

Time-dependent Green's function in \mathbb{R}^1

$$\left[i\hbar \frac{\partial}{\partial t} - H(t) \right] \psi(r,t) = \underbrace{S(r,t)}_{\text{"source" term}}$$

$$\left[i\hbar \frac{\partial}{\partial t} - H(t) \right] \underline{\underline{F(r,t; r', t')}} = \underbrace{i\hbar \delta(t-t') \delta^3(r-r')}_{\text{convention}}$$

time-dep Green's function

r,t : field point, r',t' : source point.

If F is found

$$\psi(r,t) = \underbrace{\psi_h(r,t)} + \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt' \int d^3r' F(r,t; r', t') S(r', t')$$

$$\left[i\hbar \frac{\partial}{\partial t} - H(t) \right] \psi_h(r,t) = 0$$

again the solution is not unique before we take B.C. into account.

\Rightarrow if ~~known~~ F known, we can break the driving term into a sum of δ -function contributions

outgoing time-dep. Green's function

$$k_+(r,t; r', t') = \theta(t-t') \langle r | U(t, t') | r' \rangle$$

$$\theta(z) = \begin{cases} 0 & z < 0 \\ 1 & z > 0 \end{cases} \quad \frac{\partial \theta}{\partial z} = \delta(z) \quad \int_{-a}^b dz \frac{\partial \theta}{\partial z} F(z) = \theta F(b) - \int_0^b \theta \frac{\partial}{\partial z} F(z) = - \int_0^b \frac{\partial}{\partial z} F(z) = -F(b) + F(0) = F(0)$$

$$i\hbar \frac{\partial}{\partial t} U(t, t') = H(t) U(t, t')$$

B.C. $\underline{U(t', t') = 1}$

$$i\hbar \frac{\partial}{\partial t} k_+ = i\hbar \delta(t-t') \langle r | U(t, t') | r' \rangle + \theta(t-t') \langle H \hat{U} U | r' \rangle$$

$$\underbrace{i\hbar \delta(t-t') \langle r | r' \rangle}_{\downarrow i\hbar \delta(t-t') \delta^3(r-r')} \quad \because \underbrace{H(t) \psi(r,t)}_{\text{x-repans}} = H(t) \langle r | U(t, t') | r' \rangle = \langle r | \hat{H} | \psi(t) \rangle$$

$$\Rightarrow \left[i\hbar \frac{\partial}{\partial t} - H(t) \right] k_+(r,t; r', t') = i\hbar \delta(t-t') \delta^3(r-r')$$

In dealing the path-integral $K(r, t, r', t') = \langle r | U(t, t') | r' \rangle$

we called K the propagator,

the outgoing Green's function $K_+ = \Theta(t-t') K$

is also called propagator, (outgoing) propagator advanced

but K is not a Green's function.

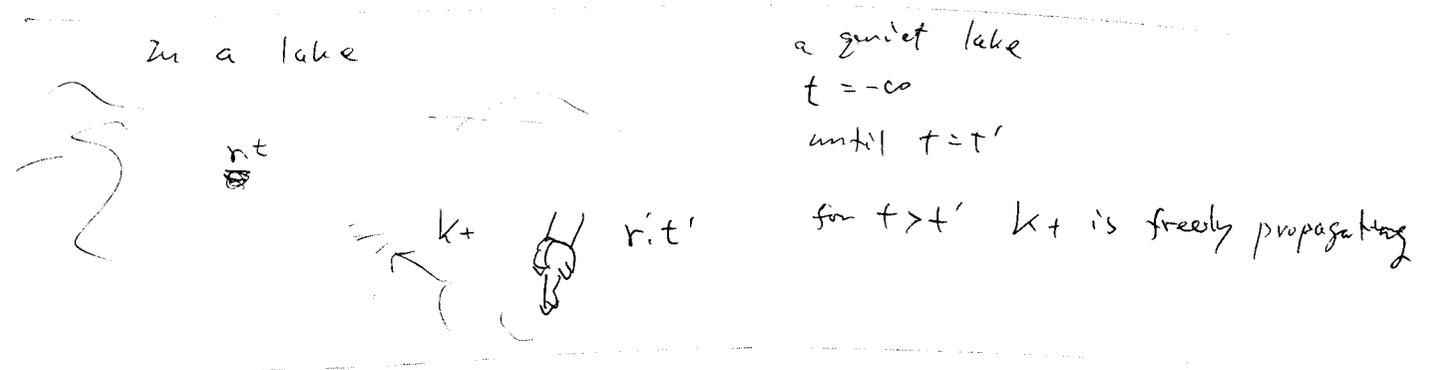
① K_+ vanish for $t < t'$.

② K_+ is a solution of the t -dep Schrödinger $\hat{H}\psi = E\psi$.

(RHS vanish for $t > t'$)

③ let $t \rightarrow t'$ from positive side, $K_+ \rightarrow \delta^3(r-r')$.

$\Rightarrow K_+$ is a solution of the t -dep Schrödinger $\hat{H}\psi = E\psi$ for $t > t'$ with the singular initial conditions, $\psi(r, t') = \delta^3(r-r')$ at $t=t'$



$$\psi(r, t) = \psi_h(r, t) + \int_{-\infty}^{\infty} dt' \int d^3r' K_+(r, t, r', t') S(r', t')$$

quiet $\psi_h = 0$, otherwise the $\Theta(t-t')$ function makes it

$$\int_{-\infty}^t dt' \int d^3r' K(r, t, r', t') S(r', t')$$

Green's eqn \rightarrow In Hilbert space, more general.
 $K_{\pm}(r, t, r', t') = \langle r | \hat{K}_{\pm}(t, t') | r' \rangle$

$$\hat{K}_{\pm}(t, t') = \pm \Theta(\pm(t-t')) U(t, t')$$

satisfy $[i\hbar \frac{\partial}{\partial t} - \hat{H}(t)] \hat{K}_{\pm}(t, t') = i\hbar \delta(t-t')$

Time-independent Hamiltonian

$$\hat{K}_{\pm}(t) = \pm \theta(\pm t) U(t)$$

$$(i\hbar \frac{\partial}{\partial t} - \hat{H}) \hat{K}_{\pm} = i\hbar \delta(t)$$

$$K_{\pm}(r, r', t) = \langle r | \hat{K}_{\pm}(t) | r' \rangle$$

free particle. $\hat{H} = \hat{p}^2 / 2m$

$$K_{0\pm}(r, r', t) = \pm \theta(\pm t) \left(\frac{m}{2\pi i \hbar t} \right)^{3/2} \exp\left(\frac{i}{\hbar} \frac{m(r-r')^2}{2t} \right)$$

$U(t, t') \rightarrow U(t-t')$
 { outgoing, advanced
 incoming, retarded

Energy-dependent Green's function in QM

$$(E - \hat{H}) \psi(r) = S(r)$$

time-independent source

eg. $\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(r)$, \hat{H} the operator acting on kets

$$(E - \hat{H}) G(r, r', E) = \delta^3(r-r')$$

just a parameter \rightarrow Energy-dependent Green's function
 not necessarily an eigenvalue of \hat{H} .

$$\psi(r) = \psi_h(r) + \int d^3r' G(r, r', E) S(r')$$

$$(E - \hat{H}) \psi_h(r) = 0$$

\rightarrow an eigenfunction of \hat{H} of energy E , (if E not eigenvalue, $\psi_h = 0$)

go to lake again



first lake was quiet for $t = -\infty \rightarrow 0$, dissipation ϵ
 $t = 0 \rightarrow \infty$ repeatedly periodic perturbation
 \Rightarrow to a standing wave with ω , $t \rightarrow \infty, \epsilon \rightarrow 0$
 $\omega \leftrightarrow E$
 when $\omega \approx \omega_h$ resonance \rightarrow



P.2: the propagator (is the Green's function)

$$\begin{aligned}
 K(x'', t; x', t_0) &= \langle x'', t | x', t_0 \rangle \\
 &= \langle x'' | \exp(-i\hat{H}(t-t_0)) | x' \rangle
 \end{aligned}$$

$$\begin{aligned}
 \left[-\left(\frac{\hbar^2}{2m}\right) \nabla''^2 + V(x'') - i\hbar \frac{\partial}{\partial t} \right] K(x'', t; x', t_0) \\
 = -i\hbar \delta^3(x'' - x') \delta(t - t_0)
 \end{aligned}$$

and $K(x'', t; x', t_0) = 0$ for $t < t_0$

It can be worked out

$$K(x'', t; x', t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \exp\left\{ \frac{im(x'' - x')^2}{2\hbar(t-t_0)} \right\}$$

Higher-order Born Approximate

$$V|\psi\rangle = T|\phi\rangle$$

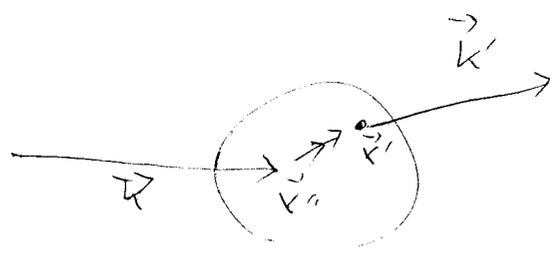
$$T = V + V \frac{1}{E - H_0 + i\epsilon} V + V \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V + \dots$$

$$f^{(1)}(\vec{k}', \vec{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \vec{k}' | V | \vec{k} \rangle$$

$$f^{(2)}(\vec{k}', \vec{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \vec{k}' | V \frac{1}{E - H_0 + i\epsilon} V | \vec{k} \rangle$$

$$f^{(2)} = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \int d^3x' d^3x'' \langle \vec{k}' | \vec{x}' \rangle V(x') \langle x' | \frac{1}{E - H_0 + i\epsilon} | x'' \rangle V(x'') \langle x'' | \vec{k} \rangle$$

$$= -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' d^3x'' e^{-i\vec{k}' \cdot x'} V(x') \frac{2m}{\hbar^2} G_+(x', x'') V(x'') e^{i\vec{k} \cdot x''}$$



$$\frac{\hbar^2}{2m} \langle \vec{x} | \frac{1}{E - H_0 + i\epsilon} | \vec{x}' \rangle = \frac{\hbar^2}{2m} \int d^3p' d^3p'' \langle x | p' \rangle \langle p' | \frac{1}{E - \frac{p'^2}{2m} + i\epsilon} | p'' \rangle \langle p'' | x' \rangle$$

$$= \frac{\hbar^2}{2m} \int d^3p' d^3p'' \frac{e^{i\frac{p' \cdot x}{\hbar}}}{(2\pi\hbar)^{\frac{3}{2}}} \frac{\delta^3(p' - p'')}{E - \frac{p'^2}{2m} + i\epsilon} \frac{e^{-i\frac{p'' \cdot x'}{\hbar}}}{(2\pi\hbar)^{\frac{3}{2}}}$$

$$= \frac{\hbar^2}{2m} \int \frac{d^3p'}{(2\pi\hbar)^3} \frac{e^{i\frac{p' \cdot (x - x')}{\hbar}}}{E - \frac{p'^2}{2m} + i\epsilon} = -\frac{1}{4\pi} \frac{e^{i\vec{k}(x - x')}}{|x - x'|}$$

The G_+ is nothing but the Green's function

$$(\nabla^2 + k^2) G_+(\vec{x}, \vec{x}') = \delta^3(\vec{x} - \vec{x}')$$

or the Lippmann-Schwinger E.g $H_0 | \phi \rangle = E | \phi \rangle$

$$| \psi \rangle = | \phi \rangle + \frac{1}{E - H_0 + i\epsilon} V | \psi \rangle$$

$$H \rightarrow H_0 + V$$

$$(H_0 + V) | \psi \rangle = E | \psi \rangle$$

Scattering, time-dep formulation

$$(i\hbar \frac{\partial}{\partial t} - H_0) | \psi(t) \rangle = V | \psi(t) \rangle$$

Like Solving the D.E with an inhomogeneous term by the Green's function
 This operator Schrödinger Eq is solved by introducing the Green's operator $\vec{G}_+(t, t')$, which satisfies $(i\hbar \frac{\partial}{\partial t} - H_0) \vec{G}_+(t, t') = \delta(t - t')$

In general, we have to solve

$$(\nabla^2 + k^2) \psi(r) = V(r) \psi(r)$$

suppose there exists a function $G(r)$ such that

$$(\nabla^2 + k^2) G(r) = \delta^3(r), \quad \text{Green's function of}$$

the operator $\nabla^2 + k^2$. then any function

$$\psi(r) = \underbrace{\psi_0(r)}_{(\nabla^2 + k^2) \psi_0 = 0} + \int d^3r' G(r-r') U(r') \psi(r') \quad \text{is the solution.}$$

$$G_{\pm}(r) = -\frac{1}{4\pi} \frac{e^{\pm i k r}}{r}$$

G_+ : outgoing
 G_- : incoming
 Green's functions

~~$\nabla^2 = \left(\frac{1}{r} \frac{d^2}{dr^2} r \right)$ spherical coordinate.~~
 $\nabla^2 = \nabla \cdot \vec{\nabla} = \partial_x^2 + \partial_y^2 + \partial_z^2$

~~$\nabla^2 G_{\pm}(r) = -\frac{1}{4\pi r} (-k^2) e^{\pm i k r} - \frac{1}{4\pi} \frac{\partial^2}{\partial r^2} \left(\frac{1}{r} \right) e^{\pm i k r}$~~
 $= -4\pi \delta^3(\vec{r})$

$\propto \vec{E}(r)$ of a point charge at origin
 $\nabla \cdot \vec{\nabla} \left(\frac{1}{r} \right) \propto \nabla \cdot \vec{E} = \rho(r) = A \delta^3(r)$

$$\int dV \nabla \cdot \vec{\nabla} \left(\frac{1}{r} \right) = A$$

$$= \oint_{da} -\frac{\hat{r}}{r^2} \cdot da$$

$$-\frac{4\pi R^2}{R^2} = A$$

For $r \neq 0$

$$\nabla^2 G_{\pm} = -\frac{1}{4\pi} \partial_x \left(-\frac{x}{r^2} e^{\pm i k x} \pm i k_x \frac{1}{r} e^{\pm i k x} \right)$$

$$= -\frac{1}{4\pi} \left[-\frac{x}{r^2} e^{\pm i k x} + \frac{2x^2}{r^4} e^{\pm i k x} \pm i k_x x \frac{1}{r^2} e^{\pm i k x} - k_x^2 \frac{1}{r} e^{\pm i k x} \right]$$

$$\partial_x^2 \left(-\frac{1}{4\pi} \frac{1}{r} e^{\pm i k x} \right)$$

$$= -\frac{1}{4\pi} \left[-\frac{3}{r^3} + \frac{2}{r^2} \pm 2i k_x \frac{x}{r^2} - \frac{k_x^2}{r} \right] e^{\pm i k x}$$

$$= -\frac{1}{4\pi} \partial_x \left(-\frac{x}{r^2} e^{\pm i k x} \pm i k_x \frac{1}{r} e^{\pm i k x} \right)$$

$$= \dots -\frac{1}{4\pi} \left(-\frac{x}{r^2} (\pm i k_x) e^{\pm i k x} - \frac{x}{r^2} (\pm i k_x) e^{\pm i k x} \right) + \dots$$

$$= \dots + \frac{2}{4\pi} \frac{x \vec{r} \cdot \vec{k}}{r^2} e^{\pm i k x} + \dots$$

Wenn $r \neq 0$,

$\nabla^2 = \frac{1}{r} \frac{d^2}{dr^2} r$ in spherical coordinates

$$\nabla^2 \left(\frac{e^{\pm ikr}}{r} \right) = \frac{1}{r} \frac{d^2}{dr^2} (e^{\pm ikr}) = -k^2 \frac{e^{\pm ikr}}{r}$$

$$\Rightarrow (\nabla^2 + k^2) \left(\frac{e^{\pm ikr}}{r} \right) = 0$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

In Cartesian coordinates.

$$\begin{aligned} \nabla^2 &= \sum \partial_x^2 \\ &= \partial_x \left(-\frac{x}{(x^2+y^2+z^2)^{\frac{3}{2}}} e^{\pm ikr} + \frac{\pm ikx}{(x^2+y^2+z^2)^{\frac{1}{2}}} e^{\pm ikr} \right) \\ &= \left(\frac{1}{(x^2+y^2+z^2)^{\frac{3}{2}}} e^{\pm ikr} + \frac{3x^2}{(x^2+y^2+z^2)^{\frac{5}{2}}} e^{\pm ikr} + \frac{ikx}{(x^2+y^2+z^2)^{\frac{3}{2}}} e^{\pm ikr} - \frac{kx^2}{(x^2+y^2+z^2)^{\frac{1}{2}}} e^{\pm ikr} \right) \\ &\Rightarrow -\frac{3}{r^3} e^{\pm ikr} + \frac{3x^2}{r^5} e^{\pm ikr} + \frac{2ikx}{r^3} e^{\pm ikr} - \frac{k^2}{r} e^{\pm ikr} \end{aligned}$$

$$\begin{aligned} \partial_x \left(\frac{e^{\pm ik\sqrt{x^2+y^2+z^2}}}{\sqrt{x^2+y^2+z^2}} \right) &= \partial_x \left(-\frac{x}{(x^2+y^2+z^2)^{\frac{3}{2}}} e^{\pm ikr} + \frac{\pm ikz}{2\sqrt{x^2+y^2+z^2}} \frac{e^{\pm ikr}}{\sqrt{x^2+y^2+z^2}} \right) \\ &= \partial_x \left(-\frac{x}{(r^2)^{\frac{3}{2}}} e^{\pm ikr} + \frac{\pm ikz}{(r^2)^{\frac{1}{2}}} e^{\pm ikr} \right) \\ &= \left(-\frac{1}{(r^2)^{\frac{3}{2}}} e^{\pm ikr} + 3 \frac{x^2}{(r^2)^{\frac{5}{2}}} e^{\pm ikr} - \frac{x}{(r^2)^{\frac{3}{2}}} \frac{\pm ikz}{(r^2)^{\frac{1}{2}}} e^{\pm ikr} \right. \\ &\quad \left. \pm \frac{ikz}{(r^2)^{\frac{1}{2}}} e^{\pm ikr} + \frac{ikz}{(r^2)^{\frac{1}{2}}} \frac{2x^2}{(r^2)^{\frac{1}{2}}} e^{\pm ikr} - \frac{k^2}{(r^2)^{\frac{1}{2}}} \frac{x^2}{(r^2)^{\frac{1}{2}}} e^{\pm ikr} \right) \\ &\Rightarrow \left(-\frac{3}{r^3} e^{\pm ikr} + \frac{3x^2}{r^5} e^{\pm ikr} + \frac{2ikz}{r^3} e^{\pm ikr} + \frac{ikz}{r^3} e^{\pm ikr} + \frac{2ikz}{r^4} e^{\pm ikr} - \frac{k^2}{r^3} e^{\pm ikr} \right) \\ &\quad \left(+ \frac{ikz}{r^4} e^{\pm ikr} + \frac{2ikz}{r^2} e^{\pm ikr} - \frac{k^2}{r^3} e^{\pm ikr} \right) \end{aligned}$$

$$\Rightarrow (\nabla^2 + k^2) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r} = -4\pi\delta^3(\mathbf{r})$$

Shift the origin to \mathbf{r}'

$$\Rightarrow (\nabla^2 + k^2) \frac{e^{+ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = -4\pi\delta^3(\mathbf{r}-\mathbf{r}')$$

The Schrödinger Eq can be written in a similar form

$$(\nabla^2 + k^2) \psi_k(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r}) \psi_k(\mathbf{r})$$

$$\Rightarrow \psi_k^+(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi} \int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \frac{2m}{\hbar^2} V(\mathbf{r}') \psi_k^+(\mathbf{r}') d^3\mathbf{r}'$$

In Born approximation

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \tilde{V}(\mathbf{k}' - \mathbf{k})$$

Coulomb scattering

$$V(r) = \frac{ze^2}{r}$$

$$\tilde{V}(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{r}} V(r) d^3r$$

since $\nabla^2 V(r) = -4\pi ze^2 \delta^3(r)$

in the k-space

$$-q^2 \tilde{V}(\mathbf{q}) = -4\pi ze^2$$

$$\text{or } \tilde{V}(\mathbf{q}) = \frac{4\pi ze^2}{q^2}$$

$$\Rightarrow f(\theta) = -\frac{ze^2}{\frac{\hbar^2 k^2}{2m} \frac{180^\circ}{4\pi}} \quad \ominus \quad |\mathbf{q}| = 2k \sin \frac{\theta}{2}$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \left(\frac{ze^2}{\hbar^2 c} \right)^2 \frac{1}{16 \sin^4 \frac{\theta}{2}}$$

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

their Fourier transforms are

$$G(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int e^{i\vec{g} \cdot (\vec{r} - \vec{r}')} \tilde{G}(\vec{g}) d^3g$$

$$\delta(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int e^{i\vec{g} \cdot (\vec{r} - \vec{r}')} d^3g$$

$$\left(\frac{1}{(2\pi)^3} \right) (-\vec{g}^2 + k^2) \tilde{G}(\vec{g}) d^3g = \frac{1}{(2\pi)^3} \int e^{i\vec{g} \cdot (\vec{r} - \vec{r}')} d^3g$$

$$\text{or } (-\vec{g}^2 + k^2) \tilde{G}(\vec{g}) = 1 \Rightarrow \tilde{G}(\vec{g}) = \frac{1}{k^2 - \vec{g}^2}$$

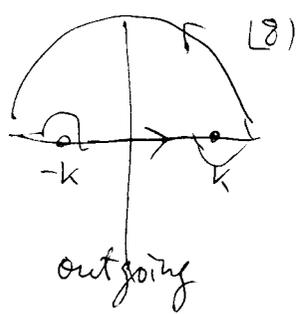
$$\text{Then } G(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{g} \cdot (\vec{r} - \vec{r}')}}{k^2 - \vec{g}^2} d^3g$$

$$= \frac{1}{(2\pi)^3} \int_0^\infty \frac{g^2 dg}{k^2 - g^2} \int_0^{2\pi} d\phi \int_{-1}^1 d\cos\theta e^{i g |\vec{r} - \vec{r}'| \cos\theta}$$

$$= \frac{1}{4\pi^2} \int_0^\infty \frac{g^2 dg}{k^2 - g^2} \frac{e^{i g |\vec{r} - \vec{r}'|} - e^{-i g |\vec{r} - \vec{r}'|}}{i g |\vec{r} - \vec{r}'|}$$

$$= \frac{1}{i 4\pi^2 |\vec{r} - \vec{r}'|} \int_0^\infty \frac{g dg}{(k^2 - g^2)} (e^{i g |\vec{r} - \vec{r}'|} - e^{-i g |\vec{r} - \vec{r}'|})$$

$$= \frac{1}{4\pi^2 i |\vec{r} - \vec{r}'|} \int_{-\infty}^\infty \frac{g dg}{(k^2 - g^2)} e^{i g |\vec{r} - \vec{r}'|}$$



$$G_+ = -\frac{1}{4\pi} \frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}$$

$$G_- = -\frac{1}{4\pi} \frac{e^{-ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}$$