

Green's functions

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The Green's function can be viewed as a kernel giving the response to a perturbation

Example: Poisson equation $-\nabla^2 \phi(\underline{r}) = \frac{1}{\epsilon_0} g(\underline{r})$

The potential at \underline{r}_1 from the charge distribution $g(\underline{r}_2)$ is

$$\phi(\underline{r}_1) = \frac{1}{4\pi\epsilon_0} \int \frac{g(\underline{r}_2)}{|\underline{r}_1 - \underline{r}_2|} d^3\underline{r}_2 \quad \text{integrating over the entire charge distribution } g(\underline{r}_2)$$

We identify $G(\underline{r}_1, \underline{r}_2) \equiv \frac{1}{4\pi\epsilon_0} \frac{1}{|\underline{r}_1 - \underline{r}_2|}$ as the kernel that converts the presence of a charge $g(\underline{r}_2) d^3\underline{r}_2$ at \underline{r}_2 into a potential at \underline{r}_1 . We can write

$$\phi(\underline{r}_1) = \int G(\underline{r}_1, \underline{r}_2) g(\underline{r}_2) d^3\underline{r}_2 \quad \text{with } G(\underline{r}_1, \underline{r}_2) \text{ the Green's function.}$$

Dirac δ -function is a distribution with the properties

$$\delta(x-t) = 0, \quad t \neq x \quad \int_a^b \delta(x-t) dt = \begin{cases} 1, & a \leq x \leq b \\ 0, & x \notin [a, b] \end{cases}$$

$$\int_a^b \delta(x-t) f(t) dt = \begin{cases} f(x), & x \in [a, b] \\ 0, & x \notin [a, b] \end{cases}$$

$\therefore f(x)$ can be expanded as $f(x) = \int_a^b \delta(x-t) f(t) dt$

Assume a second-order self-adjoint inhomogeneous ODE

$$\mathcal{L}y \equiv \frac{d}{dx} \left\{ p(x) \frac{dy}{dx} \right\} + q(x)y(x) = f(x) \quad \text{for } a \leq x \leq b$$

and homogeneous boundary conditions, e.g. $y(a) = y(b) = 0$ and/or $y' = 0$ at the end points. $\Rightarrow \mathcal{L}$ Hermitian

Consider a function $G(x, t)$ obtained as the solution of $\mathcal{L}G(x, t) = \delta(x-t)$

(NOTE: in the 6th Ed. $\mathcal{L}G(x, t) = -\delta(x-t)$)

Just be consistent!

With $G(x, t)$ we have for

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$$y(x) = \int_a^b G(x, t) f(t) dt \quad \text{that} \quad \alpha_x y(x) = \alpha_x \int_a^b G(x, t) f(t) dt = \\ = \int_a^b \alpha_x G(x, t) f(t) dt = \int_a^b \delta(x-t) f(t) dt = f(x)$$

so that if we can find $G(x, t)$ we have the solution irrespective of the inhomogeneous right hand side. $G(x, t)$ gives the response at x of the perturbation $f(t)$ at t .

Properties of Green's functions (1-D)

Integrate the (self-adjoint) equation around t with respect to x

$$\int_{t-\varepsilon}^{t+\varepsilon} \left[\frac{d}{dx} \left[p(x) \frac{dG(x, t)}{dx} \right] + q(x) G(x, t) \right] dx = \int_{t-\varepsilon}^{t+\varepsilon} \delta(t-x) dx$$

Both $\frac{dG}{dx}$ and $G(x, t)$ cannot be continuous at $x = t$ ($p(x), q(x)$ continuous functions)

Assuming $G(x, t)$ continuous as $\varepsilon \rightarrow 0$ $\int_{t-\varepsilon}^{t+\varepsilon} q(x) G(x, t) dx \rightarrow 0$

We find a discontinuity in the

derivative $\frac{dG(x, t)}{dx}$; $\lim_{\varepsilon \rightarrow 0^+} \left[\frac{dG(x, t)}{dx} \right]_{x=t+\varepsilon} - \left[\frac{dG(x, t)}{dx} \right]_{x=t-\varepsilon} = \frac{1}{p(t)}$

Let $\{\varphi_n(x)\}$ be eigenfunctions of α (self-adjoint \rightarrow complete orthonormal set)

so that $\alpha \varphi_n(x) = \lambda_n \varphi_n(x)$, $\langle \varphi_n | \varphi_m \rangle = \delta_{nm}$

Expand $G(x, t)$ in terms of $\{\varphi_n\}$ as $G(x, t) = \sum_{n, m} g_{nm} \varphi_n(x) \varphi_m^*(t)$

The δ -function $\delta(x-t) = \sum_m \varphi_m(x) \varphi_m^*(t)$

so that $\alpha \sum_{nm} g_{nm} \varphi_n(x) \varphi_m^*(t) = \sum_m \varphi_m(x) \varphi_m^*(t)$

α only operates on the x -dependence and $\alpha \varphi_n(x) = \lambda_n \varphi_n(x)$

$$\text{so } G(x,t) = \begin{cases} A y_1(x) y_2(t) & x < t \\ A y_2(x) y_1(t) & x > t \end{cases} \quad \text{Assume } y_1, y_2 \text{ real} \quad (4)$$

The discontinuity in the derivative at $x=t$

$$\left. \frac{dG}{dx} \right|_{x=t^+} - \left. \frac{dG}{dx} \right|_{x=t^-} = \frac{1}{p(t)} \quad \text{becomes } A \left\{ \overbrace{y_2'(t) y_1(t) - y_1'(t) y_2(t)}^{\text{Wronskian}} \right\} = \frac{1}{p(t)}$$

$$\text{so that } A = \left\{ p(t) \cdot W\{y_1(t), y_2(t)\} \right\}^{-1}$$

Explicit expression for $y(x)$:

$$\begin{aligned} y(x) &= \int_a^x G_>(x,t) f(t) dt + \int_x^b G_<(x,t) f(t) dt = \\ &= A y_2(x) \int_a^x y_1(t) f(t) dt + A y_1(x) \int_x^b y_2(t) f(t) dt \end{aligned}$$

For $x \rightarrow a$ the first integral becomes zero and the second term is proportional to $y_1(a)$. Similar for $x \rightarrow b$.

To show that $dy(x) = f(x)$ for this $y(x)$ note that

$$\begin{aligned} \frac{d}{dx} \left\{ y_2(x) \int_a^x y_1(t) f(t) dt \right\} &= y_2'(x) \int_a^x y_1(t) f(t) dt + y_2(x) y_1(x) f(x) \\ \text{and } \frac{d}{dx} \left\{ y_1(x) \int_x^b y_2(t) f(t) dt \right\} &= y_1'(x) \int_x^b y_2(t) f(t) dt - y_1(x) y_2(x) f(x) \end{aligned}$$

Example 10.1.1. $-y'' = f(x)$ with $y(0) = y(1) = 0$ $x \in [0,1]$

Solutions to $y'' = 0$ are $y(x) = c_0 + c_1 x$

Take $y_1 = x$ so that $y_1(0) = 0$

$y_2 = 1-x$ — " — $y_2(1) = 0$

The ODE is on standard form with $p(x) = -1$
(self-adjoint)

$$\text{so that } A = \frac{1}{(-1)[(-1)x - (1)(1-x)]} = 1$$

$$\text{so that } G(x,t) = \begin{cases} x(1-t), & 0 \leq x < t \\ (1-x)t, & t < x \leq 1 \end{cases}$$

Set $f(x) = 2x$; $y(x) = (1-x) \int_0^x t \cdot 2t dt + x \int_x^1 (1-t) 2t dt =$
 $= (1-x) \frac{2}{3} x^3 + x \left[t^2 - \frac{2}{3} t^3 \right]_x^1 = \frac{2}{3} x^3 - \frac{2}{3} x^4 + \frac{1}{3} x - x^3 + \frac{2}{3} x^4 =$
 $= \frac{1}{3} x - \frac{1}{3} x^3 \quad y(0) = 0, y(1) = 0$

$y' = \frac{1}{3} - x^2, \quad -y'' = 2x \quad \text{OK}$

Set $f(x) = \sin \pi x$; $y(x) = (1-x) \int_0^x t \sin \pi t dt + x \int_x^1 (1-t) \sin \pi t dt$
 $\int_0^x t \sin \pi t dt = \left[-\frac{t}{\pi} \cos \pi t \right]_0^x + \frac{1}{\pi} \int_0^x \cos \pi t dt = -\frac{x}{\pi} \cos \pi x + \frac{1}{\pi^2} \left[\sin \pi t \right]_0^x =$
 $= -\frac{x}{\pi} \cos \pi x + \frac{1}{\pi^2} \sin \pi x$

$\int_x^1 (1-t) \sin \pi t dt = \int_x^1 \sin \pi t dt - \int_x^1 t \sin \pi t dt = -\frac{1}{\pi} \left[\cos \pi t \right]_x^1 -$
 $- \left\{ \left[-\frac{t}{\pi} \cos \pi t \right]_x^1 + \frac{1}{\pi} \int_x^1 \cos \pi t dt \right\} =$
 $= -\frac{1}{\pi} \cos \pi + \frac{1}{\pi} \cos \pi x + \frac{1}{\pi} \cos \pi - \frac{x}{\pi} \cos \pi x + \frac{1}{\pi^2} \sin \pi x$

So that $y(x) = (1-x) \left\{ -\frac{x}{\pi} \cos \pi x + \frac{1}{\pi^2} \sin \pi x \right\} + x \left\{ \frac{1}{\pi} \cos \pi x - \frac{x}{\pi} \cos \pi x + \frac{1}{\pi^2} \sin \pi x \right\} =$
 $= -\frac{x}{\pi} \cos \pi x + \frac{x^2}{\pi} \cos \pi x + \frac{1}{\pi^2} \sin \pi x - \frac{x}{\pi^2} \sin \pi x +$
 $+ \frac{x}{\pi} \cos \pi x - \frac{x^2}{\pi} \cos \pi x + \frac{x}{\pi^2} \sin \pi x = \frac{1}{\pi^2} \sin \pi x$

$y(0) = y(1) = 0 \quad \text{and} \quad -y'' = \sin \pi x$

∴ The Green's function can be used to construct the solution for arbitrary right hand side (assuming we can do the integrals)

Non-homogeneous boundary conditions $y(a) = c_1, y(b) = c_2$
 c_1 and/or $c_2 \neq 0$

set $u = y - \frac{c_1(b-x) + c_2(x-a)}{b-a}$

$\Rightarrow u(a) = y(a) - c_1 = 0$

$u(b) = y(b) - c_2 = 0$

Initial value problems: Take $\Delta y = y'' + y = f(x)$ (6)

with $y(0) = y'(0) = 0$; $p(x) = 1$

Linearly independent solutions $y_1 = \sin x$, $y_2 = \cos x$

but $c_1 \sin x + c_2 \cos x$ gives $c_2 = 0$ at $x = 0$

Derivative $c_1 \cos x - c_2 \sin x$ gives $c_1 = 0$ at $x = 0$

so for $x < t$ $G(x, t) = 0$

For $x > t$ no constraining B.C. so set

$$G(x, t) = c_1(t) \sin x + c_2(t) \cos x, \quad x > t$$

Continuity of ~~the solution~~ $G(x, t)$ as $x \rightarrow t_{+,-}$ $0 = c_1(t) \sin t + c_2(t) \cos t$

Discontinuity of the derivative

$$\frac{\partial G}{\partial x}(t_+, t) - \frac{\partial G}{\partial x}(t_-, t) = \frac{1}{p(t)} = 1 \rightarrow c_1(t) \cos t - c_2(t) \sin t = 1$$

$$\text{We have } c_1(t) = -c_2(t) \frac{\cos t}{\sin t} \rightarrow -c_2(t) \left\{ \frac{\cos^2 t}{\sin t} + \sin t \right\} = 1$$

$$\text{and } c_2(t) = -\sin t, \quad c_1(t) = \cos t$$

Thus, $G(x, t) = \sin x \cos t - \cos x \sin t = \sin(x-t)$, $x > t$

$$\text{and } G(x, t) = \begin{cases} 0, & x < t \\ \sin(x-t), & t < x \end{cases}$$

$$y(x) = \int_0^{\infty} G(x, t) f(t) dt = \int_0^x \sin(x-t) f(t) dt$$

$G(x, t)$ not symmetric since B.C. only on one side

Boundary at infinity

$$\left(\frac{d^2}{dx^2} + k^2 \right) \psi(x) = g(x)$$

with solutions as outgoing waves

at infinity $y_1 = e^{-ikx}$, $y_2 = e^{ikx}$

$$\psi(x, t) = e^{-i\omega t} \cdot y_i \rightarrow \begin{matrix} e^{-i(kx + \omega t)} \\ y_1 \end{matrix}, \begin{matrix} e^{i(kx - \omega t)} \\ y_2 \end{matrix}$$

Outgoing wave $\rightarrow y_2$ for large, positive x

y_1 for large, negative x

So

$$G(x, x') = \begin{cases} A y_1(x') y_2(x), & x > x' \\ A y_2(x') y_1(x), & x < x' \end{cases}$$

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$$p(x) = 1 \Rightarrow A = \frac{1}{y_2' y_1 - y_1' y_2} = \frac{1}{ik + ik} = -\frac{i}{2k}$$

$$\text{and } G(x, x') = -\frac{i}{2k} \exp(i|x-x'|)$$

Integral equations

Consider the eigenvalue equation $\alpha y(x) = \lambda y(x)$ with α self-adjoint and $y(a) = y(b) = 0$ as an inhomogeneous ODE with $\lambda y(x)$ as the right hand side. Find the Green's function

$G(x, t)$ and write $y(x) = \lambda \int_a^b G(x, t) y(t) dt$

The ODE is converted to an integral equation.

It ~~also~~ satisfies the ODE since

$$\begin{aligned} \alpha_x y(x) &= \lambda \alpha_x \int_a^b G(x, t) y(t) dt = \lambda \int_a^b \alpha_x G(x, t) y(t) dt = \\ &= \lambda \int_a^b \delta(x-t) y(t) dt = \lambda y(x) \end{aligned}$$

$G(x, t)$ kernel with boundary conditions built in

Problems in two and three dimensions

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- A homogeneous PDE $\Delta \varphi(\underline{r}_1) = 0$ and its boundary conditions define a Green's function $G(\underline{r}_1, \underline{r}_2)$ as the solution to $\Delta G(\underline{r}_1, \underline{r}_2) = \delta(\underline{r}_1 - \underline{r}_2)$ subject to the relevant B.C.
- The solution $\varphi(\underline{r})$ to $\Delta \varphi(\underline{r}) = f(\underline{r})$ can be written
$$\varphi(\underline{r}_1) = \int G(\underline{r}_1, \underline{r}_2) f(\underline{r}_2) d^3 \underline{r}_2$$
 integrating over the entire space relevant to the problem
- When Δ with its B.C. define $\Delta \varphi = \lambda \varphi$ as Hermitian eigenvalue problem with eigenfctns $\varphi_n(x)$ and eigenvalues λ_n then $G(\underline{r}_1, \underline{r}_2) = G^*(\underline{r}_2, \underline{r}_1)$ symmetric
and
$$G(\underline{r}_1, \underline{r}_2) = \sum_n \frac{\varphi_n^*(\underline{r}_2) \varphi_n(\underline{r}_1)}{\lambda_n}$$
 eigenfunction expansion
- $G(\underline{r}_1, \underline{r}_2)$ continuous and differentiable for $\underline{r}_1 \neq \underline{r}_2$

Self-adjointness

$$\Delta \varphi(\underline{r}) = \nabla [p(\underline{r}) \nabla \varphi(\underline{r})] + q(\underline{r}) \varphi(\underline{r}) = f(\underline{r})$$

Eigenfunction expansion with parameter λ

Write $\Delta \varphi(\underline{r}) = \lambda \varphi(\underline{r})$ as $\Delta \varphi(\underline{r}) - \lambda \varphi(\underline{r}) = 0$

For the Green's function $\Delta \varphi(\underline{r}_1) - \lambda \varphi(\underline{r}_1) = \delta(\underline{r}_2 - \underline{r}_1)$

Eigenfunction expansion becomes
$$G(\underline{r}_1, \underline{r}_2) = \sum_n \frac{\varphi_n^*(\underline{r}_2) \varphi_n(\underline{r}_1)}{\lambda_n - \lambda}$$

The eigenvalues are found as poles of $G(\underline{r}_1, \underline{r}_2)$ (divergence).

Specific forms

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Laplace operator in 3-D with B.C. that G vanishes at infinity

$$\nabla_1^2 G(\underline{r}_1, \underline{r}_2) = \delta(\underline{r}_1 - \underline{r}_2) \quad , \quad \lim_{|\underline{r}_1| \rightarrow \infty} G(\underline{r}_1, \underline{r}_2) = 0$$

B.C. spherically symmetric and at infinity so we can assume $G(\underline{r}_1, \underline{r}_2)$ to be a function of $r_{12} = |\underline{r}_1 - \underline{r}_2|$

Integrate over spherical volume of radius a centered at \underline{r}_2

$$\int_{r_{12} < a} \nabla_1 \cdot \nabla_1 G(\underline{r}_1, \underline{r}_2) d^3 \underline{r}_1 = 1 \quad \leftarrow \text{from } \delta\text{-function}$$

Apply Gauss' theorem $\int_{r_{12}=a} \nabla_1 G(\underline{r}_1, \underline{r}_2) d\sigma_1 = 4\pi a^2 \left. \frac{dG}{dr_{12}} \right|_{r_{12}=a} = 1$

$$\therefore \frac{dG(\underline{r}_1, \underline{r}_2)}{dr_{12}} = \frac{1}{4\pi r_{12}^2} \quad \rightarrow \quad G(\underline{r}_1, \underline{r}_2) = -\frac{1}{4\pi} \frac{1}{|\underline{r}_1 - \underline{r}_2|}$$

Satisfies the B.C. at ∞

(otherwise a constant of integration can be added)

For different B.C. a suitable solution to the homogeneous equation can be added.

2-D: circular coordinates $\underline{s} = (s, \varphi)$ and infinite extent

$$\int_{s_{12}=a} \nabla_1 G(\underline{s}_1, \underline{s}_2) d\sigma_1 = 2\pi a \left. \frac{dG}{ds_{12}} \right|_{s_{12}=a} = 1 \quad \rightarrow \quad \frac{dG}{ds_{12}} = \frac{1}{2\pi s_{12}}$$

$$\text{and } G(\underline{s}_1, \underline{s}_2) = \frac{1}{2\pi} \ln |\underline{s}_1 - \underline{s}_2|$$

Table 10.1 3-D

Operator	Laplace ∇^2	Helmholtz $\nabla^2 + k^2$	Modified Helmholtz $\nabla^2 - k^2$
$G(\underline{r}_1, \underline{r}_2)$	$-\frac{1}{4\pi} \frac{1}{ \underline{r}_1 - \underline{r}_2 }$	$-\frac{\exp(ik \underline{r}_1 - \underline{r}_2)}{4\pi \underline{r}_1 - \underline{r}_2 }$	$-\frac{\exp(-k \underline{r}_1 - \underline{r}_2)}{4\pi \underline{r}_1 - \underline{r}_2 }$
B.C.	$G \rightarrow 0$ $r_{12} \rightarrow \infty$	outgoing wave	$G \rightarrow 0$ $r_{12} \rightarrow \infty$

Accommodating B.C.

1-D Laplace eq. $\frac{d^2 \varphi(x)}{dx^2} = 0$ with $G(x_1, x_2) = \frac{1}{2} |x_1 - x_2|$

we want $\varphi(0) = \varphi(1) = 0$. we can add terms of the form $f(x_1)g(x_2)$ ~~with~~ where $\frac{d^2 f}{dx_1^2} = 0$ and $\frac{d^2 g}{dx_2^2} = 0$ without affecting the continuity of G or the discontinuity of G' . f and g will be of the form $ax+b$

$$\begin{aligned} \text{Take } G(x_1, x_2) &= -\frac{1}{2}(x_1+x_2) + x_1 x_2 + \frac{1}{2}|x_1 - x_2| = \\ &= \begin{cases} -\frac{1}{2}(x_1+x_2) + x_1 x_2 + \frac{1}{2}(x_2 - x_1), & x_1 < x_2 \\ -\frac{1}{2}(x_1+x_2) + x_1 x_2 + \frac{1}{2}(x_1 - x_2), & x_2 < x_1 \end{cases} \end{aligned}$$

$$G(0, x_2) = -\frac{1}{2}x_2 + \frac{1}{2}x_2 = 0$$

$$G(1, x_2) = -\frac{1}{2}(1+x_2) + x_2 + \frac{1}{2}(1-x_2) = 0$$

Quantum Mechanical Scattering - Born Approximation

A beam of particles is moving along the negative z -axis towards a scattering potential $V(\underline{r})$ at the origin where a small fraction is scattered and goes out as a spherical wave

The Schrödinger eq. $-\frac{\hbar^2}{2m} \nabla^2 \varphi(\underline{r}) + V(\underline{r})\varphi(\underline{r}) = E\varphi(\underline{r})$ can be rearranged as

$$\nabla^2 \varphi(\underline{r}) + k^2 \varphi(\underline{r}) = \left[\frac{2m}{\hbar^2} V(\underline{r}) \varphi(\underline{r}) \right] \quad \text{with } k^2 = \frac{2mE}{\hbar^2}$$

Look for solutions having the asymptotic form

$$\varphi(\underline{r}) \sim e^{i\mathbf{k}_0 \cdot \underline{r}} + f_{\mathbf{k}}(\vartheta, \varphi) \frac{e^{ikr}}{r} \quad \leftarrow \text{spherical wave}$$

incident plane wave $\quad \leftarrow$ scattering amplitude gives cross-section

elastic scattering $|\mathbf{k}_0| = k$

$$|f_{\mathbf{k}}(\vartheta, \varphi)|^2$$

write the solution as

$$\varphi(\underline{r}_1) = \int \frac{2m}{\hbar^2} V(\underline{r}_2) \varphi(\underline{r}_2) G(\underline{r}_1, \underline{r}_2) d^3 \underline{r}_2$$

Use the Green's function for the Helmholtz operator

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$$G(\underline{r}_1, \underline{r}_2) = -\frac{1}{4\pi} \frac{e^{ik|\underline{r}_1 - \underline{r}_2|}}{|\underline{r}_1 - \underline{r}_2|}$$

which gives the correct asymptotic form

Add incident wave $e^{i\vec{k}_0 \cdot \underline{r}}$ (solution to the homogeneous eq.)

$$\text{Thus, } \psi(\underline{r}_1) = e^{i\vec{k}_0 \cdot \underline{r}_1} - \int \frac{2m}{\hbar^2} V(\underline{r}_2) \psi(\underline{r}_2) \frac{e^{ik|\underline{r}_1 - \underline{r}_2|}}{4\pi |\underline{r}_1 - \underline{r}_2|} d^3\underline{r}_2 \quad (\text{exact})$$

Lippmann-Schwinger eq.

For weak scattering, such that $e^{i\vec{k}_0 \cdot \underline{r}_1}$ dominates the solution we can approximate $\psi(\underline{r}_2)$ in the integral by $e^{i\vec{k}_0 \cdot \underline{r}_2}$ and find the Born approximation (1st order)

$$\psi_1(\underline{r}_1) = e^{i\vec{k}_0 \cdot \underline{r}_1} - \int \frac{2m}{\hbar^2} V(\underline{r}_2) \frac{e^{ik|\underline{r}_1 - \underline{r}_2|}}{4\pi |\underline{r}_1 - \underline{r}_2|} e^{i\vec{k}_0 \cdot \underline{r}_2} d^3\underline{r}_2$$

The second order is obtained by using $\psi_1(\underline{r}_1)$ in the Lippmann-Schwinger equation

$$\psi_2(\underline{r}_1) = e^{i\vec{k}_0 \cdot \underline{r}_1} - \int \frac{2m}{\hbar^2} V(\underline{r}_2) \frac{e^{ik|\underline{r}_1 - \underline{r}_2|}}{4\pi |\underline{r}_1 - \underline{r}_2|} \psi_1(\underline{r}_2) d^3\underline{r}_2 =$$

$$= \psi_1(\underline{r}_1) + \left(\frac{2m}{\hbar^2}\right)^2 \int V(\underline{r}_2) \frac{e^{ik|\underline{r}_1 - \underline{r}_2|}}{4\pi |\underline{r}_1 - \underline{r}_2|} d^3\underline{r}_2 \int V(\underline{r}_3) \frac{e^{ik|\underline{r}_2 - \underline{r}_3|}}{4\pi |\underline{r}_2 - \underline{r}_3|} e^{i\vec{k}_0 \cdot \underline{r}_3} d^3\underline{r}_3$$

and so on