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Helmholz equation

Solution in arbitrary basis:

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

we know that

$$\psi(\bar{r}) = \frac{1}{4\pi} \int \rho(\bar{r}') \, G(\bar{r}, \bar{r}') \, dr' + \text{surface terms} \qquad ②$$

0 if V = all space

We know that $G(\bar{r}, \bar{r}')$ solves:

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

Assume that $\{\phi_n(\bar{r})\}$ are a set of orthonormal functions that solve the homogeneous equation so that

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

$\phi_n(\bar{r})$ can be Bessel functions or sines, etc.

Now we can expand $\psi(\bar{r})$ [the solution of (1) with $\rho(\bar{r})=0$] in terms of $\{\phi_n(\bar{r})\}$ so that

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

Also we can write:

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

and

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

completitude property

Plugging (7), (6), in (3):

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

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

Using (4) in (8) $\left[\nabla^2 \phi_n = -k_n^2 \phi_n \right]$:

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

$$= \sum_n \phi^*_n(\bar{r}') \phi_n(\bar{r})$$

Comparing coefficients of the orthogonal ϕ_n's:

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

$$a_n(\bar{r}')\left[k^2 - k_n^2\right] = \phi^*_n(\bar{r}')$$

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

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 $\{\phi_n(\bar{r})\} \longrightarrow \{e^{ikx}\}$

We have:

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

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

solve the homogeneous eq.

Then

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

Then

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

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

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

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

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

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

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

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

$$\therefore \quad a_{k'}(x') = \frac{e^{-ik'x'}}{2\pi (k^2 - k'^2)} \qquad 14$$

Plugging (14) in (12):

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

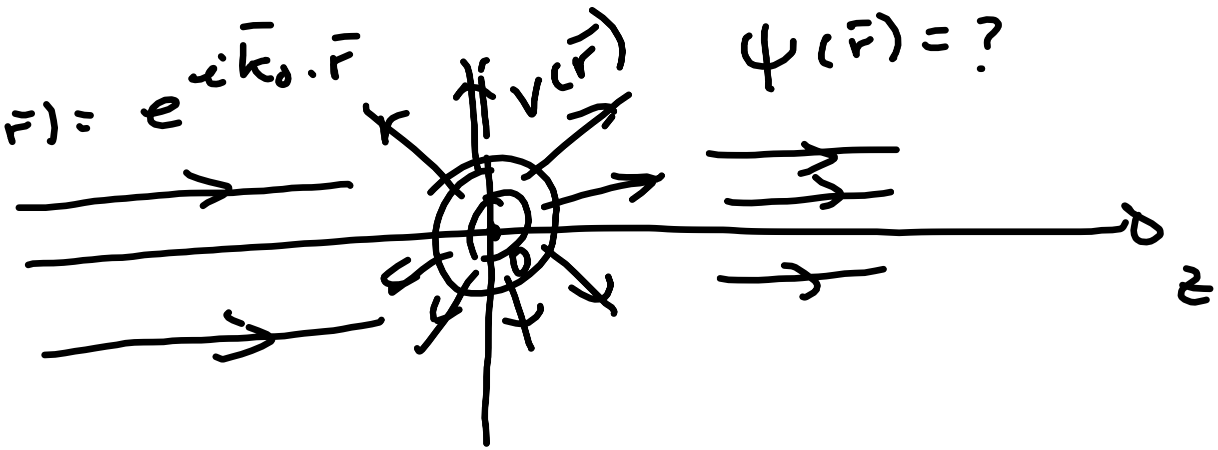
$$= \frac{1}{2\pi}\int \frac{e^{-ik'(x'-x)}}{k^2-k'^2}\, dk' =$$

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

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

Example: Quantum Mechanical Scattering.

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



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

For free particles $E = \dfrac{\hbar^2 k^2}{2m} \equiv \dfrac{p^2}{2m}$ (2)

Replacing ② in ① and multiplying by $\frac{2m}{\hbar^2}$:

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

"source" of perturbation

③ is the inhomogeneous Helmholtz equation. Then

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

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

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

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

$\psi(\bar{r})$ has to be found self-consistently

but if $V(\bar{r})$ is very weak we can use the

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

Then

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

Convolution

$$(f * g)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) \underbrace{f(x-y)}_{\text{weight function.}} \, dy \quad (1)$$

convolution of f with g.

$f(x)$ and $g(x)$ have to be "well-behaved" functions of x with Fourier transforms $F(k)$ and $G(k)$.

Examples:

$$\phi(\bar{r}) = \frac{1}{4\pi\varepsilon_0} \int_{-\infty}^{\infty} \rho(\bar{r}') \, G(\bar{r}-\bar{r}') \, dr'$$

convolution of ρ with G.

for $\rho(r)$ in isotropic space

$$\langle y^2 \rangle = \int y^2 \underbrace{f(y)}_{\text{weight function with } x=0} dy$$

average value of y^2 is a convolution of y^2 with the weight function.

Let's use FT to evaluate $(f * g)(x)$:

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

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

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

(1) shows that the anti FT of the product of FT is the convolution of the original functions.

Properties:

- If $x=0$ (1) and (2) become

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

$$\int e^{-ik(x-x')}\, dk = \underset{\times 2\pi}{\delta(x-x')}$$

- Perseval relations:

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

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

Then

$$\int_{-\infty}^{\infty} F(k)\, G^*(k)\, dk = \int_{-\infty}^{\infty} f(x)\, g^*(x)\, dx \qquad 3$$

If $G^*(k) = F^*(k) \Rightarrow$

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

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

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

Application: Momentum representation

In Quantum Mechanics:

$$|\psi(x)|^2 dx = \psi^*(x)\,\psi(x)\,dx$$

represents the probability of finding a particle between x and $x+dx$

Then

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

since the particle has to be somewhere.

Now we can evaluate

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

What is $g(p)$ which will allow us to get $\langle p \rangle$ (average value of p) by evaluating

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

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

then:

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

$$FT\ \psi(x) = g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx}\, dx \quad (*)$$

$$\lambda = \frac{h}{p} \quad \text{(de Broglie assumption)}$$

λ: wavelength, h: Planck's c., p: momentum

$$k = \frac{2\pi}{\lambda} \quad \text{then} \quad \frac{2\pi}{k} = \frac{h}{p} \quad \therefore \boxed{p = \frac{h}{2\pi} k = \hbar k} \quad (**)$$

k: wave number

Combining (**) and (*):

$$g(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-i\frac{px}{\hbar}}\, dx$$

and

$$g^*(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi^*(x)\, e^{\frac{ipx}{\hbar}}\, dx .$$

$$\langle p \rangle = \int_{-\infty}^{\infty} g^*(p)\, p\, g(p)\, dp \overset{?}{=} \int_{-\infty}^{\infty} \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi(x)\, dx$$

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$$\langle p \rangle = \int_{-\infty}^{\infty} \frac{1}{2\pi\hbar} \iint \psi^*(x')\, e^{ipx'/\hbar}\, p\, \psi(x)\, e^{-ipx/\hbar}\, dp\, dx\, dx'$$

$$= \frac{1}{2\pi\hbar} \iint \psi^*(x')\, \psi(x) \underbrace{\int_{-\infty}^{\infty} p\, e^{ip(x'-x)/\hbar}\, dp}_{?}\, dx\, dx'$$

$$\hbar \int_{-\infty}^{\infty} e^{ik(x'-x)} dk = 2\pi \hbar \, \delta(x'-x)$$

$$\frac{d}{dx} \int_{-\infty}^{\infty} e^{ip(x'-x)/\hbar} dp = 2\pi \hbar \, \delta'(x'-x)$$

$$\shortparallel$$

$$-\int_{-\infty}^{\infty} \frac{ip}{\hbar} e^{ip(x'-x)/\hbar} dp$$

Then

$$\langle p \rangle = \frac{2\pi i \hbar^2}{2\pi \hbar} \iint \psi^*(x') \psi(x) \delta'(x'-x) \, dx \, dx' =$$

$$= -i\hbar \int \psi^*(x') \frac{\partial \psi}{\partial x'} dx' = \langle p \rangle$$