Green function for the inhomogeneous wave equation: 11/25

Last time we found $G^{\pm}(\bar{x}, \bar{x}', t, t')$.

How are these functions used?

If at $t \to -\infty$ there is a wave $\psi_{in}(\bar{x}, t)$ that satisfies the homogeneous wave equation

$$\nabla^2 \psi_{in} - \frac{1}{c^2} \frac{\partial^2 \psi_{in}}{\partial t^2} = 0 \qquad (1)$$

The solution to ① is a plane wave:

$$\psi_{in}(\bar{x}, t) \propto e^{-i(\bar{k}\cdot\bar{x} - \omega t)}$$

If at time t_0 we turn on a source $f(\bar{x}, t)$ then:

$$\psi(\bar{x}, t) = \psi_{in}(\bar{x}, t) + \frac{1}{4\pi}\iint_{t_0}^{\infty} G^{+}(\bar{x}, \bar{x}', t, t')\, f(\bar{x}', t')\, d^3x'\, dt'$$

$\int$ all space. t_0 vanishes for any $t < t'$!

Helmholz equation

Solution in an arbitrary basis:

$$\nabla^2 \psi(\bar{r}) + k^2 \psi(\bar{r}) = \rho(\bar{r}) \qquad (1)$$

We know that

$$\psi(\bar{r}) = \frac{1}{4\pi} \int \rho(\bar{r}') G(\bar{r}, \bar{r}')\, dr' + \underbrace{\text{surface terms}}_{0 \text{ if } V \to \infty.} \qquad (2)$$

We also know that G solves:

$$\nabla^2 G(\bar{r}, \bar{r}') + k^2 G(\bar{r}, \bar{r}') = \delta(\bar{r} - \bar{r}') \qquad (3)$$

Assume that there is a set of orthogonal functions $\{\phi_n(\bar{r})\}$ that solve the homogeneous Helmholtz eq.:

$$\nabla^2 \phi_n(\bar{r}) + k_n^2 \phi_n(\bar{r}) = 0 \qquad (4)$$

Now we will expand $\psi(\bar{r})$ in terms of $\phi_n(\bar{r})$. Then:

$$\psi^{\text{homogeneous}}(\bar{r}) = \sum_n A_n \phi_n(\bar{r}) \qquad (5)$$

We also can write:

$$G(\bar{r},\bar{r}') = \sum_{m=0}^{\infty} a_m(\bar{r}')\,\phi_m(\bar{r}) \qquad (6)$$

$$\delta(\bar{r}-\bar{r}') = \sum_{m=0}^{\infty} \phi_m^*(\bar{r})\,\phi_m(\bar{r}')$$ completitude property. (7)

Plugg (7) and (6) in (3):

$$\nabla^2\left[\sum_{m=0}^{\infty} a_m(\bar{r}')\,\phi_m(\bar{r})\right] + k^2\sum_{m=0}^{\infty} a_m(\bar{r}')\,\phi_m(\bar{r})$$

$$= \sum_{m=0}^{\infty} \phi_m^*(\bar{r})\,\phi_m(\bar{r}') \qquad (8)$$

From (4) $\nabla^2\phi_m(\bar{r}) = -k_m^2\,\phi_m(\bar{r})$

$$\sum_{n=0}^{\infty} a_n(\bar{r}')(-k_n^2)\phi_n(\bar{r}) + k^2 \sum_{n=0}^{\infty} a_n(\bar{r}')\phi_n(\bar{r})$$

$$= \sum_{n=0}^{\infty} \phi_n^*(\bar{r}')\phi_n(\bar{r})$$

Since $\phi_n(\bar{r})$ are orthogonal I get that

$$a_n(\bar{r}')(k^2 - k_n^2) = \phi_n^*(\bar{r}')$$

$$a_n(\bar{r}') = \frac{\phi_n^*(\bar{r}')}{(k^2 - k_n^2)} \qquad 9$$

Plugging 9 in 6 :

$$G(\bar{r},\bar{r}') = \sum_{n=0}^{\infty} \frac{\phi_n^*(\bar{r}')\,\phi_n(\bar{r})}{k^2-k_n^2} \qquad (10)$$

If $\{\phi_n(\bar{r})\} \rightarrow \{e^{-ikx}\}$

We have:

$$(\nabla^2+k^2)\,G(x,x') = \delta(x-x') \qquad (11)$$

and $\nabla^2 e^{-ikx} + k^2 e^{-ikx} = 0$

Then

$$\psi^{\text{homogeneous}}_{(x)} = \frac{1}{\sqrt{2\pi}} \int a_k e^{-ikx} dk$$

Then

$$G(x, x') = \int a_k(x') e^{-ikx} dk \qquad (12)$$

$$\delta(\bar{x} - \bar{x}') = \frac{1}{2\pi} \int e^{-i(x-x')k} dk \qquad (13)$$

Plugging (12) and (13) in (11):

$$(\nabla^2 + k^2) \int a_{k'}(x') e^{-ik'x} dk' = \frac{1}{2\pi} \int e^{-i(x-x')k'} dk'$$

$$-\int \left(a_{k'}(x')\, k'^2 e^{-ik'x} + k^2 a_{k'}(x')\, e^{-ik'x}\right) dk' =$$

$$= \frac{1}{2\pi} \int e^{-i(x-x')k'} dk'$$

$$\int a_{k'}(x')\,(k^2 - k'^2)\, e^{-ik'x}\, dk' = \frac{1}{2\pi} \int e^{-ix'k'} e^{-ixk'} dk'$$

$$a_{k'}(x')\,(k^2 - k'^2) = \frac{e^{-ix'k'}}{2\pi}$$

$$a_{k'}(x') = \frac{e^{-ix'k'}}{2\pi\,(k^2 - k'^2)} \qquad 14$$

Plugging (14) in (12):

$$G(x,x') = \frac{1}{2\pi}\int \frac{e^{-ik'x'}}{k^2-k'^2}\, e^{ik'x}\, dk' =$$

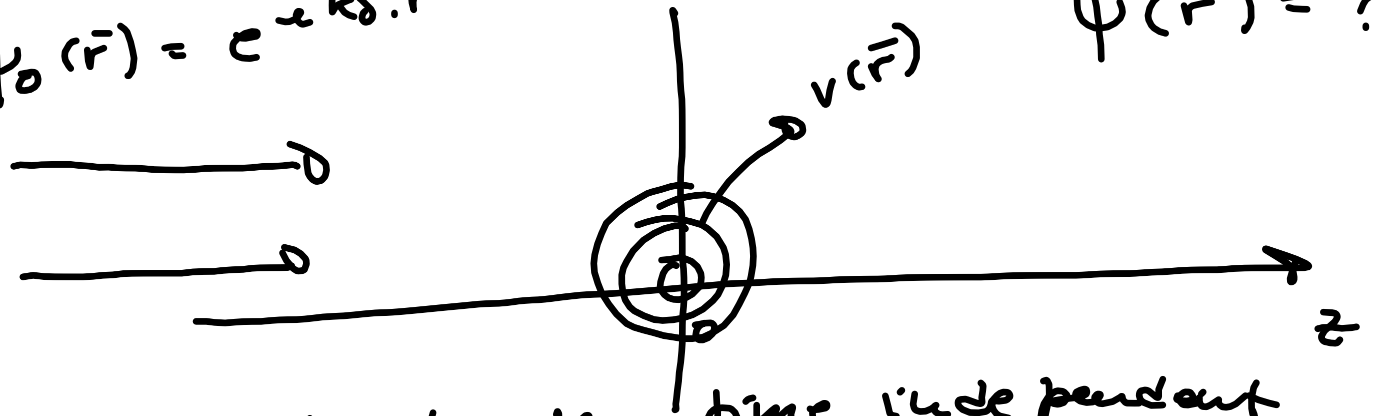
$$= \frac{1}{2\pi}\int \frac{e^{-ik'(x'-x)}}{k^2-k'^2}\, dk' =$$

$$= \frac{e^{ik|x-x'|}}{4\pi|x-x'|}$$

this is the same $G(x,x')$ that we found before.

Example: Quantum Mechanical Scattering.

$\psi_0(\bar{r}) = e^{-i\bar{k}_0\cdot\bar{r}}$ $\psi(\bar{r}) = ?$



We need to solve the time independent Schrödinger eq:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\bar{r}) + V(\bar{r})\,\psi(\bar{r}) = E\,\psi(\bar{r}) \qquad (1)$$

For a free particle $V(\bar{r}) = 0$ and (1) becomes

$$-\frac{\hbar^2}{2m} \nabla^2 e^{i\bar{k}_0 \cdot \bar{r}} = E\, e^{i\bar{k}_0 \cdot \bar{r}}$$

$$\frac{\hbar^2 k_0^2}{2m} = E \qquad (2) \qquad \hbar k = p \text{ momentum}$$

$$E = \frac{p^2}{2m}$$ all kinetic energy.

Let's plugs (2) in (1) and multiply by $\left(-\frac{2m}{\hbar^2}\right)$

$$\nabla^2 \psi(\bar{r}) + k^2 \psi(\bar{r}) = -\underbrace{\left(-\frac{2m}{\hbar^2} V(\bar{r})\, \psi(\bar{r})\right)}_{f(\bar{r})} \quad (3)$$

$f(\bar{r})$ "source" of the perturbation ($V(\bar{r})$).

(3) is the inhomogeneous Helmholz equation. Then,

$$\psi(\bar{r}) = \frac{1}{4\pi} \int f(\bar{r}')\, G(\bar{r}, \bar{r}')\, dr' \quad (4)$$

with

$$G(\bar{r}, \bar{r}') = \frac{e^{-i\bar{k}\cdot(\bar{r}-\bar{r}')}}{|\bar{r}-\bar{r}'|} \quad (5)$$

Replacing (5) and (3) in (4):

$$\psi(\bar{r}) = -\frac{2m}{4\pi\hbar^2}\int V(\bar{r}')\,\psi(\bar{r}')\,\frac{e^{-i\bar{k}\cdot(\bar{r}-\bar{r}')}}{|\bar{r}-\bar{r}'|}\,d^3r' \qquad (6)$$

(6) should be solved self-consistently.

You start with $\psi(\bar{r}') = \psi_0(\bar{r}') = e^{i\bar{k}\cdot\bar{r}'}$

find $\psi(\bar{r})$ plug it back in (6) and continue

until $|\psi_N(\bar{r}) - \psi_{N-1}(\bar{r})| < \varepsilon$ (N = iteration).

If $V(\bar{r})$ is very weak we can say that

$\psi(\bar{r}) = \psi_0(\bar{r})$ + small corrections (Born approximation).

$$\psi(\bar{r}) \approx e^{i\bar{k}_0\cdot\bar{r}} - \frac{2m}{4\pi k^2}\int V(\bar{r})\,\underbrace{e^{i\bar{k}_0\cdot\bar{r}'}}_{\psi_0(\bar{r}')}\,\frac{e^{-i\bar{k}\cdot(\bar{r}-\bar{r}')}}{|\bar{r}-\bar{r}'|}\,d^3r'$$

Convolution

$$(f * g)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y)\, f(x-y)\, dy \qquad (1)$$

Convolution of f with g and

$f(x-y)$: weight function.

$f(x)$ and $g(x)$ are well-behaved functions with FT given by $F(k)$ and $G(k)$.

Examples of convolutions:

- $\phi(\bar{r}) = \frac{1}{4\pi\epsilon_0}\int_{-\infty}^{\infty} \rho(\bar{r}')\, G(\bar{r}-\bar{r}')\, d^3r'$

ϕ is the convolution of ρ with G and G is the weight-function.

- $\langle y^2 \rangle = \int y^2 f(y)\, dy$

the weight function $f(y)$ is the distribution function: $f(y)=1$ if the distribution of y is uniform in the interval.
Or $f(y) = e^{-\alpha y^2}$ if the distribution is gaussian, etc.

We can use FT to evaluate convolutions.

Consider $(f * g)(x)$:

(i)

$$(f*g)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y)\, f(x-y)\, dy =$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} g(y) \int_{-\infty}^{\infty} F(k)\, e^{-ik(x-y)}\, dk\, dy =$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k) \Bigg[\underbrace{\int_{-\infty}^{\infty} g(y)\, e^{iky}\, dy}_{\sqrt{2\pi}\, G(k)} \Bigg] e^{-ikx}\, dk =$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, G(k)\, e^{-ikx}\, dk \qquad ②$$

We see that the antifourier transform of the product of the FT is the convolution of the original functions.

Properties: if $x=0$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(-y)\, g(y)\, dy = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, G(k)\, dk$$

- Perseval relation:

Calculate

$$\int_{-\infty}^{\infty} F(k)\, G^*(k)\, dk = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx} dx \,.$$

$$\cdot \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g^*(x')\, e^{+ikx'} dx'\, dk =$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g^*(x') f(x)\, dx\, dx' \underbrace{\int_{-\infty}^{\infty} e^{-ik(x-x')} dk}_{2\pi\,\delta(x-x')}$$

$$= \int_{-\infty}^{\infty} g^*(x) f(x)\, dx \quad (3)$$

If $G^*(k) \equiv F^*(k)$:

$$\int_{-\infty}^{\infty} F(k)\, F^*(k)\, dk = \int_{-\infty}^{\infty} |F(k)|^2\, dk$$

and if $\int_{-\infty}^{\infty} |F(k)|^2\, dk = 1$ then we see

that from 5:

$$\int_{-\infty}^{\infty} |f(x)|^2\, dx = 1$$

Application: Momentum representation.

In quantum mechanics:

$$|\psi(x)|^2 dx = \psi^*(x)\,\psi(x)\,dx \rightarrow$$ probability of finding the particle represented by $\psi(x)$ in the interval $(x, x+dx)$.

$\psi(x)$: wave function.

Then

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$ since the particle has to be somewhere.

Now we can evaluate $\langle x \rangle$:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx$$

What will be the function $g(p)$ [p is the momentum and $p = \hbar k$ where k is the conjugate variable of x via FT], which will allow us to obtain $\langle p \rangle$ the average momentum of the particle so that

$$\langle p \rangle = \int_{-\infty}^{\infty} g^*(p)\, p\, g(p)\, dp \ ?$$ with

$|g(p)|^2 dp$ the probability of the particle having momentum between p and $p+dp$

and with

$$\int_{-\infty}^{\infty} |g(p)|^2 \, dp = 1.$$