first inspect the equation above. We wrote each of the terms in the equation of green's function as the inverse Fourier transform of their Fourier transforms. We denoted the Fourier transform of our green's function as G_n and we know that the Fourier transform of a delta function is equal to 1.
Now we note by comparison of the 2 sides of the equation above that

$$G_n = -\frac{1}{k^2}$$

This allows us to write our integral equation for our green's function as

$$G(r) = \frac{-1}{(2\pi)^3}\iiint \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2} d^3k$$

This integration should be done over the entire k space. We choose to do it over spherical coordinates for simplicity.

$$\begin{aligned}
G(r) &= \frac{-1}{(2\pi)^3}\int_0^\infty \int_0^{2\pi} \int_0^\pi \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2} k^2 \sin(\theta) d\theta d\phi dk \\
&= \frac{-1}{(2\pi)^2}\int_0^\infty \int_0^\pi e^{ikr\cos(\theta)} \sin(\theta) d\theta dk \\
&= \frac{-1}{(2\pi)^2}\int_0^\infty \frac{e^{ikr} - e^{-ikr}}{ikr} dk \\
&= -\frac{1}{2\pi^2 r}\int_0^\infty \frac{\sin(kr)}{k} dk \\
&= -\frac{1}{2\pi^2 r}\frac{\pi}{2} \\
&= -\frac{1}{4\pi r} = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r'}|}
\end{aligned}$$

We note that this approach is a much more general approach as it is the one used to obtain Green's functions for other operators such as the d'lambertian.

4 Helmholtz's equation and the Integral form of Schrodinger's equation

The Helmholtz equation can be motivated if we look at the time independent Schrodinger's equation in 3D.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \tag{34}$$

By using the change of variables $k^2 = \frac{2mE}{\hbar^2}$ and $Q = \frac{2m}{\hbar^2}V\psi$, we get:

$$(\nabla^2 + k^2)\psi(\vec{r}) = Q(\vec{r})$$

Where Helmholtz's equation is $(\nabla^2 + k^2)\psi(\vec{r}) = 0$.
We now want to get the Green's function for Helmholtz's equation.

$$(\nabla^2 + k^2)G(\mathbf{r} - \mathbf{r'}) = \delta(\mathbf{r} - \mathbf{r'}) \tag{35}$$

Where we used $G(\mathbf{r} - \mathbf{r'})$ instead of $G(\mathbf{r}, \mathbf{r'})$ because the Helmholtz operator ($\mathcal{L} \equiv \nabla^2 + k^2$) is translationally invariant. We can, even further, work on getting just $G(\mathbf{r})$, and then substitute every $\mathbf{r}$ for $\mathbf{r} - \mathbf{r'}$ since they have the same functional form. We will use the Fourier transform method as previously established.

$$G(\mathbf{r}) = \frac{1}{(2\pi)^3}\iiint\limits_{all-space} G(\mathbf{s})e^{i\mathbf{s}\cdot\mathbf{r}}d^3s$$

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3}\iiint\limits_{all-space} e^{i\mathbf{s}\cdot\mathbf{r}}d^3s$$

Substituting in the equation we get:

$$\frac{1}{(2\pi)^3}\iiint\limits_{all-space}(-s^2 + k^2)\tilde{G}(\mathbf{s})e^{i\mathbf{s}\cdot\mathbf{r}}d^3s = \frac{1}{(2\pi)^3}\iiint\limits_{all-space} e^{i\mathbf{s}\cdot\mathbf{r}}d^3s$$

Which gives the Fourier transform of $G(\mathbf{r})$ as:

$$\tilde{G}(\mathbf{s}) = \frac{1}{k^2 - s^2}$$

Meaning $G(\mathbf{r})$ can be written as:

$$G(\mathbf{r}) = \frac{1}{(2\pi)^3}\iiint\limits_{all-space} \frac{1}{k^2 - s^2}e^{i\mathbf{s}\cdot\mathbf{r}}d^3s$$

We can switch to spherical coordinates and choose our polar axis to be in the direction of $\mathbf{r}$ such that we would have polar symmetry, and we can go ahead and compute that integral which gives

2π right away

$$
\begin{aligned}
G(\mathbf{r}) &= \frac{1}{(2\pi)^2}\int_0^\infty ds \frac{s^2}{k^2-s^2}\int_0^\pi e^{isr\cos\theta}\sin\theta d\theta \\
&= -\frac{1}{(2\pi)^2}\frac{1}{ir}\int_0^\infty ds \frac{s^2}{s(k^2-s^2)}\left[e^{-isr}-e^{isr}\right] \\
&= \frac{i}{8\pi^2 r}\left[\int_{-\infty}^\infty ds \frac{se^{-isr}}{k^2-s^2} - \int_{-\infty}^\infty ds \frac{se^{isr}}{k^2-s^2}\right] \\
&= \frac{i}{8\pi^2 r}[I_1 - I_2]
\end{aligned}
$$

Where the integral with a negative exponential is I_1, and I_2 is the integral with a positive exponential.
These integrals are singular at finite points on the real axis, so their value is technically not defined. There are multiple ways we can get limiting solutions. The most popular way is by calculating the Cauchy Principal Value, but when doing this, the Green's function that comes out has terms that look like e^{ikr} and e^{-ikr}. However, due purely to physical considerations, we only want solutions that have terms following e^{ikr}. These are plane waves that are going away from the system. The reason for this, is that the integral form for Schrodinger's equation is studied to better understand scattering of particles. A method called Born's approximation is utilized, where its basic thinking is to observe particle-waves far away from the potential after they have been scattered off a certain system to approximately understand what the system you are scattering off looks like. The Born approximation is done by Taylor expanding the $\frac{1}{r}$ term we get in the final Green's function.

To get the e^{ikr}, we apply a different regularization method developed by Richard Feynman, called the $i\epsilon$-prescription. We push the poles that are on the real axis up/down to get the poles in such a way as to obtain the e^{ikr} term when calculating the residue, then take the limit as ϵ goes to 0.

We first compute the I_1 term. By Jordan's lemma, we know that this real integral can be computed as a contour integral on the lower half plane (since $r > 0$ and the argument of the complex exponential is then negative), such that the integral on C_R (the arc) will vanish. We will calculate the contour integral on the path shown in figure 1.

$$
\begin{aligned}
\lim_{\epsilon\to 0}\left[\oint \frac{ze^{-izr}}{(z-(-k-i\epsilon))(z-(k+i\epsilon))}dz\right] &= \lim_{\epsilon\to 0}\left[\int_{C_R}\frac{ze^{-izr}}{(z-(-k-i\epsilon))(z-(k+i\epsilon))}dz\right. \\
&\quad \left. + \int_{-R}^{R}\frac{ze^{-izr}}{(z-(-k-i\epsilon))(z-(k+i\epsilon))}dz\right] \\
&= -\int_\infty^\infty \frac{ze^{-izr}}{k^2-z^2}dz
\end{aligned}
$$

Where we took $R \to \infty$ and used Jordan's lemma to vanish the integral on C_R.
The contour integral is then evaluated by calculating the residues and multiplying by $2\pi i$ (there is a negative because the denominator is swapped and another negative sign from going around the contour clockwise).

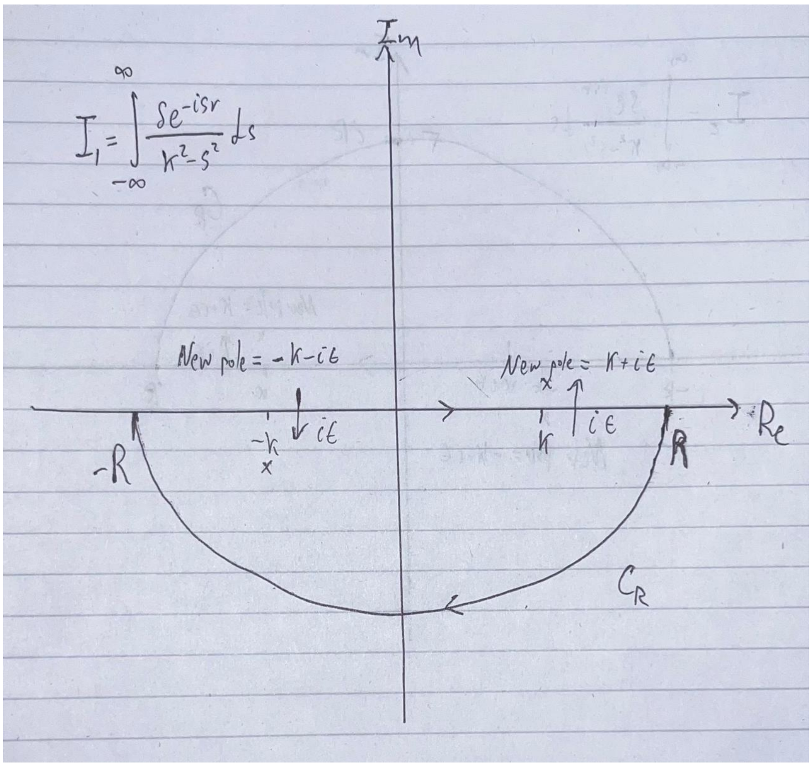

Figure 1: Contour of I_1

$$
\begin{aligned}
I_1 &= -\lim_{\epsilon\to 0}\left[-2\pi i \ \mathrm{Res}(f(z), -k-i\epsilon)\right] = 2\pi i \lim_{\epsilon\to 0}\left[\frac{(-k-i\epsilon)e^{-ir(-k-i\epsilon)}}{-k-i\epsilon-k-i\epsilon}\right] \\
&= 2\pi i \frac{e^{irk}}{2} = i\pi e^{ikr}
\end{aligned}
$$

Calculating I_2 is almost identical, we will traverse the contour as shown in figure 2:

$$
\begin{aligned}
\lim_{\epsilon\to 0}\left[\oint \frac{ze^{izr}}{(z-(-k-i\epsilon))(z-(k+i\epsilon))}dz\right] &= \lim_{\epsilon\to 0}\left[\int_{C_R} \frac{ze^{izr}}{(z-(-k-i\epsilon))(z-(k+i\epsilon))}dz\right. \\
&\quad \left. + \int_{-R}^{R} \frac{ze^{izr}}{(z-(-k-i\epsilon))(z-(k+i\epsilon))}dz\right] \\
&= -\int_{\infty}^{\infty} \frac{ze^{izr}}{k^2-z^2}dz
\end{aligned}
$$

Where we took $R\to\infty$ and used Jordan's lemma to vanish the integral on C_R.
The contour integral is then evaluated by calculating the residues and multiplying by $2\pi i$ (there is only one negative sign because the denominator is swapped, and the contour is traversed counter-clockwise).

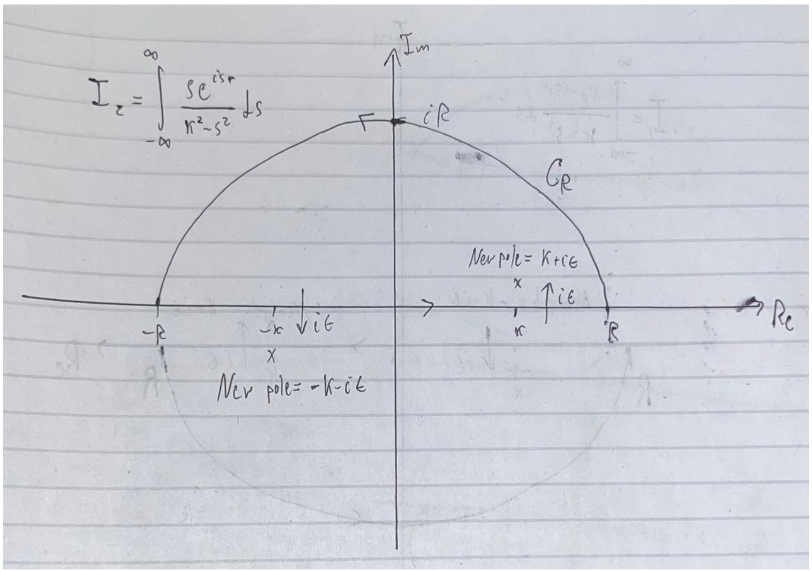

Figure 2: Contour of I_2

$$I_2 = \lim_{\epsilon \to 0} \left[-2\pi i \text{ Res}(f(z), k + i\epsilon)\right] = -2\pi i \lim_{\epsilon \to 0} \left[\frac{(k + i\epsilon)e^{ir(k+i\epsilon)}}{k + i\epsilon + k + i\epsilon}\right]$$
$$= -2\pi i \frac{e^{irk}}{2} = -i\pi e^{ikr}$$

We can see that we succeeded in only generating e^{ikr} terms.
The Green's function is then:

$$G(\mathbf{r}) = \frac{i}{8\pi^2 r}\left[i\pi e^{ikr} - (-i\pi e^{ikr})\right] = -\frac{e^{ikr}}{4\pi r} = -\frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|} \tag{36}$$

We can get $G(\mathbf{r} - \mathbf{r}')$ by promoting the function as we said.

$$G(\mathbf{r} - \mathbf{r}') = -\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}$$

Now, the general solution to Schrodinger's equation can be written as a homogenous term (solution to $(\nabla^2 + k^2)\psi(\mathbf{r}) = 0$) added to the convolution of Q with the Green's function. The homogenous terms go as $Ae^{ikr} + Be^{-ikr}$, we also only choose terms that have e^{ikr}, we will just call the homogenous term $\psi_0(\mathbf{r})$. The general solution is:

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int -\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}Q(\mathbf{r}')d^3r' = \psi_0(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}V(\mathbf{r}')\psi(\mathbf{r}')d^3r' \tag{37}$$

The Born approximation consists of Taylor expanding the $\frac{1}{|\mathbf{r}-\mathbf{r}'|}$ term to get solutions for $\psi(\mathbf{r})$ very far away from the source of the potential (system we are scattering off of).

5 Appendix

5.1 Inhomogenous Boundary Conditions

When using Green's functions, we unfortunately require that we impose homogenous boundary conditions on our problem, so that when we are convolving our Green's function with the forcing term, the final solution would have the same boundary conditions. If the Green's function had a value at the boundaries, the value of the solution at the boundaries would not generally be the same. In a problem with inhomogenous boundary conditions, we address it as we did in the course. We will split our solution into 2 terms, one that solves $\mathcal{L}y_1(x) = 0$ and has inhomogenous boundary conditions, and $\mathcal{L}y_2(x) = f(x)$ with homogenous boundary conditions which we can then solve using Green's functions. The solution to $y_1(x)$ can then be obtained using any method like the ones we encountered in this course or otherwise. The final solution is then $y(x) = y_1(x) + y_2(x)$.

5.2 Translational Invariance

Intuitively, the Green's function would be translationally invariant and hence only depend on the seperation from the source term when the operator $\mathcal{L}$ does not depend on position, which occurs frequently in encountered problems if $\mathcal{L}$ only contains a mix of derivatives and constants, like the laplacian and d'lambertian. We can formalize this argument using the translation operator $T(\vec{a})$, which operates by adding $\vec{a}$ to every position vector.

Theorem:
If $\mathcal{L}$ commutes with $T(\vec{a})$ ($\mathcal{L}T(\vec{a})$=$T(\vec{a})\mathcal{L}$) and appropriate boundary conditions are placed on the problem as to eliminate any gauge freedom in the choice of the Green's function (making the Green's function unique), the Green's function $G(\vec{x}, \vec{x}') = G(\vec{x} - \vec{x}')$

Proof:
We first show that $G(\vec{x}, \vec{x}') = G(\vec{x} + \vec{a}, \vec{x}' + \vec{a})$

$$\begin{aligned}
&\mathcal{L}G(\vec{x}, \vec{x}') = \delta(\vec{x} - \vec{x}') \\
&T(\vec{a})[\mathcal{L}G(\vec{x}, \vec{x}')] = T(\vec{a})\delta(\vec{x} - \vec{x}') \\
&\mathcal{L}[T(\vec{a})G(\vec{x}, \vec{x}')] = \delta(\vec{x} + \vec{a} - (\vec{x}' + \vec{a})) = \delta(\vec{x} - \vec{x}') \\
&\mathcal{L}[G(\vec{x} + \vec{a}, \vec{x}' + \vec{a})]) = \delta(\vec{x} - \vec{x}')
\end{aligned}$$

If the PDE is well-posed, the Green's function is unique (up to the addition of a homogenous solution which is eliminated by the imposition of appropriate boundary conditions). Hence, $G(\vec{x}, \vec{x}') = G(\vec{x} + \vec{a}, \vec{x}' + \vec{a})$.
We can then choose $\vec{a}$=-$\vec{x}'$, which gives us $G(\vec{x}, \vec{x}') = G(\vec{x} + -\vec{x}', \vec{x}' + -\vec{x}') = G(\vec{x} - \vec{x}', 0) = G(\vec{x} - \vec{x}')$

5.3 Abel's Identity

Let us consider a second order linear homogenous differential equation

$$\alpha(x)\frac{d^2y}{dx^2} + \beta(x)\frac{dy}{dx} + \gamma(x)y = 0$$

with 2 solutions $y_1(x),\ y_2(x)$.
Their Wronskian is defined as, $W(y_1, y_2) = y_1(x)y_2'(x) - y_1'(x)y_2(x)$.

We will take the derivative of W:

$$\begin{aligned} W' &= y_1'y_2' + y_1y_2'' - y_1'y_2' - y_1''y_2 = y_1y_2'' - y_1''y_2 \\ &= -y_1(\frac{\beta}{\alpha}y_2' + \frac{\gamma}{\alpha}y_2) + y_2(\frac{\beta}{\alpha}y_1' + \frac{\gamma}{\alpha}y_1) \\ &= -\frac{\beta}{\alpha}(y_1y_2' - y_1'y_2) = -\frac{\beta}{\alpha}W \end{aligned}$$

Which gives:

$$W(y_1, y_2)(x) = W(y_1, y_2)(x_0)e^{-\int_{x_0}^{x} \frac{\beta(u)}{\alpha(u)}du}$$

However, we will only need $W' = -\frac{\beta}{\alpha}W$ in our report.

5.4 Jordan's Lemma

Jordan's lemma is needed to know when you can integrate functions multiplied by complex exponentials to calculate real infinite integrals on the real axis using contour integrals and the residue theorem. Such integrals are very powerful in calculating inverse Fourier transforms, which is the standard way we use to compute Green's functions in higher dimensions. It also guides us in choosing whether to preform such a contour integral in the upper half plane or the lower half plane, depending on the sign of the complex exponential.

Theorem I:
Given that a function $f(z)$ is analytic at all points in the upper half plane that have $|z| > R_0$ $(0 \leq \theta \leq \pi)$, and for all points on a semicircle with $R > R_0$, there is positive real number M_R, such that $|f(z)| \leq M_R$ and $\lim_{R\to\infty} M_R = 0$.

Then, for every positive constant a,

$$\lim_{R\to\infty} \int_{C_R} f(z)e^{iaz}dz = 0 \tag{38}$$

Proof I:

We can parametrize the C_R integral and show that its modulus is bounded, and show that that bound goes to 0 as R goes to ∞.
We will first prove a lemma called Jordan's inequality.
Jordan's Inequality:

$$\int_0^{\pi} e^{-R\sin\theta}d\theta = 2\int_0^{\pi/2} e^{-R\sin\theta}d\theta$$

This is possible since $\sin\theta$ is symmetric around $\pi/2$. We also know that for $0 \leq \theta \leq \pi/2$, $\sin\theta \geq \frac{2\theta}{\pi}$.
Which tell us that $e^{-R\sin\theta} \leq e^{-2R\theta/\pi}$.
So, we have that:

$$\int_0^{\pi/2} e^{-R\sin\theta}d\theta \leq \int_0^{\pi/2} e^{-2R\theta/\pi}d\theta = \frac{\pi}{2R}(1 - e^{-R}) \leq \frac{\pi}{2R}$$

$$\int_{C_R} f(z)e^{iaz} = \int_0^{\pi} f(Re^{i\theta})e^{iaRe^{i\theta}} iRe^{i\theta} d\theta$$

$$\left| \int_{C_R} f(z)e^{iaz} dz \right| \leq M_R R \int_0^{\pi} e^{-aR\sin\theta} d\theta < \frac{M_R \pi}{a}$$

Since as $R \to \infty$, $M_R \to 0$, we can see that $\int_{C_R} \to 0$

If $a < 0$, the inequality won't hold, so we need to take the contour integral on the lower half plane (so that $-\pi \leq \theta \leq 0$).

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