Chapter 10
Fourier Transform

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(Date: October 26, 2010)

10.1. Fourier transformation and inverse Fourier transform

Jean Baptiste Joseph Fourier (21 March 1768 – 16 May 1830) was a French mathematician and physicist best known for initiating the investigation of Fourier series and their applications to problems of heat transfer and vibrations. The Fourier transform and Fourier's Law are also named in his honour. Fourier is also generally credited with the discovery of the greenhouse effect.

http://en.wikipedia.org/wiki/Joseph_Fourier

10.1.1 Definition-1

The Fourier transform is defined by

$$F(\omega) = \mathbf{F}[f(t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} f(t) dt .$$

$$f(t) = \mathbf{F}^{-1}[F(\omega)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} F(\omega) d\omega \,.$$

where ***F*** is the operator for the Fourier transform and ***F***$^{-1}$ is the operator for the inverse Fourier transform.

((**Proof**))

$$I_1 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} d\omega F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} d\omega \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t'} f(t') dt' ,$$

or

$$I_1 = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t') dt' \int_{-\infty}^{\infty} e^{i\omega(t-t)'} d\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t') 2\pi\delta(t-t') dt' = f(t) \,.$$

((Note))

We note the Dirac delta function which is given by

$$\int_{-\infty}^{\infty} e^{i\omega(t-t')} d\omega = 2\pi\delta(t-t') \,.$$

10.1.2 Defintion of Fourier transform in Mathematica

In the Mathematica, the Fourier transform (default) is defined as the conventional one (denoted as type-I),

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} f(t) dt$$

and

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} F(\omega) d\omega \,.$$

We use the following Mathematica commands for the calculation of Fourier transform (type I);

FourierTransform[*f*[*t*], *t*, ω]	Fourier transform of *f*(*t*)
InverseFourierTransform[*F*[ω], ω, *t*]	Inverse Fourier transform of *F*(ω)

However, the definition of the Fourier transform (denoted as type II) in the *x*-*k* representation of the quantum mechanics (which will be discussed later) is different from that for the type I;

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

and

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

where *x* is the position and *k* is the wave number. In the calculation of such a Fourier transform we need to use the Mathematica commands in the following way.

FourierTransform[*f* [*x*], *x*, *k*, FourierParameters→{0,-1}]
InverseFourierTransform[*F*(*k*), *k*, *x*, FourierParameters→{0,-1}]

((**Note**))
In physics, the plane waves travelling in the positive *x* direction can be described by

$$\psi(x,t) = \langle x|\psi\rangle = \int dk \int d\omega \langle k|\psi\rangle \exp[i(kx - \omega t)]$$

This implies that we need to use the conventional (the type-1) Fourier transform for *t* and ω, and to use the type-II Fourier transform over *x* and *k*.

10.1.3 Examples

```
Clear["Global`*"]
```

```
FourierTransform[UnitStep[t] - UnitStep[t - T], t, ω] // FullSimplify
```

$$-\frac{i\left(-1+e^{i T \omega}\right)}{\sqrt{2\pi}\,\omega}$$

```
FourierTransform[Sin[ω0 t], t, ω]
```

$$i\sqrt{\frac{\pi}{2}}\,\text{DiracDelta}[\omega-\omega 0]-i\sqrt{\frac{\pi}{2}}\,\text{DiracDelta}[\omega+\omega 0]$$

```
FourierTransform[Cos[ω0 t], t, ω]
```

$$\sqrt{\frac{\pi}{2}}\,\text{DiracDelta}[\omega-\omega 0]+\sqrt{\frac{\pi}{2}}\,\text{DiracDelta}[\omega+\omega 0]$$

$$\text{FourierTransform}\left[\text{Exp}\left[-\frac{t}{\tau}\right], t, \omega\right]$$

$$\sqrt{2\pi}\,\text{DiracDelta}\left[\frac{i}{\tau}+\omega\right]$$

$$\text{FourierTransform}\left[\text{Exp}\left[-\frac{t}{\tau}\right]\text{UnitStep}[t], t, \omega\right]$$

$$\frac{i\,\tau}{\sqrt{2\pi}\,(i+\tau\,\omega)}$$

```
FourierTransform[Exp[- ⅈ ω0 t] (UnitStep[t] - UnitStep[t - T]), t, ω]
```

$$\frac{i}{\sqrt{2\pi}\,(\omega-\omega 0)}-\frac{i\,e^{i\,T\,(\omega-\omega 0)}}{\sqrt{2\pi}\,(\omega-\omega 0)}+\sqrt{\frac{\pi}{2}}\,\mathrm{DiracDelta}[\omega-\omega 0]-e^{i\,T\,(\omega-\omega 0)}\sqrt{\frac{\pi}{2}}\,\mathrm{DiracDelta}[\omega-\omega 0]$$

```
FourierTransform[1 / t, t, ω]
```

$$i\sqrt{\frac{\pi}{2}}\,\mathrm{Sign}[\omega]$$

```
FourierTransform[1 / t^2, t, ω]
```

$$-\sqrt{\frac{\pi}{2}}\,\omega\,\mathrm{Sign}[\omega]$$

```
FourierTransform[1 / (1 + t^4), t, ω]
```

$$\left(\frac{1}{4}+\frac{i}{4}\right)e^{-\frac{(1+i)\,\omega}{\sqrt{2}}}\sqrt{\pi}\left(e^{\sqrt{2}\,\omega}\left(-i+e^{i\sqrt{2}\,\omega}\right)\mathrm{HeavisideTheta}[-\omega]+\left(1-i\,e^{i\sqrt{2}\,\omega}\right)\mathrm{HeavisideTheta}[\omega]\right)$$

```
InverseFourierTransform[Exp[- (t0)^2 (ω - ω0)^2], ω, t]
```

$$\frac{e^{-\frac{1}{4}t\left(\frac{t}{t0^2}+4\,i\,\omega 0\right)}}{\sqrt{2}\,\mathrm{Abs}[t0]}$$

```
FourierTransform[Exp[-ⅈ ω0 t], t, ω]
```

$$\sqrt{2\pi}\,\mathrm{DiracDelta}[\omega-\omega 0]$$

```
InverseFourierTransform[Exp[-α t - ⅈω0 t] * UnitStep[t], t, ω]
```

$$\frac{1}{\sqrt{2\pi}\,(\alpha+i\,\omega+i\,\omega 0)}$$

10.2. Properties of Fourier transform

10.2.1 derivative

$$F(\omega)=\mathbf{F}[f(t)]=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{i\omega t}f(t)\,dt$$

We now consider the Fourier transform of the derivative

$$\mathbf{F}[\frac{df}{dt}] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} \frac{df}{dt} dt = -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} i\omega e^{i\omega t} f(t) dt = -i\omega \mathbf{F}[f]$$

$$\mathbf{F}[\frac{d^2 f}{dt^2}] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} \frac{d^2 f}{dt^2} dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (-i\omega)^2 e^{i\omega t} f(t) dt = -\omega^2 \mathbf{F}[f]$$

10.2.2 Delay

$$\mathbf{F}[f(t-t_0)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} f(t-t_0) dt$$

Make the substitution $\tau = t - t_0$ to obtain

$$\mathbf{F}[f(t-t_0)] = \frac{1}{\sqrt{2\pi}} e^{i\omega t_0} \int_{-\infty}^{\infty} e^{i\omega \tau} f(\tau) d\tau = e^{i\omega t_0} \mathbf{F}[f(t)]$$

10.2.3 Inverse of real function

$$\mathbf{F}[f(-t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} f(-t) dt$$

where $f(t)$ is pure real. Substitution of $\tau = -t$ gives

$$\begin{aligned} \mathbf{F}[f(-t)] &= -\frac{1}{\sqrt{2\pi}} \int_{\infty}^{-\infty} e^{-i\omega \tau} f(\tau) d\tau \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega \tau} f(\tau) d\tau \\ &= F(\omega)^* \end{aligned}$$

10.2.4 Even and odd functions

If $f(t)$ is pure real and is an even function of t;

$$f(-t) = f(t)$$

Since

$$\mathbf{F}[f(-t)] = F(\omega)^*$$
$$\mathbf{F}[f(t)] = F(\omega)$$

we have

$$F(\omega)^* = F(\omega)$$

Thus $F(\omega)$ is a pure real function of ω.

If $f(t)$ is pure real and is an odd function of t;

$$f(-t) = -f(t)$$

we have

$$F(\omega)^* = -F(\omega)$$

Thus $F(\omega)$ is a pure imaginary function of ω.

10.2.5 The form of $F(\omega)$ for pure real $f(t)$

If $f(t)$ is pure real, then we have

$$F(-\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} f(t) dt = F(\omega)^*$$

10.3 Wave equations

We consider the solution of the wave equations in the electromagnetic field.

$$\nabla^2 \mathbf{E} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E}$$
$$\nabla^2 \mathbf{B} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{B}$$

We consider the special case when ***E*** or ***B*** depend only on x. In this case the equation for the field becomes

$$\frac{\partial^2}{\partial t^2} f = c^2 \frac{\partial^2}{\partial x^2} f$$

where f is understood any component of the vector ***E*** or ***B*** in the Maxwell's equation.

We use the Fourier transformation technique.

$$F(x,\omega)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{i\omega t}f(x,t)dt$$

$$f(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-i\omega t}F(x,\omega)d\omega$$

$$\frac{\partial^2}{\partial x^2}f-\frac{1}{c^2}f=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-i\omega t}[\frac{\partial^2}{\partial x^2}F(x,\omega)+\frac{\omega^2}{c^2}F(x,\omega)]d\omega=0$$

Then we have

$$\frac{\partial^2}{\partial x^2}F(x,\omega)+k^2F(x,\omega)=0$$

where $k=\frac{\omega}{c}$

The solution of this equation is

$$F(x,\omega)=G(\omega)e^{\pm ikx}=G(\omega)e^{\pm i\frac{\omega x}{c}}$$

where $G(\omega)$ is an arbitrary function of ω. Finally we get

$$f(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}F(x,\omega)e^{-i\omega t}d\omega=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}G(\omega)e^{-i\omega(t\pm\frac{x}{c})}d\omega=g(t\pm\frac{x}{c})$$

where

$$g(t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}G(\omega)e^{-i\omega t}d\omega$$

Therefore, $f(x,t)$ is a function of $t\pm\frac{x}{c}$.

((**Mathematica**))

```
Clear["Global`*"]
```

```
eq1 = D[F[x, ω], {x, 2}] + ω^2/c^2 F[x, ω] == 0
```

$$\frac{\omega^2 F[x,\omega]}{c^2} + F^{(2,0)}[x,\omega] == 0$$

```
eq2 = DSolve[eq1, F[x, ω], x] // TrigToExp
```

$$\left\{\left\{F[x,\omega] \to \frac{1}{2} e^{-\frac{i x \omega}{c}} C[1] + \frac{1}{2} e^{\frac{i x \omega}{c}} C[1] + \frac{1}{2} i e^{-\frac{i x \omega}{c}} C[2] - \frac{1}{2} i e^{\frac{i x \omega}{c}} C[2]\right\}\right\}$$

```
F[x_, ω_] = Exp[-i ω/c x] G[ω];
```

We assume the Gaussian ditribution function for G[ω].

```
G[ω_] = 1/(Sqrt[2 π] σ) Exp[-1/(2 σ^2) (ω - ω0)^2];
```

```
f[x_, t_] =
 InverseFourierTransform[F[x, ω], ω, t,
   FourierParameters → {0, -1}] // Simplify
```

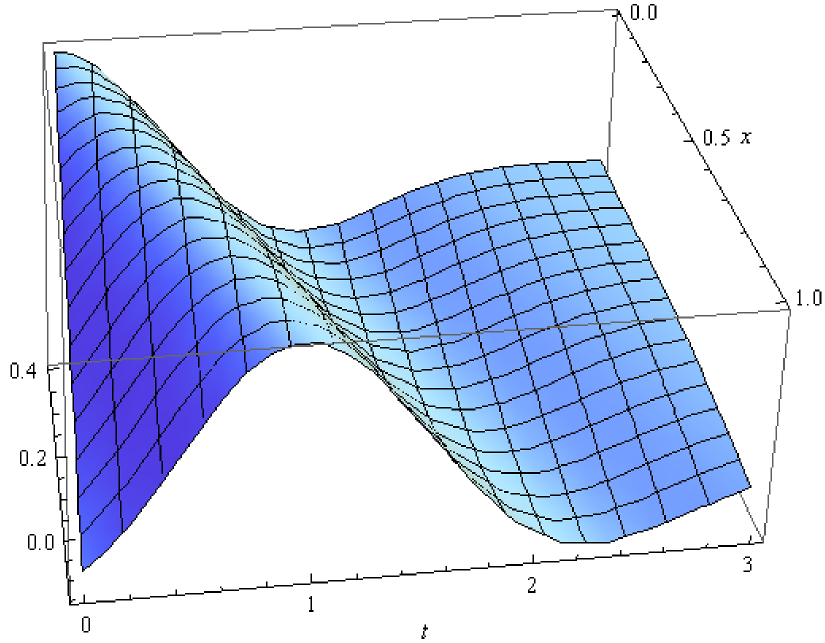
$$\frac{e^{-\frac{(c\,t-x)\left(c\,t\,\sigma^2 - x\,\sigma^2 - 2\,i\,c\,\omega 0\right)}{2\,c^2}}\,\mathrm{Abs}[\sigma]}{\sqrt{2\pi}\,\sigma}$$

```
f1[x_, t_] = Re[f[x, t]] /. {σ → 1, k → 1, ω0 → 2, c → 1} //
  Simplify[#, {x ∈ Reals, t ∈ Reals}] &
```

$$\frac{e^{-\frac{1}{2}(t-x)^2}\,\mathrm{Cos}[2\,t - 2\,x]}{\sqrt{2\pi}}$$

The wave function is described by a function of t - $\frac{x}{c}$ for the propagating along the positive x axis.

```
Plot3D[f1[x, t], {x, 0, 1}, {t, 0, 3}, AxesLabel → Automatic]
```



10.4 Convolution
10.4.1 Definition

We define the convolution

$$f * g = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t-\tau)g(\tau)d\tau = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(t-\tau)f(\tau)d\tau$$

Then we have

$$\mathbf{F}[f * g] = \mathbf{F}[f]\mathbf{F}[g] = F(\omega)G(\omega)$$

or

$$(f * g)(t) = \mathbf{F}^{-1}[F(\omega)G(\omega)]$$

((**Proof**))

$$I = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} d\omega F(\omega) G(\omega)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} d\omega \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' e^{i\omega t'} f(t') \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt'' e^{i\omega t''} g(t'')$$

or

$$I = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' f(t') \int_{-\infty}^{\infty} dt'' g(t'') \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(-t+t'+t'')} d\omega$$

or

$$I = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' f(t') \int_{-\infty}^{\infty} dt'' g(t'') \delta(-t+t'+t'')$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt' f(t') g(t-t') = f * g$$

((**Note**))

Conventionally the convolution of two functions is defined by

$$f \otimes g = \int_{-\infty}^{\infty} f(t-\tau) g(\tau) d\tau = \int_{-\infty}^{\infty} g(t-\tau) f(\tau) d\tau = \sqrt{2\pi} f * g \, .$$

$$\mathbf{F}[f * g] = F(\omega) G(\omega) = \frac{1}{\sqrt{2\pi}} \mathbf{F}[f \otimes g]$$

or

$$\mathbf{F}[f \otimes g] = \sqrt{2\pi} \mathbf{F}[f * g]$$

10.4.2 Example-1

We now consider the convolution of two functions, g(t) and

$$f(t) = \delta(t+a) + \delta(t-a)$$

From the definition,

$$f*g = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t-t')g(t')dt'$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}[\delta(t-t'+a)+\delta(t-t'-a)]g(t')dt'$$

$$= \frac{1}{\sqrt{2\pi}}[g(t-a)+g(t+a)]$$

$$\mathbf{F}^{-1}[F(\omega)G(\omega)] = f*g$$

where

$$F(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\omega t} f(t)dt = \frac{1}{\sqrt{2\pi}}(e^{i\omega a}+e^{-i\omega a}) = \sqrt{\frac{2}{\pi}}\cos(a\omega)$$

10.4.3 Convolve (Mathematica program)

Convolve[*f*, *g*, *x*, *y*];

to gives the convolution of two functions *f* and *g*;

$$(f\otimes g)(y) = \int_{-\infty}^{\infty} f(x)g(y-x)dx = \int_{-\infty}^{\infty} f(y-x)g(x)dx$$

We calculate the convolution of *f* and *g* using several methods.

$$f(x) = e^{-x}Unitstep[x]$$
$$g(x) = \sin x$$

(i) The use of Convolve[*f*, *g*, *x*, *y*]

(ii) Direct calculation of $\int_{-\infty}^{\infty} f(x)g(y-x)dx = \int_{-\infty}^{\infty} f(y-x)g(x)dx$.

(iii) The use of the inverse Fourier transform.

((**Mathematica**))

```
Clear["Global`*"]
```

Calculation of convolution using the Convolve

```
Clear[f, g]
f[x_] := Exp[-x] UnitStep[x]; g[x_] := Sin[x]
Convolve[f[x], g[x], x, y]
```

$$\frac{1}{2} (-\text{Cos}[y] + \text{Sin}[y])$$

Calculation of convolution using the definition of integral

$$\int_{-\infty}^{\infty} f[y - x]\, g[x]\, dx$$

$$\frac{1}{2} (-\text{Cos}[y] + \text{Sin}[y])$$

$$\int_{-\infty}^{\infty} f[x]\, g[y - x]\, dx$$

$$\frac{1}{2} (-\text{Cos}[y] + \text{Sin}[y])$$

Calculation of convolution using the InverseFourierTransform

```
F = FourierTransform[f[x], x, k]
```

$$\frac{i}{(i + k) \sqrt{2 \pi}}$$

```
G = FourierTransform[g[x], x, k]
```

$$i \sqrt{\frac{\pi}{2}}\ \text{DiracDelta}[-1 + k] - i \sqrt{\frac{\pi}{2}}\ \text{DiracDelta}[1 + k]$$

$$\sqrt{2 \pi}\ (\text{InverseFourierTransform}[F\, G, k, y])$$

$$\frac{1}{2} (-\text{Cos}[y] + \text{Sin}[y])$$

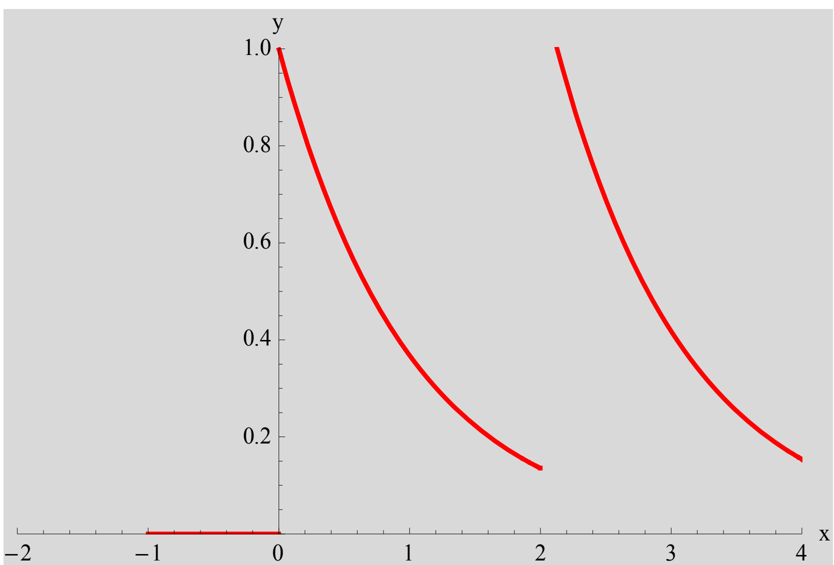
10.4.4 Example-I (Mathematica)

We consider the convolution of two functions;

$$f(x) = \delta(x) + \delta(x-2), \qquad g(x) = \exp(-x)H(x)$$

where $H(x)$ is a Heaviside step function. $H(x)$ = 1 for x>0 and 0for x<0.

```
Clear["Global`*"];

f[x_] := Exp[-x] UnitStep[x];
g[x_] = DiracDelta[x] + DiracDelta[x - 2];

s1 = Convolve[f[y], g[y], y, x];

Plot[s1, {x, -1, 4}, PlotRange → {{-2, 4}, {0, 1}},
 PlotStyle → {Red, Thick}, Background → LightGray,
 AxesLabel → {"x", "y"} ]
```



10.4.5 Example-II (Mathematica)

We consider the convolution of two functions;

$$f(x) = \sum_{k=-10}^{10} \delta(x-k), \quad g(x) = \exp(-3x)H(x)$$

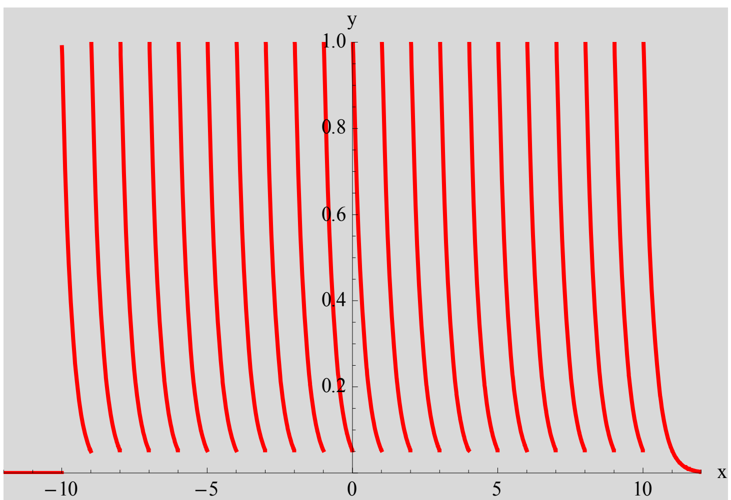
where $H(x)$ is a Heaviside step function. $H(x)$ = 1 for x>0 and 0for x<0.

((**Mathematica**))

```
Clear["Global`*"]

f[x_] = Sum[DiracDelta[x - k], {k, -10, 10}];

g[x_] = Exp[-3 x] UnitStep[x];
```

e^{-3x} UnitStep[x]

```
s1 = Convolve[f[y], g[y], y, x];

Plot[s1, {x, -12, 12}, PlotPoints → 100,
 PlotRange → {{-12, 12}, {0, 1}}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"x", "y"}]
```



((Note)) There is a convenient function in the Mathematica.

DiracComb[*t*]:

represents the Dirac comb function giving a delta function at every integer point.

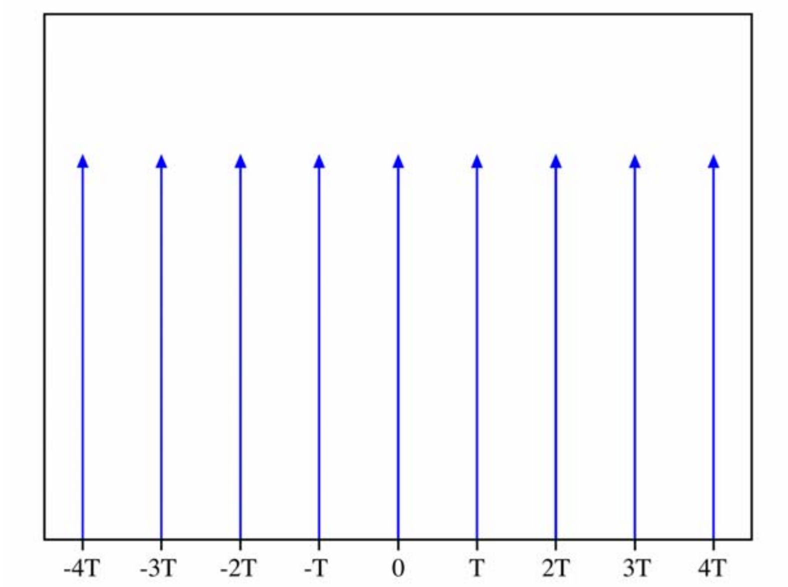


Fig. A Dirac comb is an infinite series of Dirac delta functions spaced at intervals of *T*.

The Dirac comb is defined by

$$f(t) = \sum_{n=-\infty}^{\infty} \delta(t - nT)$$

We consider the convolution of a function $g(t)$ and the Dirac comb $f(t)$,

$$\begin{aligned}(f \otimes g)(t) &= \int_{-\infty}^{\infty} f(\tau) g(t-\tau) d\tau \\ &= \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \delta(\tau - nT) g(t-\tau) d\tau \\ &= \sum_{n=-\infty}^{\infty} g(t - nT)\end{aligned}$$

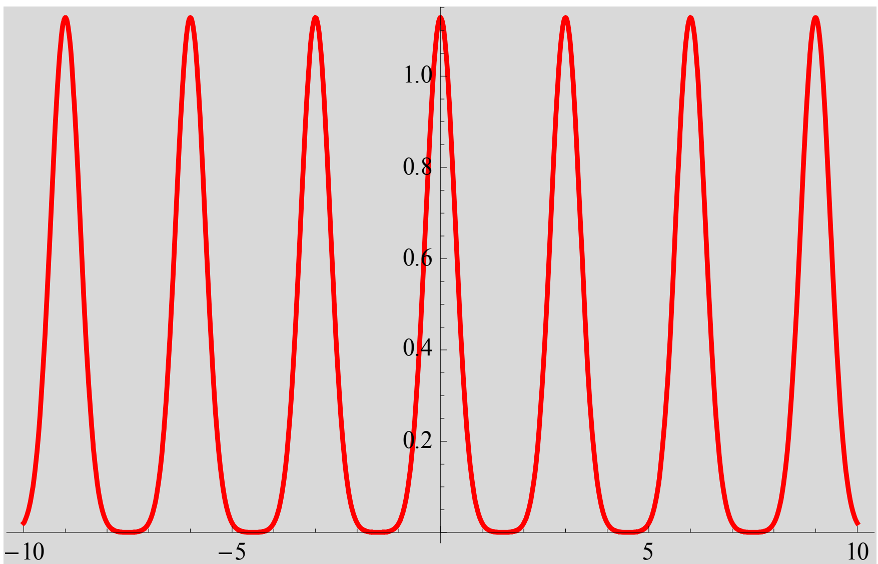
10.4.6 Example-III (Mathematica)

The function $f(t)$ is a periodic function of Gaussian pulses with period T, as described by

$$f(t) = \frac{\alpha}{\sqrt{\pi}} \sum_{n=-\infty}^{\infty} \exp[-\alpha^2 (t - nT)^2]$$

This function can be looked as the convolution of a single Gaussian pulse with a train of Dirac delta function.

```
Clear["Global`*"]

f1[t_] := α/√π Exp[-α² t²];

f2[t_, m_] := Sum[DiracDelta[t - n T], {n, -m, m}];

h1 = Convolve[f1[x], f2[x, 10], x, t] // Simplify;

Plot[h1 /. {T → 3, α → 2}, {t, -10, 10}, PlotStyle → {Red, Thick},
 Background → LightGray]
```

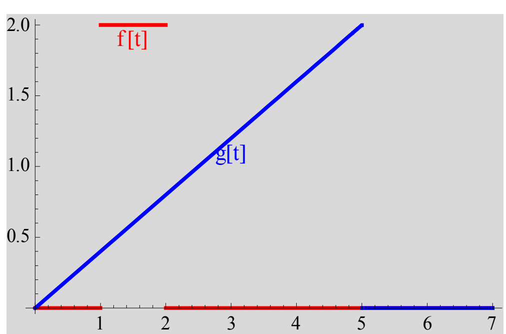


10.4.7 Example-IV (Mathematica)

We consider the convolution of two functions $f(t)$ and $g(t)$,

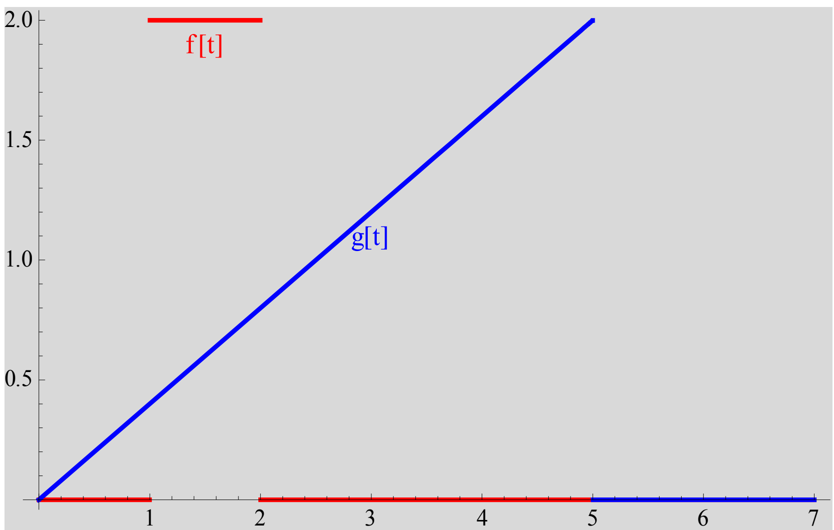
$$h(t) = f(t) \otimes g(t) = \int_{-\infty}^{\infty} f(t-\tau) g(\tau) d\tau = \int_{-\infty}^{\infty} f(\tau) g(t-\tau) d\tau$$

where $f(t)$ and $g(t)$ are given as follows.

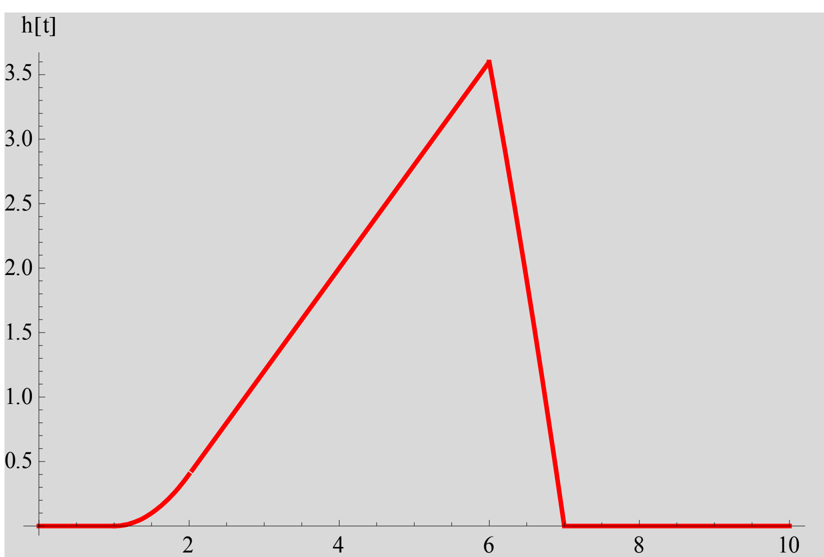


((**Mathematica**))

```
Clear["Global`*"]

f[t_] := 2 (UnitStep[t - 1] - UnitStep[t - 2]);
g[t_] := 2/5 t (UnitStep[t ] - UnitStep[t - 5]);

Plot[{f[t], g[t]}, {t, 0, 7},
 PlotStyle → {{Red, Thick}, {Blue, Thick}},
 Background → LightGray,
 Epilog → { Text[Style["f[t]", 12, Red], {1.5, 1.9}],
   Text[Style["g[t]", 12, Blue], {3, 1.1}]}]
```




```
h[t_] = Convolve[f[x], g[x], x, t];

Plot[h[t], {t, 0, 10}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"t", "h[t]"}]
```



10.4.8 Example-V; Periodic burst (Mathematica))

We consider the convolution of two functions $f(t)$ and $g(t)$, which is defined as

$$h(t) = f(t) \otimes g(t) = \int_{-\infty}^{\infty} f(t-\tau) g(\tau) d\tau = \int_{-\infty}^{\infty} f(\tau) g(t-\tau) d\tau$$

where $f(t)$ and $g(t)$ are given by

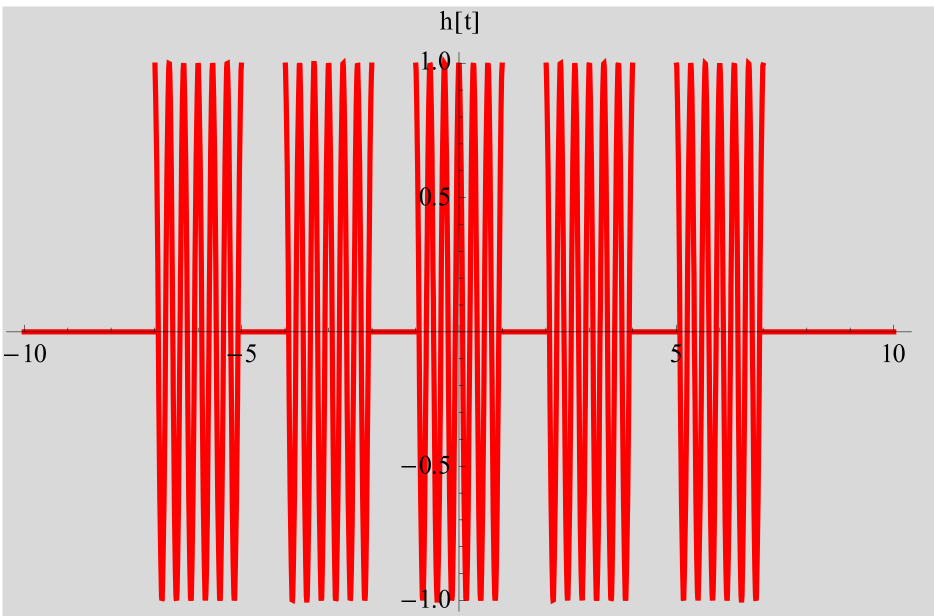
$$f(t) = \cos(\omega_0 t)[H(t+t_0) - H(t-t_0)]$$

$$g(t) = \delta(t+2t_1) + \delta(t+t_1) + \delta(t) + \delta(t-t_1) + \delta(t-2t_1)$$

and $t_0 = 1$, $\omega_0 = 6\pi$, and $t_1 = 3$, where H(t) is a Heaviside step function and $\delta(t)$ is the Dirac delta function.

((**Mathematica**))

```
Clear["Global`*"]

f[t_] := Cos[ω0 t] ( UnitStep[t + t0] - UnitStep[t - t0])

g[t_] := DiracDelta[t + 2 t1] + DiracDelta[t + t1] +
  DiracDelta[t] + DiracDelta[t - t1] + DiracDelta[t - 2 t1]

h[t_] := Convolve[f[x], g[x], x, t];

t0 = 1; ω0 = 6 π; t1 = 3;

Plot[Evaluate[h[t]], {t, -10, 10}, PlotStyle → {Red, Thick},
 AxesLabel → {"t", "h[t]"}, Background → LightGray]
```



10.5. Parseval's relation

10.5.1 Definition

$$\int_{-\infty}^{\infty} F(\omega)G^*(\omega)d\omega = \int_{-\infty}^{\infty} f(t)g^*(t)dt$$

((**Proof**))

$$I = \int_{-\infty}^{\infty} f(t)g^*(t)dt = \int_{-\infty}^{\infty} dt \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} F(\omega) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' e^{i\omega' t} G^*(\omega')$$

or

$$I = \int_{-\infty}^{\infty} d\omega F(\omega) \int_{-\infty}^{\infty} d\omega' G^*(\omega') \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{it(\omega'-\omega)} = \int_{-\infty}^{\infty} d\omega F(\omega) \int_{-\infty}^{\infty} d\omega' G^*(\omega') \delta(\omega - \omega')$$

or

$$I = \int_{-\infty}^{\infty} d\omega F(\omega) G^*(\omega) .$$

((Note)) $f = g$

$$\int_{-\infty}^{\infty} |F(\omega)|^2 d\omega = \int_{-\infty}^{\infty} |f(t)|^2 dt$$

If a function $f(t)$ is normalized to unity, its transform $F(\omega)$ is likewise normalized to unity.

10.5.2 Example-1

Arfken 15-5-5: Single slit diffraction problem

(a) A rectangular pulse is described by

f[x] = 1 for |x|<a, and 0 for |x|>a.

Show that the Fourier exponential transform is

$$F[k] = \sqrt{\frac{\pi}{2}} \frac{\mathrm{Sin}[a\,k]}{k}$$

This is the single slit diffraction problem of physical optics. The slit is described by f[x]. The diffraction pattern amplitude is given by the Fourier transform F[k].

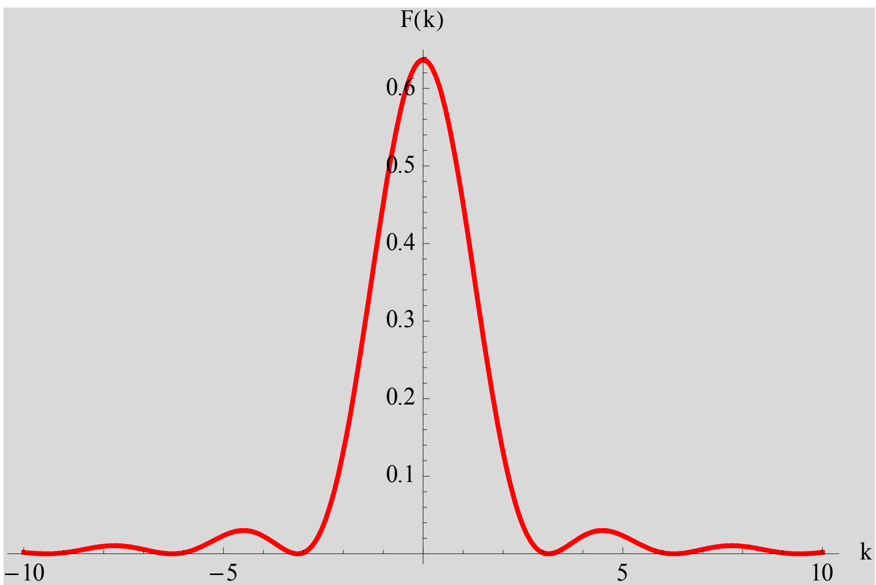
(b) Use the Parseval relation to evaluate

$$\int_{-\infty}^{\infty} \frac{\mathrm{Sin}[k]^2}{k^2} dk .$$

```
Clear["Global`*"]

f[x_] = Simplify[UnitStep[x - a] - UnitStep[x + a], a > 0];

F[k_] = FourierTransform[f[x], x, k,
  FourierParameters → {0, -1}]
```

$$-\frac{\sqrt{\frac{2}{\pi}}\ \mathrm{Sin}[a\ k]}{k}$$

```
Plot[F[k]^2 /. a → 1, {k, -10, 10}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"k", "F(k)"}]
```



Parseval relation

$$\mathrm{Simplify}\left[\int_{-\infty}^{\infty} F[k]^2\, dk,\ a > 0\right]$$

2 a

$$\mathrm{Simplify}\left[\int_{-a}^{a} 1\, dx,\ a > 0\right]$$

2 a

10.5.3 Example-2

Arfken 15-5-7

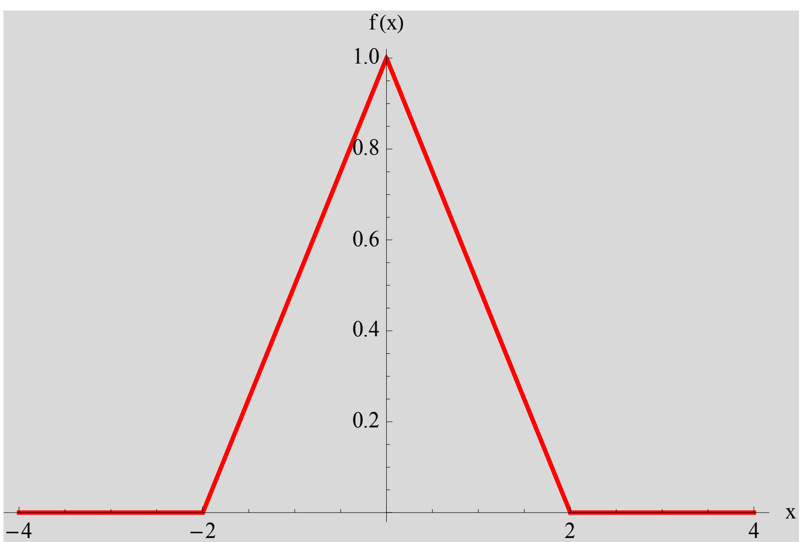
(a) Given f[x] = 1 - |x|/2, -2⩽x⩽2 and zero elsewhere, show that the Fourier transform of f[x] is

$$F[k] = \sqrt{\frac{\pi}{2}}\ \left(\frac{\text{Sin}[k]}{k}\right)^2.$$

(b) Using the Parseval relation, evaluate

$$\int_{-\infty}^{\infty}\left(\frac{\text{Sin}[k]}{k}\right)^4 dk$$

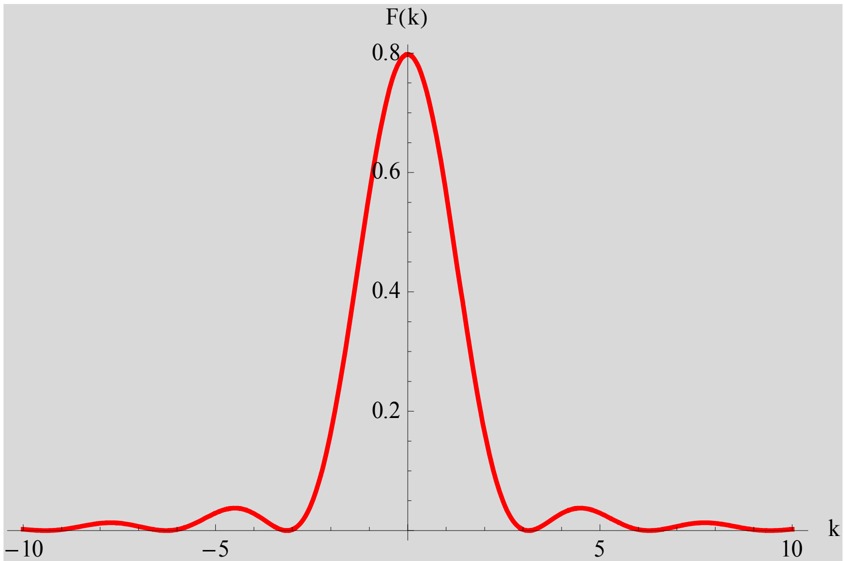
```
Clear["Global`*"]

f[x_] = (1 - Abs[x / 2]) (-UnitStep[x - 2] + UnitStep[x + 2]);

Plot[f[x], {x, -4, 4}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"x", "f(x)"}]
```




```
F[k_] =
 FourierTransform[f[x], x, k, FourierParameters → {0, -1}] //
  FullSimplify
```

$$\frac{\sqrt{\frac{2}{\pi}}\ \text{Sin}[k]^2}{k^2}$$

```
Plot[F[k], {k, -10, 10}, PlotStyle → {Red, Thick},
 Background → LightGray, AxesLabel → {"k", "F(k)"}]
```



(b) Parseval relation

$$\int_{-\infty}^{\infty} \text{Abs}[F[k]]^2 \, dk$$

$$\frac{4}{3}$$

$$\int_{-\infty}^{\infty} f[x]^2 \, dx$$

$$\frac{4}{3}$$

10.5.4 Example-4

Use the Parseval relation to show that

$$\int_{-\infty}^{\infty} \frac{1}{(\omega^2 + a^2)^2} d\omega = \frac{\pi}{2a^3}.$$

((Mathematica))

```
F[ω_] = 1/(ω^2 + a^2);
```

```
Simplify[∫_{-∞}^{∞} F[ω]^2 dω, a > 0]
```

$$\frac{\pi}{2\,a^3}$$

```
f1 = Simplify[InverseFourierTransform[F[ω], ω, t], {a > 0, t > 0}]
```

$$\frac{e^{-a\,t}\sqrt{\frac{\pi}{2}}}{a}$$

```
f2 = Simplify[InverseFourierTransform[F[ω], ω, t], {a > 0, t < 0}]
```

$$\frac{e^{a\,t}\sqrt{\frac{\pi}{2}}}{a}$$

```
Simplify[∫_0^∞ f1^2 dt + ∫_{-∞}^0 f2^2 dt, a > 0]
```

$$\frac{\pi}{2\,a^3}$$

10.5.5 Example-5 Arfken

```
F1[ω_] = ω/(ω^2 + a^2);

Simplify[∫_{-∞}^{∞} F1[ω]^2 dω, a > 0]
```

$$\frac{\pi}{2\,a}$$

```
g = InverseFourierTransform[F1[ω], ω, t];

g1 = Simplify[g, {t > 0, a > 0}]
```

$$-i\, e^{-a\,t} \sqrt{\frac{\pi}{2}}$$

```
g2 = Simplify[g, {t < 0, a > 0}]
```

$$i\, e^{a\,t} \sqrt{\frac{\pi}{2}}$$

```
Simplify[∫_0^∞ Abs[g1]^2 dt + ∫_{-∞}^0 Abs[g2]^2 dt, a > 0]
```

$$\frac{\pi}{2\,a}$$

10.6. Correlations

A quantitative measure of the degree of correlation between two functions $f(t)$ and g(t), is provided by the cross correlation

$$C[f,g](t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t+\tau) g^{*}(\tau) d\tau$$

$$\mathbf{F}[C[f,g](t)] = F(\omega) G^{*}(\omega)$$

where the complex conjugate of one factor ensures that the correlation between complex exponentials. This is similar to the convolution theorem, but complex conjugation of one factor does have important consequences.

((**Proof**))

$$\mathbf{F}[C[f,g](t)] = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt e^{i\omega t}\int_{-\infty}^{\infty} f(t+\tau)g^*(\tau)d\tau$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} e^{i\omega(t+\tau)} f(t+\tau)e^{-i\omega\tau} g^*(\tau)d\tau$$
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\omega s} f(s)ds \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-i\omega\tau} g^*(\tau)d\tau$$
$$= F(\omega)G^*(\omega)$$

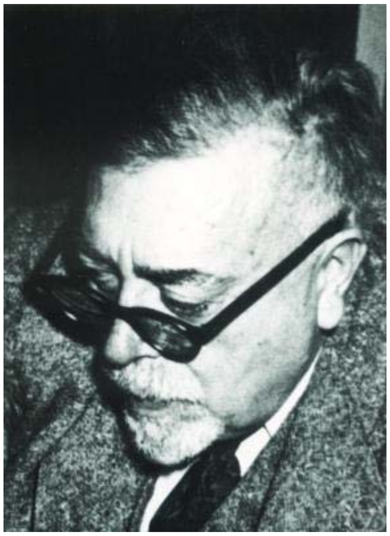
An important special case is the autocorrelation function.

$$C[f,f](t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t+\tau)f^*(\tau)d\tau$$
$$\mathbf{F}[C[f,f](t)] = F(\omega)F^*(\omega) = |F(\omega)|^2$$

which is proportional to the power spectrum.

((Wiener-Khinchin theorem))

Norbert Wiener (November 26, 1894, Columbia, Missouri – March 18, 1964, Stockholm, Sweden) was an American mathematician. A famous child prodigy, Wiener later became an early studier of stochastic and noise processes, contributing work relevant to electronic engineering, electronic communication, and control systems. Wiener is regarded as the originator of cybernetics, a formalization of the notion of feedback, with many implications for engineering, systems control, computer science, biology, philosophy, and the organization of society.



http://en.wikipedia.org/wiki/Norbert_Wiener

Aleksandr Yakovlevich Khinchin (Russian: Алекса́ндр Я́ковлевич Хи́нчин, French: *Alexandre Khintchine*; July 19, 1894 – November 18, 1959) was a Soviet mathematician and one of the most significant people in the Soviet school of probability theory. He was born in the village of Kondrovo, Kaluga Governorate, Russian Empire. While studying at Moscow State University, he became one of the first followers of the famous Luzin school. Khinchin graduated from the university in 1916 and six years later he became a full professor there, retaining that position until his death.

http://en.wikipedia.org/wiki/Aleksandr_Yakovlevich_Khinchin

Autocorrelation function

$$C(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} E^*(\tau) E(t+\tau) d\tau .$$

The Fourier transform of $E(t)$ is defined by

$$E(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} E_\omega e^{-i\omega t} d\omega .$$

Its complex conjugate is given by

$$E^*(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} E_\omega{}^* e^{i\omega t} d\omega .$$

Plugging $E(t)$ and $E^*(t)$ into the autocorrelation function gives

$$C(t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}E_{\omega}{}^{*}e^{i\omega\tau}d\omega][\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}E_{\omega'}e^{-i\omega'(t+\tau)}d\omega']d\tau$$

$$=\frac{1}{2\pi}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}E_{\omega}{}^{*}e^{i\omega\tau}E_{\omega'}e^{-i\omega'(t+\tau)}d\omega'd\omega d\tau$$

$$=\frac{1}{2\pi}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}E_{\omega}{}^{*}E_{\omega'}e^{-i\omega' t}d\omega'd\omega\int_{-\infty}^{\infty}e^{i(\omega-\omega')\tau}d\tau$$

$$=\frac{1}{2\pi}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}E_{\omega}{}^{*}E_{\omega'}e^{-i\omega' t}d\omega'd\omega 2\pi\delta(\omega-\omega')$$

$$=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}E_{\omega}{}^{*}E_{\omega}e^{-i\omega t}d\omega$$

$$=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left|E_{\omega}\right|^{2}e^{-i\omega t}d\omega$$

or

The Fourier transform

$$F[C(t)]=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dtC(t)e^{i\omega t}=\frac{1}{2\pi}\int_{-\infty}^{\infty}dte^{i\omega t}\int_{-\infty}^{\infty}\left|E_{\omega'}\right|^{2}e^{-i\omega' t}d\omega'$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left|E_{\omega'}\right|^{2}d\omega'\int_{-\infty}^{\infty}dte^{i(\omega-\omega')t}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left|E_{\omega'}\right|^{2}d'\omega' 2\pi\delta(\omega-\omega')$$

$$=\left|E_{\omega}\right|^{2}$$

Thus the autocorrelation is simply given by the Inverse Fourier transform of the absolute square of E_{ω}. The Wiener-Khinchin theorem is a special case of the cross-correlation theorem with $f = g$.

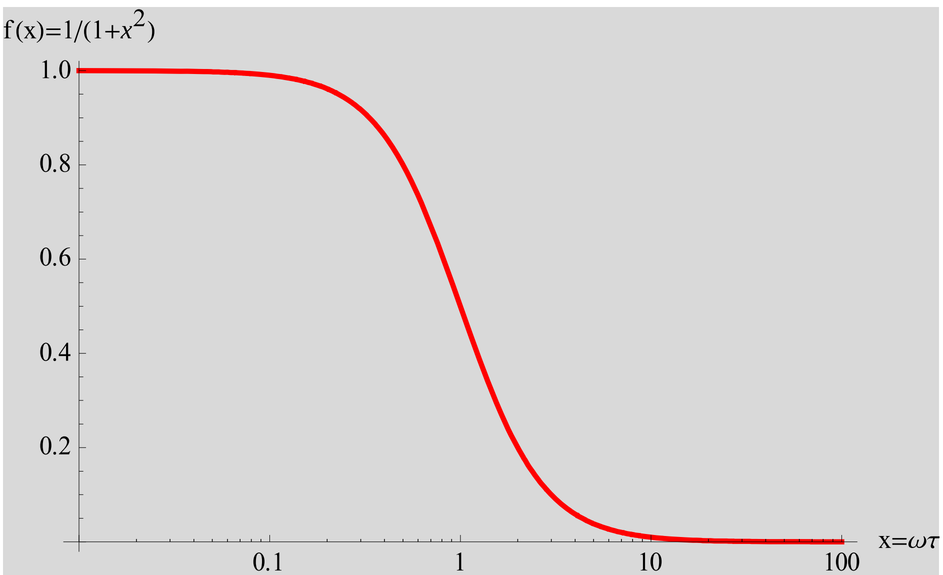
((**Example**)) "**White noise**"
C. Kittel: Elementary Statistical Physics (Dover Publication, Mineola, NY, 2004)

Suppose that

$$C(t)=\sqrt{2\pi}e^{-|t|/\tau_0}$$

The Fourier transform:

$$
\begin{aligned}
F[C(t)] &= |E_\omega|^2 \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt C(t) e^{i\omega t} \\
&= \int_{-\infty}^{\infty} dt e^{-|t|/\tau_0} e^{i\omega t} \\
&= \int_{-\infty}^{0} dt e^{t/\tau_0} e^{i\omega t} + \int_{0}^{\infty} dt e^{-t/\tau_0} e^{i\omega t} \\
&= \frac{1}{i\omega + \frac{1}{\tau_0}} - \frac{1}{i\omega - \frac{1}{\tau_0}} = \frac{2\tau_0}{1 + (\omega\tau_0)^2}
\end{aligned}
$$



As shown in the above figure, the power spectrum is flat on a log scale out to $\omega\tau_0 = 1$, and then decreases as $1/(\omega\tau_0)^2$ at high frequencies. We say roughly that the spectrum for the correlation function is "white" out to a cutoff $\omega\tau_0 = 1$

10.7 Fourier transform of Dirac delta function

(1) One dimensional case

Fourier transform:

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

Inverse Fourier transform:

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

When $f(x) = 1$,

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} dx = \sqrt{2\pi}\delta(k)$$

or

$$\int_{-\infty}^{\infty} e^{-ikx} dx = 2\pi\delta(k)$$

By replacing $k \to -k$ and using the property of the Dirac delta function; $\delta(-k) = \delta(k)$, we have

$$\int_{-\infty}^{\infty} e^{ikx} dx = (2\pi)\delta(-k) = 2\pi\delta(k)$$

((Mathematica))

```
Clear["Global`*"]

f[x_] = 1;

F[k_] = FourierTransform[1, x, k, FourierParameters → {0, -1}]

√(2 π) DiracDelta[k]

InverseFourierTransform[F[k], k, x, FourierParameters → {0, -1}]

1
```

(2) Two dimensional case

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{ik_x x + ik_y y} = (2\pi)^2 \delta(k_x)\delta(k_y) = (2\pi)^2 \delta(\mathbf{k})$$

$$\to (2\pi)^2 DiracDeltra[\{k_x, k_y\}]$$

(3) Three dimensional case

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz e^{ik_x x + ik_y y + ik_z z} = (2\pi)^3 \delta(k_x)\delta(k_y)\delta(k_z)$$

$$= (2\pi)^3 \delta(\mathbf{k})$$

$$\rightarrow (2\pi)^3 \mathit{DiracDeltra}[\{k_x, k_y.k_z\}]$$

(4) Physical meaning

We consider the function defined by

$$f(\theta, N) = \sum_{n=-N}^{N} \exp(in\theta) = \frac{\sin(N + \frac{1}{2})\theta}{\sin\frac{\theta}{2}}$$

$$g(\theta, N) = |f(\theta, N)|^2 = \frac{\sin^2(N + \frac{1}{2})\theta}{\sin^2\frac{\theta}{2}}$$

What is the dependence of $g(\theta, N)$ on θ, when N becomes infinity? The answer is that $g(\theta, N)$ approaches the Dirac delta function $\delta(\theta)$; $g(\theta, N) \rightarrow 0$ for finite θ.

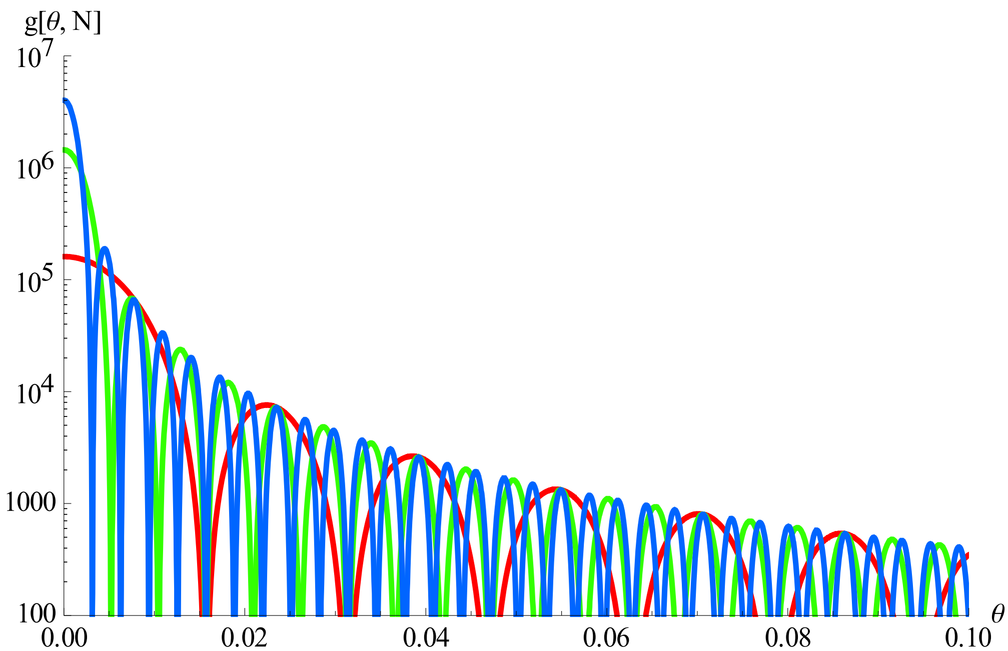


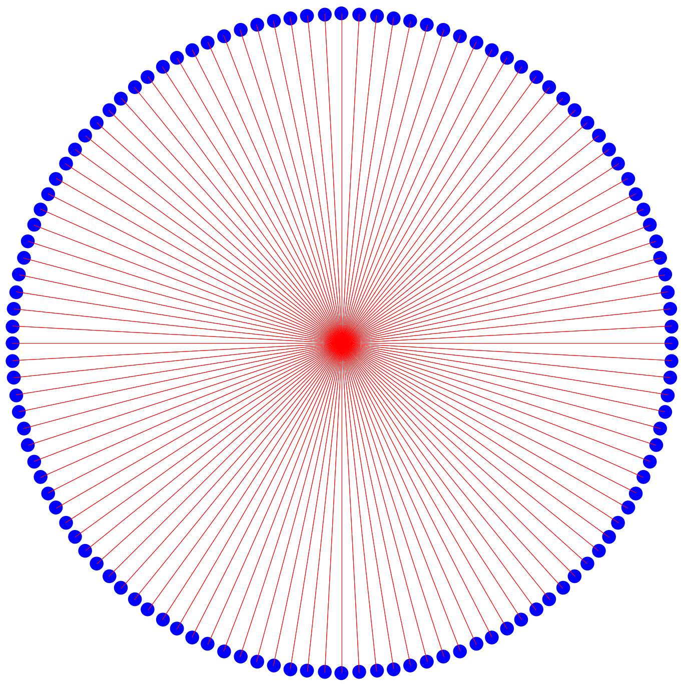
Fig. $g(\theta, N)$ as a function of θ, where N = 1000 (blue), N = 600 (green), and N = 200 (red).

((**Smearing of phase**))

We make a plot of the coordinate (x, y) with x = Re[exp($in\theta$)] and y = Im[exp($in\theta$)] for n = 0, 1, 2,..., N-1, where N is a very large integer. In the limit of N →0, there should be a pair of points with (x, y) and (-x,-y) on the unit circle. So the complete cancellalation occurs, leading to

$$X = \mathrm{Re}[\sum_{n=0}^{N} \exp(in\theta)] = 0$$

$$Y = \mathrm{Im}[\sum_{n=0}^{N} \exp(in\theta)] = 0$$



((Note))

We calculate

$$f(x) = \int_{-\eta}^{\eta} e^{ikx} dk = \frac{2\sin(\eta x)}{x},$$

in the limit of very large positive value η. We make a plot of this function when the parameter η is varied between η = 20 and 100. We find that this function has a peak at x = 0,

$$f(0) = 2\eta .$$

This function becomes zero at

$$x = \pm\frac{n\pi}{\eta} \quad (n = \text{integer}).$$

The integral of $f(x)$ is obtained as

$$\int_{-\infty}^{\infty} f(x)dx = 2\pi$$

which is independent of η.

In conclusion, we get the Dirac delta function as

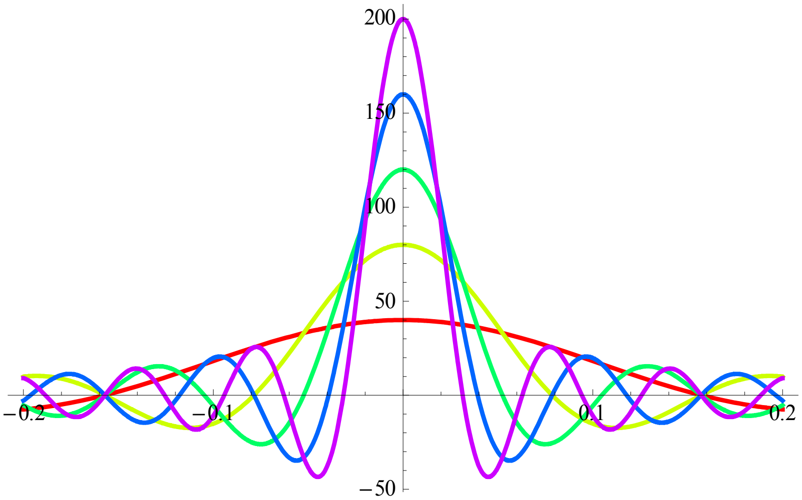
$$\int_{-\infty}^{\infty} e^{ikx} dk = 2\pi\delta(x) .$$

((**Mathematica**))

```
Clear["Global`"]; Clear[f1];

f[x_] := Integrate[Exp[ⅈ k x], {k, -η, η}] // Simplify[#, {η > 0}] &

f[x]
```

$$\frac{2\,\mathrm{Sin}[x\,\eta]}{x}$$

```
Plot[Evaluate[Table[f[x], {η, 20, 100, 20}]], {x, -0.2, 0.2},
 PlotStyle → Table[{Hue[0.2 i], Thick}, {i, 0, 5}], PlotRange → All]
```




```
Integrate[f[x], {x, -∞, ∞}] // Simplify[#, η > 0] &
```

2π

```
f[0]
```

2η

10.8. Three dimensional case (*r*-*k* space)

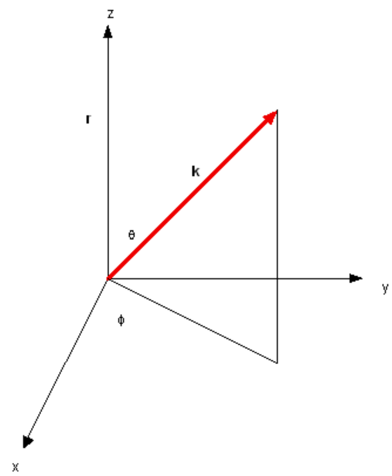
$$F(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) d\mathbf{r}$$

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\mathbf{k}\cdot\mathbf{r}} F(\mathbf{k}) d\mathbf{k}$$

((**Example**))

When $F(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{k^2}$, what is the form of $f(\boldsymbol{r})$?

$$f(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{(2\pi)^{3/2}} \frac{1}{k^2} d\mathbf{k} = \frac{1}{(2\pi)^3} \int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2} d\mathbf{k}$$



$\mathbf{k}\cdot\mathbf{r} = kr\cos\theta$ (we assume that $\boldsymbol{r}$ is directed to the z axis).

$$d\mathbf{k} = k^2 \sin\theta dk d\theta d\phi$$

$$f(\mathbf{r}) = \frac{1}{(2\pi)^3} \int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2} d\mathbf{k} = \frac{1}{(2\pi)^3} \iiint e^{ikr\cos\theta} \frac{k^2}{k^2} \sin\theta dk d\theta d\phi$$

or

$$f(\mathbf{r}) = \frac{1}{(2\pi)^2} \int_0^\infty dk \int_0^\pi e^{ikr\cos\theta} \sin\theta d\theta$$

$$f(\mathbf{r}) = \frac{1}{4\pi^2 ir} \int_0^\infty dk (\frac{e^{ikr} - e^{-ikr}}{k}) = \frac{1}{4\pi^2 ir} \int_{-\infty}^\infty dk \frac{e^{ikr}}{k}$$

We calculate $I = \int_{-\infty}^{\infty} dk \frac{e^{ikr}}{k}$ by using the Cauchy's theorem.

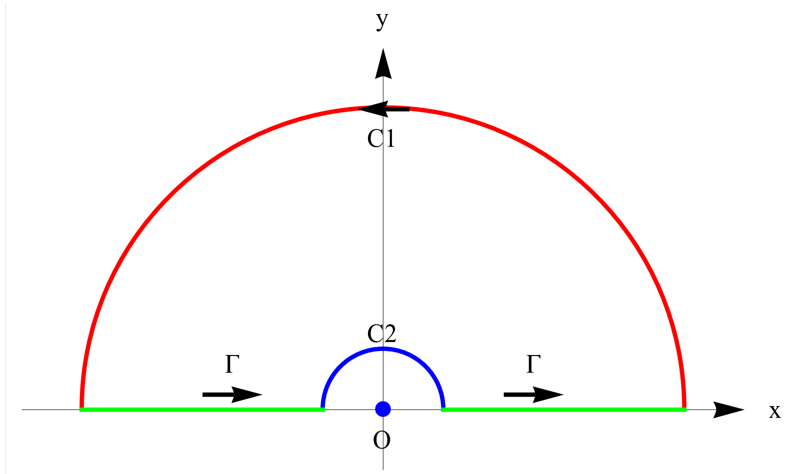


Fig. Upper half-plane contour for r>0.

$$P\int_{-\infty}^{\infty} dk \frac{e^{ikr}}{k} + \int_{C1} dz \frac{e^{izr}}{z} + \int_{C2} dz \frac{e^{izr}}{z} = 0$$

or

$$P\int_{-\infty}^{\infty} dk \frac{e^{ikr}}{k} = -\int_{C_2} dz \frac{e^{izr}}{z} = \pi i \operatorname{Res}(z=0) = \pi i$$

since

$$\int_{C1} dz \frac{e^{izr}}{z} = 0 \qquad \text{(Jordan's lemma, } r>0\text{).}$$

Then we have

$$f(\mathbf{r}) = \frac{1}{4\pi^2 ir}\pi i = \frac{1}{4\pi r}$$

10.9 Green's function (Helmholtz)

We now consider the form of the Green's function.

$$(\Delta + k^2)G_0(\mathbf{r}) = -\delta(\mathbf{r})$$

The Fourier transform of $G_0(\mathbf{r})$ is defined as

$$G_0(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{r} e^{-\mathbf{iq\cdot r}} G_0(\mathbf{r})$$

The inverse Fourier transform is also defined as

$$G_0(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q} e^{\mathbf{iq\cdot r}} G_0(\mathbf{q})$$

where

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d\mathbf{q} e^{\mathbf{iq\cdot r}}$$

Then

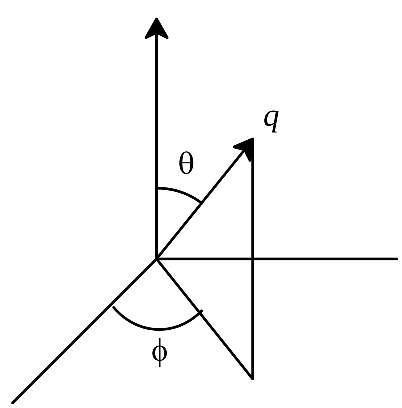
$$\frac{1}{(2\pi)^{3/2}} \int d\mathbf{q} (\Delta + k^2) e^{\mathbf{iq\cdot r}} G_0(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q} (-q^2 + k^2) e^{\mathbf{iq\cdot r}} G_0(\mathbf{q})$$
$$= -\delta(\mathbf{r}) = -\frac{1}{(2\pi)^3} \int d\mathbf{q} e^{\mathbf{iq\cdot r}}$$

or

$$G_0(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{q^2 - k^2}$$

Thus the Green's function is rewritten as

$$G_0^{(\pm)}(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d\mathbf{q} e^{\mathbf{iq\cdot r}} \frac{1}{q^2 - (k^2 \pm i\varepsilon)}$$



For convenience, we assume that the direction of ***r*** is the *z* axis. The angle between ***r*** and ***q*** is θ.

$$\mathbf{q}\cdot\mathbf{r} = qr\cos\theta$$

$$d\mathbf{q} = 2\pi q^2 dq \sin\theta d\theta$$

$$G_0^{(\pm)}(\mathbf{r}) = \frac{1}{(2\pi)^3}\int\int 2\pi q^2 dq\sin\theta d\theta e^{\mathbf{i}qr\cos\theta}\frac{1}{q^2-(k^2\pm i\varepsilon)}$$

Note

$$\int \sin\theta d\theta e^{\mathbf{i}qr\cos\theta} = -\frac{i}{qr}[e^{iqr}-e^{-iqr}],$$

we have

$$G_0^{(\pm)}(\mathbf{r}) = G_0^{(\pm)}(r) = \frac{1}{(2\pi)^3}\int q^2 dq(-\frac{2\pi i}{qr})\frac{e^{iqr}-e^{-iqr}}{q^2-(k^2\pm i\varepsilon)}$$

since $G_0^{(\pm)}(\mathbf{r})$ depends only on *r*.

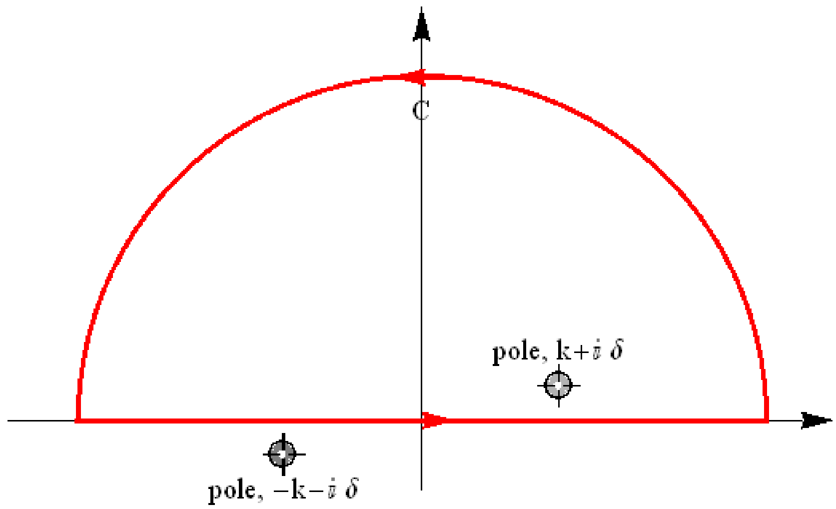
or

$$G_0^{(\pm)}(r) = \frac{1}{4\pi^2 ir}\int_0^\infty qdq\frac{e^{iqr}-e^{-iqr}}{q^2-(k^2\pm i\varepsilon)} = \frac{1}{4\pi^2 ir}\int_{-\infty}^\infty qdq\frac{e^{iqr}}{q^2-(k^2\pm i\varepsilon)}$$

(a)
This function with (+iε) has a single pole at

$$q = \pm\sqrt{k^2+i\varepsilon} = \pm k(1+\frac{i\varepsilon}{2k}) = \pm(k+\frac{i\varepsilon}{2}) = \pm(k+i\delta)$$

with $\delta = \varepsilon/2$.



Since r>0, the path of integration can be closed by an infinite semicircle in the upper half-plane (Jordan's lemma).

$$G_0^{(+)}(r) = \frac{1}{4\pi^2 ir}\oint_C qdq\frac{e^{iqr}}{q^2-(k^2+i\varepsilon)}$$
$$= \frac{1}{4\pi^2 ir}2\pi i\,\mathrm{Res}(q=k+i\delta) = \frac{1}{4\pi r}e^{ikr}$$

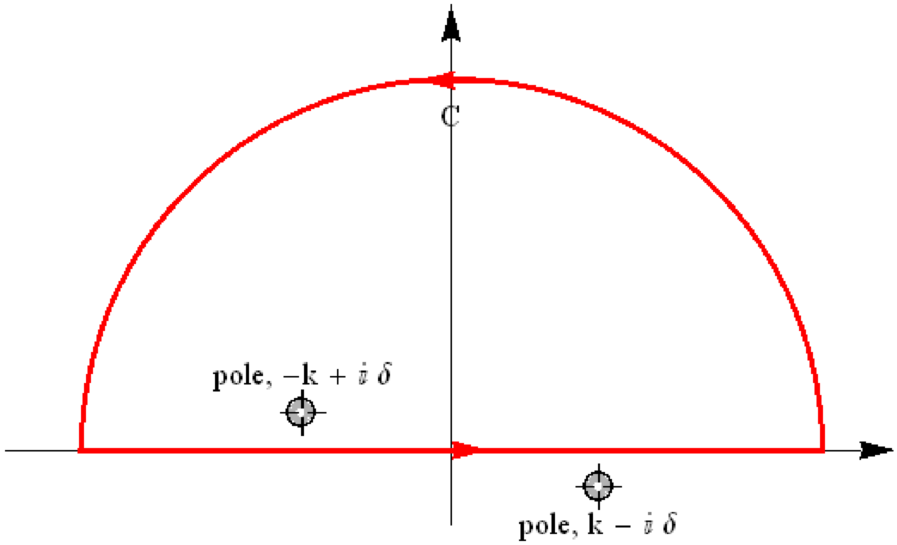
(retarded Green's function).

Similarly,

$$G_0^{(-)}(r) = \frac{1}{4\pi^2 ir}\oint_C qdq\frac{e^{iqr}}{q^2-(k^2-i\varepsilon)}$$
$$= \frac{1}{4\pi^2 ir}2\pi i\,\mathrm{Res}(q=-k+i\delta) = \frac{1}{4\pi r}e^{-ikr}$$

((**Advanced Green's function**))

Note that there is a simple pole at $q = -k+i\delta$ in the upper-half plane (r>0).



10.8. Green's function (modified Helmholtz)

We now consider the form of the Green's function.

$$(\Delta - k^2)G_0(\mathbf{r}) = -\delta(\mathbf{r})$$

The Fourier transform of $G_0(\mathbf{r})$ is defined as

$$G_0(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}}\int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} G_0(\mathbf{r}) .$$

The inverse Fourier transform is also defined as

$$G_0(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\int d\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{r}} G_0(\mathbf{q}) ,$$

where

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{r}} .$$

Then

$$\begin{aligned}\frac{1}{(2\pi)^{3/2}}\int d\mathbf{q}(\Delta - k^2)e^{i\mathbf{q}\cdot\mathbf{r}} G_0(\mathbf{q}) &= \frac{1}{(2\pi)^{3/2}}\int d\mathbf{q}(-q^2 - k^2)e^{i\mathbf{q}\cdot\mathbf{r}} G_0(\mathbf{q}) \\ &= -\delta(\mathbf{r}) = -\frac{1}{(2\pi)^3}\int d\mathbf{q} e^{i\mathbf{q}\cdot\mathbf{r}}\end{aligned},$$

or

$$G_0(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{q^2 + k^2} .$$

Thus the Green's function is rewritten as

$$G_0(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d\mathbf{q} e^{\mathbf{iq\cdot r}} \frac{1}{q^2 + k^2}$$

$$G_0(\mathbf{r}) = \frac{1}{(2\pi)^3} \int\int 2\pi q^2 dq \sin\theta d\theta e^{\mathbf{i}qr\cos\theta} \frac{1}{q^2 + k^2} .$$

Note

$$\int \sin\theta d\theta e^{\mathbf{i}qr\cos\theta} = -\frac{i}{qr}[e^{iqr} - e^{-iqr}] ,$$

we have

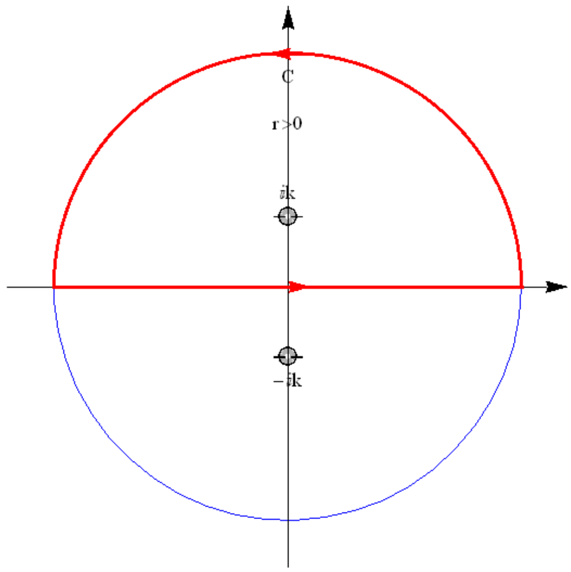
$$G_0(\mathbf{r}) = G_0(r) = \frac{1}{(2\pi)^3} \int q^2 dq (-\frac{2\pi\mathbf{i}}{qr}) \frac{e^{iqr} - e^{-iqr}}{q^2 + k^2} ,$$

since $G_0(\mathbf{r})$ depends only on *r*. This equation can be rewritten as

$$G_0(r) = \frac{1}{4\pi^2 ir} \int_0^\infty q dq \frac{e^{iqr} - e^{-iqr}}{q^2 + k^2} = \frac{1}{4\pi^2 ir} \int_{-\infty}^\infty q dq \frac{e^{iqr}}{q^2 + k^2}$$

This function has a single pole at

$$q = \pm ik$$



Since r>0, the path of integration can be closed by an infinite semicircle in the upper half-plane (Jordan's lemma).

$$G_0(r) = \frac{1}{4\pi^2 ir}\oint_C qdq\frac{e^{iqr}}{q^2+k^2} = \frac{1}{4\pi^2 ir}2\pi i\,\mathrm{Re}\,s(q = ik) = \frac{1}{4\pi r}e^{-kr}$$

((Note))

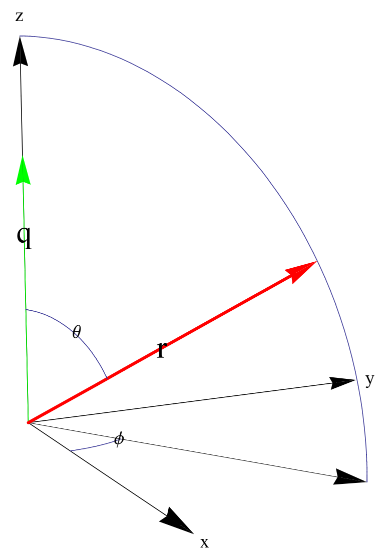
Yukawa potential $U(r)$ is described by

$$U(r) = g\frac{e^{-\kappa r}}{r}$$

where g is constant and κ>0. The Fourier transform of $U(r)$ is given by

$$u(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}}\int d\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}g\frac{e^{-\kappa r}}{r}$$

For convenience, we assume that the direction of $\boldsymbol{q}$ is the z axis. The angle between $\boldsymbol{r}$ and $\boldsymbol{q}$ is θ.



$$\mathbf{q}\cdot\mathbf{r} = qr\cos\theta\,,$$

$$d\mathbf{r} = r^2\sin\theta dr d\theta d\phi\,,$$

$$\begin{aligned}
u(\mathbf{q}) &= \frac{g}{(2\pi)^{3/2}}\int_0^\infty r^2\frac{e^{-\kappa r}}{r}dr\int_0^\pi \sin\theta d\theta\int_0^{2\pi} d\phi e^{-\mathbf{i}qr\cos\theta} \\
&= \frac{4\pi g}{(2\pi)^{3/2}}\int_0^\infty drr^2\frac{e^{-\kappa r}}{r}\frac{\sin(qr)}{qr} \\
&= \frac{4\pi g}{(2\pi)^{3/2}q}\int_0^\infty dre^{-\kappa r}\sin(qr) \\
&= \frac{g}{(2\pi)^{1/2}iq}\int_0^\infty dr[e^{-(\kappa-iq)r}-e^{-(\kappa+iq)r}] \\
&= \frac{g}{(2\pi)^{1/2}iq}\left(\frac{1}{\kappa-iq}-\frac{1}{\kappa+iq}\right) \\
&= \frac{2g}{(2\pi)^{1/2}}\left(\frac{1}{\kappa^2+q^2}\right)
\end{aligned}$$

10.9. One-dimensional diffusion

We now consider the heat diffusion equation

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{1}{\kappa}\frac{\partial\psi(x,t)}{\partial t}$$

with the initial condition $\psi(x,0) = f(x)$, where the diffusion constant k is proportional to the thermal conductivity of the material and inversely proportional to its heat capacity per unit volume.

$$\Psi(k,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-ikx}\psi(x,t)dx$$

$$\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{ikx}\Psi(k,t)dk$$

We note that

$$\frac{\partial^2\psi(x,t)}{\partial x^2}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}[-k^2e^{ikx}\Psi(k,t)]dk$$

$$\frac{1}{\kappa}\frac{\partial\psi(x,t)}{\partial t}=\frac{1}{\kappa}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{ikx}\frac{\partial\Psi(k,t)}{\partial t}dk$$

Then the differential equation becomes

$$\int_{-\infty}^{\infty}[\frac{1}{\kappa}\frac{\partial\Psi(k,t)}{\partial t}+k^2\Psi(k,t)]e^{ikx}dk=0$$

or

$$\frac{\partial\Psi(k,t)}{\partial t}+\kappa k^2\Psi(k,t)=0$$

The solution of this equation is given by

$$\Psi(k,t)=\exp[-\kappa k^2 t]\Psi(k,t=0),$$

where

$$\Psi(k,t=0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-ikx}\psi(x,t=0)dx=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-ikx'}f(x')dx'.$$

The inverse Fourier transform becomes

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \exp[-\kappa k^2 t] \Psi(k, t=0) dk$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' \exp[-\kappa k^2 t + ik(x-x')] f(x')$$

Here we note that

$$-\kappa t k^2 + ik(x-x') = -\kappa t[k - \frac{i(x-x')}{2\kappa t}]^2 - \frac{(x-x')^2}{4\kappa t}$$

Then we have

$$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' \exp\{-\kappa t[k - \frac{i(x-x')}{2\kappa t}]^2\} \exp[-\frac{(x-x')^2}{4\kappa t}] f(x')$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx' f(x') \exp[-\frac{(x-x')^2}{4\kappa t}] \int_{-\infty}^{\infty} dk \exp\{-\kappa t[k - \frac{i(x-x')}{2\kappa t}]^2\}$$

$$\int_{-\infty}^{\infty} dk \exp\{-\kappa t[k - \frac{i(x-x')}{2\kappa t}]^2\} = \int_{-\infty}^{\infty} dk \exp(-\kappa t k^2)$$

$$= \frac{1}{\sqrt{\kappa t}} \int_{-\infty}^{\infty} dk' \exp(-k'^2) = \sqrt{\frac{\pi}{\kappa t}}$$

Finally we get

$$\psi(x,t) = \frac{1}{\sqrt{4\pi\kappa t}} \int_{-\infty}^{\infty} dx' f(x') \exp[-\frac{(x-x')^2}{4\kappa t}]$$

This takes the form of a convolution integral.

Suppose that $f(x) = \psi_0 \delta(x)$. Then we have

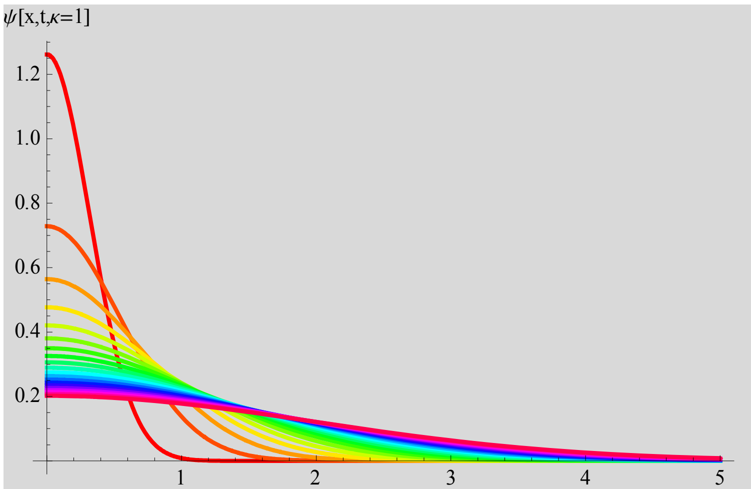
$$\psi(x,t) = \frac{1}{\sqrt{4\pi\kappa t}} \int_{-\infty}^{\infty} dx' \psi_0 \delta(x') \exp[-\frac{(x-x')^2}{4\kappa t}]$$

$$= \frac{1}{\sqrt{4\pi\kappa t}} \psi_0 \exp[-\frac{x^2}{4\kappa t}]$$

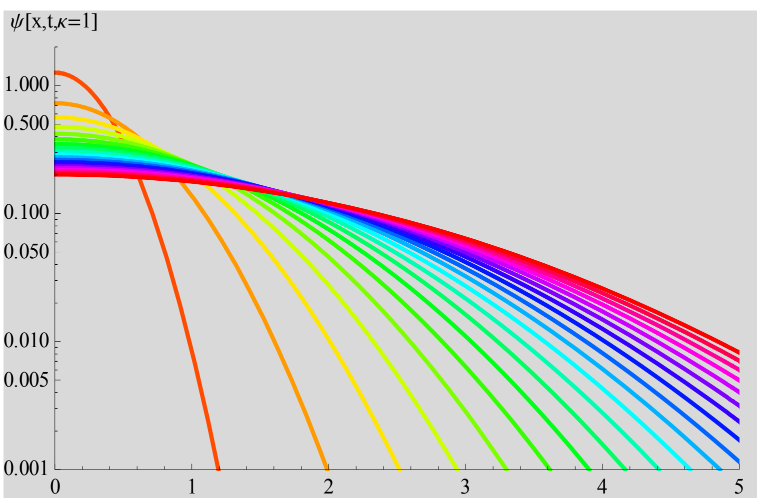
((**Mathematica**))

```
ψ[x_, t_, κ_] := Exp[-x^2/(4 κ t)] / Sqrt[4 π κ t]
```

```
ew1 = Plot[Evaluate[Table[ψ[x, t, 1], {t, 0.05, 2, 0.1}]],
  {x, 0, 5}, PlotStyle → Table[{Hue[0.05 i], Thick}, {i, 0, 20}],
  PlotRange → All , Background → LightGray,
  AxesLabel → {"t", "ψ[x,t,κ=1]"}]
```




```
ew2 = LogPlot[Evaluate[Table[ψ[x, t, 1], {t, 0.05, 2, 0.1}]],
  {x, 0, 5}, PlotStyle → Table[{Hue[0.05 i], Thick}, {i, 1, 20}],
  PlotRange → {{0, 5}, {0.001, 2}}, Background → LightGray,
  AxesLabel → {"t", "ψ[x,t,κ=1]"}]
```



10.10. Step function (iε prescription)

(i) Method-1

We now consider a step function

$$f(t) = \lim_{\varepsilon \to 0+} \Theta(t)\exp(-\varepsilon t),$$

where $\Theta(t)$ is a Heaviside step function and ε is a positive constant ($\varepsilon \to 0$)

The Fourier transform of $f(t)$:

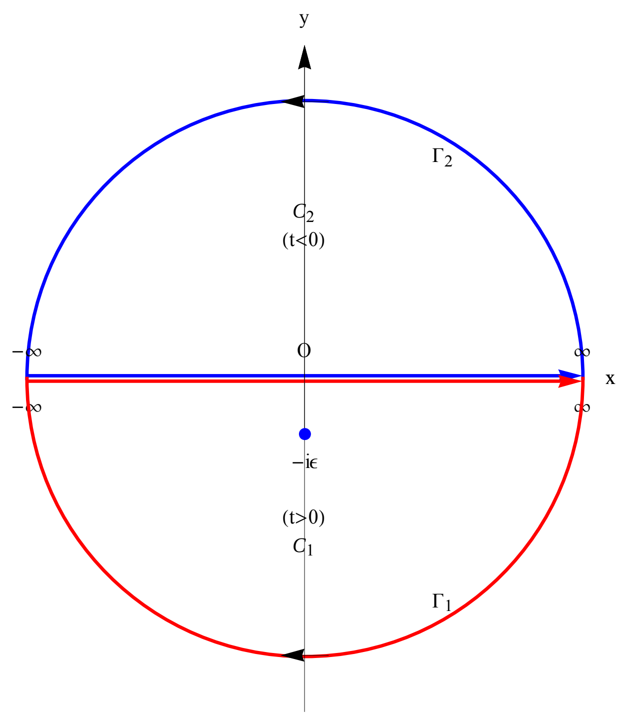
$$\begin{aligned}
F(\omega) &= \lim_{\varepsilon \to 0+} \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{i\omega t} e^{-\varepsilon t} dt \\
&= \lim_{\varepsilon \to 0+} \frac{1}{\sqrt{2\pi}} \frac{e^{i\omega t} e^{-\varepsilon t}}{i\omega - \varepsilon} \Big|_0^\infty \\
&= \lim_{\varepsilon \to 0+} \frac{1}{\sqrt{2\pi}} \frac{-1}{i\omega - \varepsilon} \\
&= \lim_{\varepsilon \to 0+} \frac{1}{\sqrt{2\pi}} \frac{i}{\omega + i\varepsilon}
\end{aligned}$$

The inverse Fourier transform:

$$\begin{aligned}
f(t) &= \frac{1}{\sqrt{2\pi}} \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} e^{-i\omega t} \frac{1}{\sqrt{2\pi}} \frac{i}{\omega + i\varepsilon} d\omega \\
&= \frac{i}{2\pi} \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega + i\varepsilon} d\omega
\end{aligned}$$

We need to calculate the integral

$$\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega + i\varepsilon} d\omega$$



From the Jordan's lemma, we have

$$I = \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega + i\varepsilon} d\omega = \oint \frac{e^{-izt}}{z + i\varepsilon} dz$$

The integrant has a simple pole in the lower half-plane just below the real axis. The closure is made either up or down according to the sign of t:

(a) For $t>0$
We need to use the lower half- plane (clock wise)

$$I = -2\pi i \operatorname{Res}(z = -i\varepsilon) = -2\pi i e^{-\varepsilon t}.$$

(b) For $t<0$
We need to use the upper half- plane. Since there is no pole in this plane, we have

$$I = 0.$$

Then

$$f(t) = \frac{i}{2\pi} \lim_{\varepsilon \to 0+} (-2\pi i e^{-\varepsilon t}) = 1 \quad \text{for } t>0, \text{ and } f(t) = 0 \text{ for } t<0.$$

in other words,

$$f(t) = \Theta(t)$$

(ii) Method-II

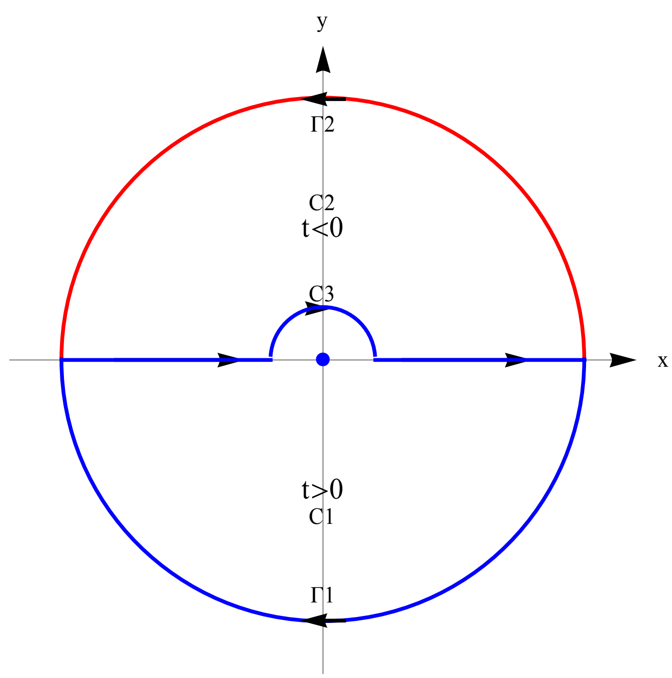
Alternatively we show that

$$\boxed{\frac{P}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{-i\omega t}}{\omega}d\omega = \frac{1}{2}[1 - 2\Theta(t)]}$$

where P denotes the principal-value integral.

To show this formula, we consider the integral around the contour C_1 (t>0) and the contour C_2 (t<0)

$$\oint \frac{e^{-izt}}{z}dz$$



For t>0 (the lower half-plane)

$$\oint_{C_1}\frac{e^{-izt}}{z}dz = P\int_{-\infty}^{\infty}\frac{e^{-i\omega t}}{\omega}d\omega + \oint_{C_3}\frac{e^{-izt}}{z}dz + \oint_{\Gamma_1}\frac{e^{-izt}}{z}dz = -2\pi i \operatorname{Re}s[z=0]$$

where the integral around the contour Γ_1 is zero according to the Jordan's lemma. The radius of the contour C_3 is infinitesimally small. There is a simple pole at $z = 0$ inside the contour C_1. The rotation of the contour C_1 is clock-wise. Noting that

$$\oint_{C_3} \frac{e^{-izt}}{z} dz = -\pi i \operatorname{Res}[z=0]$$

we have

$$P\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega} d\omega = -\pi i \operatorname{Res}[z=0] = -\pi i \qquad \text{for } t>0.$$

For $t<0$ (the upper half-plane)

$$\oint_{C_2} \frac{e^{-izt}}{z} dz = P\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega} d\omega + \oint_{C_3} \frac{e^{-izt}}{z} dz + \oint_{\Gamma_2} \frac{e^{-izt}}{z} dz = 0$$

where the integral around the contour Γ_2 is zero according to the Jordan's lemma. The radius of the contour C_3 is infinitesimally small. There is no pole inside the contour C_2. The rotation of the contour C_2 is counter clock-wise. Noting that

$$\oint_{C_3} \frac{e^{-izt}}{z} dz = -\pi i \operatorname{Res}(z=0),$$

we have

$$P\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega} d\omega = \pi i, \qquad \text{for } t<0$$

Then we have

$$\boxed{\Theta(t) = \frac{1}{2} - \frac{1}{2\pi i} P\int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\omega} d\omega}.$$

What is the Fourier transform of $\Theta(t)$ using this expression?

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t}\Theta(t) dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} \frac{1}{2} dt - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} dt \frac{1}{2\pi i} P\int_{-\infty}^{\infty} \frac{e^{-i\omega' t}}{\omega'} d\omega'$$

or

$$F(\omega)=\frac{1}{\sqrt{2\pi}}\pi\delta(\omega)-\frac{1}{\sqrt{2\pi}}\frac{1}{2\pi i}P\int_{-\infty}^{\infty}\frac{1}{\omega'}d\omega'\int_{-\infty}^{\infty}dte^{it(\omega-\omega')}$$

$$=\frac{1}{\sqrt{2\pi}}\pi\delta(\omega)-\frac{1}{\sqrt{2\pi}}\frac{1}{2\pi i}P\int_{-\infty}^{\infty}\frac{1}{\omega'}d\omega' 2\pi\delta(\omega-\omega')$$

$$=\frac{1}{\sqrt{2\pi}}[\pi\delta(\omega)+iP\frac{1}{\omega}]$$

Since $F(\omega)=\lim_{\varepsilon\to 0+}\frac{1}{\sqrt{2\pi}}\frac{i}{\omega+i\varepsilon}$, we obtain

$$F(\omega)=\lim_{\varepsilon\to 0+}\frac{1}{\sqrt{2\pi}}\frac{i}{\omega+i\varepsilon}=\frac{1}{\sqrt{2\pi}}[\pi\delta(\omega)+iP\frac{1}{\omega}]$$

or

$$\lim_{\varepsilon\to 0+}\frac{1}{\omega+i\varepsilon}=P\frac{1}{\omega}-\pi i\delta(\omega).$$

Similarly we have

$$\lim_{\varepsilon\to 0+}\frac{1}{\omega-i\varepsilon}=P\frac{1}{\omega}+\pi i\delta(\omega).$$

or

$$\lim_{\varepsilon\to 0+}[\frac{1}{\omega-i\varepsilon}-\frac{1}{\omega+i\varepsilon}]=2\pi i\delta(\omega)$$

((Note)) We have several formula , which are derived from the above discussion.

$$\mathbf{F}^{-1}[\frac{1}{\sqrt{2\pi}}[\pi\delta(\omega)+iP\frac{1}{\omega}]=\mathbf{F}^{-1}[\frac{1}{\sqrt{2\pi}}\frac{i}{\omega+i\varepsilon}]=\Theta(t).$$

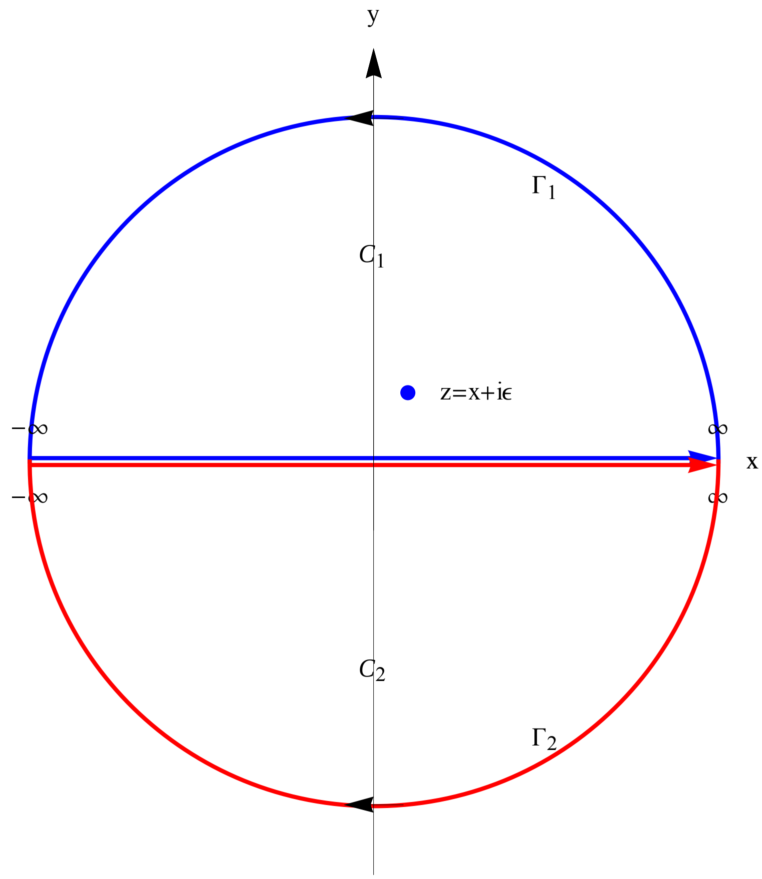
$$\mathbf{F}^{-1}[\frac{1}{\sqrt{2\pi}}\frac{i}{\omega-\omega_0+i\varepsilon}]]=e^{-i\omega_0 t}\Theta(t).$$

$$\mathbf{F}^{-1}[\frac{1}{\sqrt{2\pi}}\frac{i}{\omega+\omega_0+i\varepsilon}]]=e^{i\omega_0 t}\Theta(t).$$

10.11 Kramers-Kronig relations

The **Kramers–Kronig relations** are mathematical properties, connecting the real and imaginary parts of any complex function which is analytic in the upper half-plane. These relations are often used to relate the real and imaginary parts of response functions in physical systems because causality implies the analyticity condition is satisfied, and conversely, analyticity implies causality of the corresponding physical system. The relation is named in honor of Ralph Kronig and Hendrik Anthony Kramers.

http://en.wikipedia.org/wiki/Kramers%E2%80%93Kronig_relation



From the Cauchy relation

$$\frac{1}{2\pi i}\oint_{C_1}\frac{f(\zeta)}{\zeta - z}d\varsigma = f(z) = \frac{1}{2\pi i}\int_{\Gamma_1}\frac{f(\zeta)}{\zeta - z}d\varsigma + \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{f(x')}{x'-z}dx'$$

where the contour C_1 is in the upper half plane. There is a simple point at $\zeta = z$ inside the contour C_1. The function $f(\zeta)$ is regular inside of the contour C_1. According to the Jordan's lemma, the integral around the upper half-circle Γ_1 reduces to zero when the radius tends to infinity. In this formula, we put

$$z = x + i\varepsilon$$

where $\varepsilon>0$. Then we have

$$f(x+i\varepsilon)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{f(x')}{x'-x-i\varepsilon}dx'$$

Here we use the formula,

$$\lim_{\varepsilon\to 0+}\frac{1}{x'-x-i\varepsilon}=P\frac{1}{x'-x}+\pi i\delta(x-x')$$

$$\begin{aligned}
f(x)&=\lim_{\varepsilon\to 0}f(x+i\varepsilon)\\
&=\frac{1}{2\pi i}\{P\int_{-\infty}^{\infty}\frac{f(x')}{x'-x}dx'+\pi i\int_{-\infty}^{\infty}\delta(x-x')f(x')dx'\}\\
&=\frac{1}{2\pi i}P\int_{-\infty}^{\infty}\frac{f(x')}{x'-x}dx'+\frac{1}{2}f(x)
\end{aligned}$$

or

$$f(x)=\frac{1}{\pi i}P\int_{-\infty}^{\infty}\frac{f(x')}{x'-x}dx'$$

We assume that

$$f(x)=\mathrm{Re}[f(x)]+i\,\mathrm{Im}[f(x)]$$

Then

$$\begin{aligned}
\mathrm{Re}[f(x)]+i\,\mathrm{Im}[f(x)&=\frac{1}{\pi i}P\int_{-\infty}^{\infty}\frac{\mathrm{Re}[f(x')]+i\,\mathrm{Im}[f(x')]}{x'-x}dx'\\
&=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{-i\,\mathrm{Re}[f(x')]+\mathrm{Im}[f(x')]}{x'-x}dx'
\end{aligned}$$

The real part:

$$\mathrm{Re}[f(x)]=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\mathrm{Im}[f(x')]}{x'-x}dx'$$

The imaginary part:

$$\mathrm{Im}[f(x)=-\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\mathrm{Re}[f(x')]}{x'-x}dx'$$

These are called dispersion relation and very useful in optics and in statistical mechanics.

10.12 $|x\rangle$ and $|p\rangle$ representation (quantum mechanics)

(a) $|x\rangle$ representation

The wave function $\psi(x)$ can be described by

$$\psi(x) = \langle x|\psi\rangle$$

or

$$\psi^*(x) = \langle x|\psi\rangle^* = \langle \psi|x\rangle$$

$|x'\rangle$ is the eigenket of $\hat{x}$ with the eigenvalue x'.
$|x'\rangle$ is the state vector that a particle is located at $x = x'$.

$|\langle x|\psi\rangle|^2 dx$: probability of finding a particle between x and x+dx.

$$\hat{x}|x'\rangle = x'|x'\rangle \qquad \langle x''|\hat{x}|x'\rangle = \langle x''|x'|x'\rangle = x'\langle x''|x'\rangle = x'\delta(x''-x')$$

Note that the eigenstate $|x\rangle$ obeys the orthonormality condition

$$\langle x''|x'\rangle = \delta(x''-x')$$

where $\delta(x''-x')$ is the Dirac delta function.

The closure relation:

$$\int_{-\infty}^{\infty} dx|x\rangle\langle x| = \hat{1}.$$

The inner product is rewritten as

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

The state $|x\rangle$ is also rewritten as

$$|x\rangle = \left(\int_{-\infty}^{\infty} dx'|x'\rangle\langle x'|\right)|x\rangle$$
$$= \int_{-\infty}^{\infty} dx'|x'\rangle\langle x'|x\rangle$$
$$= \int_{-\infty}^{\infty} dx'|x'\rangle\delta(x-x')$$

$$\langle x|\psi\rangle = \int_{-\infty}^{\infty} \langle x|x'\rangle\langle x'|\psi\rangle dx'$$
$$= \int_{-\infty}^{\infty} \delta(x-x')\langle x'|\psi\rangle dx'$$

10.13 $|p\rangle$ representation

$$\psi(p) = \langle p|\psi\rangle$$

$|p\rangle$**:** state that a particle has a linear momentum *p*.

$$\hat{p}|p'\rangle = p'|p'\rangle \qquad \langle p''|\hat{p}|p'\rangle = \langle p''|p'|p'\rangle = p'\langle p''|p'\rangle = p'\delta(p''-p')$$

$|\langle p|\psi\rangle|^2 dp$: probability of finding a particle having a linear momentum between *p* and *p* +d*p*.

$$|p\rangle = \left(\int_{-\infty}^{\infty} dp'|p'\rangle\langle p'|\right)|p\rangle$$
$$= \int_{-\infty}^{\infty} dp'|p'\rangle\langle p'|p\rangle = \int_{-\infty}^{\infty} dp'|p'\rangle\delta(p'-p) = |p\rangle$$

$$\langle p'|p\rangle = \delta(p-p')$$

Closure relation

$$\int_{-\infty}^{\infty} dp|p\rangle\langle p| = \hat{1}$$

10.14 Transformation function

$$\hat{p}|p'\rangle = p'|p'\rangle$$

Note that in general, (**formula**)

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

(which will be discussed later, translation operator)

$$\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|x'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x')$$

We now consider the transformation function

$$\begin{aligned}\langle x|\hat{p}|p\rangle &= p\langle x|p\rangle \\ &= \int dx'\langle x|\hat{p}|x'\rangle\langle x'|p\rangle \\ &= \int dx'\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x')\langle x'|p\rangle \\ &= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle\end{aligned}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle$$

or

using the above formula

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

we put $|\psi\rangle = |p\rangle$

$$\langle x|\hat{p}|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle$$

The solution is

$$\langle x|p\rangle = C\exp(\frac{ipx}{\hbar}),$$

where C is the constant which is determined from the normalization condition.

$$\langle x|x'\rangle = \int \langle x|p\rangle\langle p|x'\rangle dp$$
$$= |C|^2 \int \exp(\frac{ipx}{\hbar})\exp(-\frac{ipx'}{\hbar})dp$$
$$= |C|^2 \int \exp[\frac{ip}{\hbar}(x-x')]dp$$
$$= |C|^2 2\pi\delta(\frac{x-x'}{\hbar})$$

or

$$\langle x|x'\rangle = \delta(x-x')$$
$$= |C|^2 2\pi\delta(\frac{x-x'}{\hbar}) = |C|^2 2\pi\hbar\delta(x-x'),$$

from the property of the Dirac delta function (we will discussed later)

or

$$|C| = \frac{1}{\sqrt{2\pi\hbar}}.$$

Here we use

$$C = \frac{1}{\sqrt{2\pi\hbar}}.$$

The transformation function

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{ipx}{\hbar}),$$

or

$$\langle p|x\rangle = \langle x|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}}\exp(-\frac{ipx}{\hbar}).$$

10.15 Fourier transform in the *x*-*k* representation

We can define the Fourier transform using the transformation function

$$\langle p|\psi\rangle = \int \langle p|x\rangle\langle x|\psi\rangle dx = \frac{1}{\sqrt{2\pi\hbar}}\int \exp(-\frac{ipx}{\hbar})\langle x|\psi\rangle dx$$

$$\langle x|\psi\rangle = \int \langle x|p\rangle\langle p|\psi\rangle dp = \frac{1}{\sqrt{2\pi\hbar}}\int \exp(\frac{ipx}{\hbar})\langle p|\psi\rangle dp$$

Using the Fourier transform, we can confirm the formula

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

In fact,

$$\begin{aligned}
\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\int \frac{\hbar}{i}\frac{\partial}{\partial x}\exp(\frac{ipx}{\hbar})\langle p|\psi\rangle dp \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int p\exp(\frac{ipx}{\hbar})\langle p|\psi\rangle dp \\
&= \int p\langle x|p\rangle\langle p|\psi\rangle dp \\
&= \int \langle x|\hat{p}|p\rangle\langle p|\psi\rangle dp = \langle x|\hat{p}|\psi\rangle
\end{aligned}$$

we define the transformation function

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

or

$$\langle p|x\rangle = \langle p|x\rangle^{*} = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}$$

In summary, we have

$$\langle p|\psi\rangle = \int_{-\infty}^{\infty}\langle p|x\rangle\langle x|\psi\rangle dx = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}\langle x|\psi\rangle dx$$

and

$$\langle x|\psi\rangle = \int_{-\infty}^{\infty}\langle x|p\rangle\langle p|\psi\rangle dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{ipx/\hbar}\langle p|\psi\rangle dp$$

Here we introduce *k*, as $p = \hbar k$

$$\begin{aligned}\langle p|p'\rangle &= \delta(p-p') \\ &= \delta[\hbar(k-k')] \\ &= \frac{1}{\hbar}\delta(k-k') = \frac{1}{\hbar}\langle k|k'\rangle\end{aligned}$$

Then we have the following relation

$$|p\rangle = \frac{1}{\sqrt{\hbar}}|k\rangle$$

$$\langle x|p\rangle = \frac{1}{\sqrt{\hbar}}\langle x|k\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

or

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx}$$

and

$$\langle k|x\rangle = \langle x|k\rangle^* = \frac{1}{\sqrt{2\pi}}e^{-ikx}$$

From the closure relation

$$\int_{-\infty}^{\infty} dp|p\rangle\langle p| = \hat{1}$$

we can derive the expression of the closure relation for $|k\rangle$.

$$\int_{-\infty}^{\infty} dk|k\rangle\langle k| = \hat{1}$$

since

$$\int_{-\infty}^{\infty} \hbar dk\left(\frac{1}{\sqrt{\hbar}}\right)^2 |k\rangle\langle k|dp = \hat{1}$$

In summary:

Fourier transform in the *x*-*k* space

$$\langle k|\psi\rangle = \int_{-\infty}^{\infty} \langle k|x\rangle\langle x|\psi\rangle dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx}\langle x|\psi\rangle dx$$

and

$$\langle x|\psi\rangle = \int_{-\infty}^{\infty} \langle x|k\rangle\langle k|\psi\rangle dk = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\langle k|\psi\rangle dk$$

10.16 Wave packet in quantum mechanics
10.16.1 Gaussian wave packet

A free particle (electron) in quantum mechanics is described by a plane wave

$$\exp[ik(x - x0) - \frac{\hbar k^2}{2m}t]$$

Combining waves of adjacent momentum with an amplitude weighting factor $\chi(k)$, we form a wave packet,

$$\psi(x,t) = \int_{-\infty}^{\infty} dk\chi(k)\exp[k(x - x_0) - \frac{\hbar k^2}{2m}t]$$

with

$$\chi(k) = A\exp[-\frac{(k-k_0)^2}{2\sigma^2}] \qquad \text{(Gaussian)}$$

$$\psi(x,t=0) = \int_{-\infty}^{\infty} dk\chi(k)\exp[k(x - x_0)]$$

$$= \sqrt{2\pi}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\chi(k)\exp[k(x - x_0)]$$

(a) What is the form of $\psi(x, t = 0)$?

$$\psi(x,t=0) = \sqrt{2\pi}\sigma A\exp[ik_0(x - x_0) - \frac{1}{2}\sigma^2(x - x_0)^2].$$

(b) Using the known value of χ(k), integrate to get the explicit form of $\psi(x, t)$. Note that this wave packet diffuses or spread out with time.

$$\psi(x,t) = A\frac{\sqrt{2\pi}\sigma}{\sqrt{1+\frac{i\hbar t\sigma^2}{m}}}\exp[\frac{ik_0(x-x_0-\frac{k_0\hbar t}{2m})-\frac{1}{2}\sigma^2(x-x_0)^2}{1+\frac{i\hbar t\sigma^2}{m}}]$$

or

$$|\psi(x,t)|^2 = \frac{\sigma}{\sqrt{\pi}\sqrt{1+\frac{\hbar^2 t^2\sigma^4}{m^2}}}\exp[-\frac{\sigma^2(x-x_0-\frac{k_0\hbar t}{m})^2}{1+\frac{\hbar^2 t^2\sigma^4}{m^2}}]$$

where the wave function is normalized;

$$A = \frac{1}{\sqrt{2\sigma}\pi^{3/4}}.$$

10.16.2 Physical meaning

The position of particle:

$$\langle x\rangle = x_0 + \frac{k_0 t\hbar}{m}$$

The velocity of particle:

$$\frac{d\langle x\rangle}{dt} = \frac{\hbar k_0}{m} = v_0$$

The spreading of the wave packet:

$$\Delta x = \frac{1}{\sqrt{2}\sigma}\sqrt{1+\frac{t^2\hbar^2}{m^2}\sigma^4}$$

The amplitude of $|\psi(x,t)|^2$:

$$Amplitude = \frac{\sigma}{\sqrt{\pi}}\frac{1}{\sqrt{1+\frac{t^2\hbar^2}{m^2}\sigma^4}}.$$

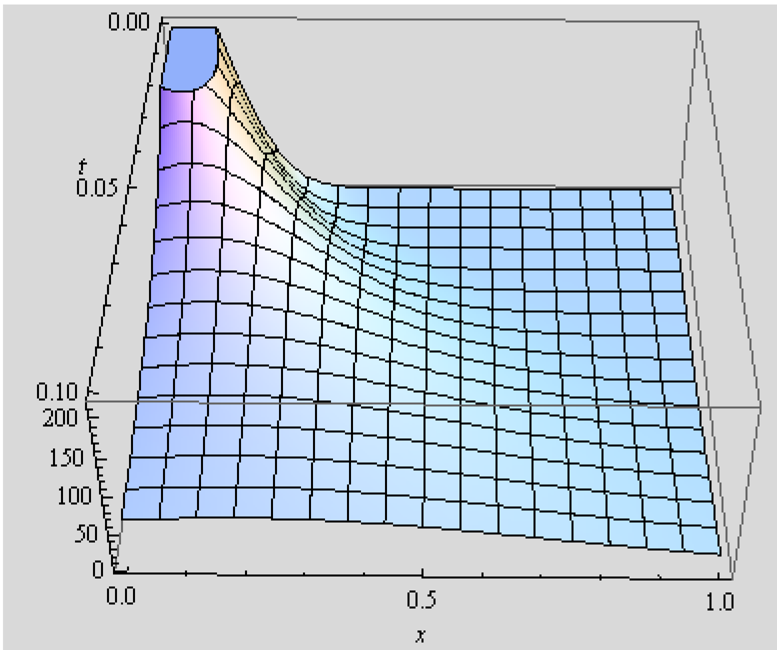
The evolution of the wave packet is not confined to a simple displacement at a velocity v_0. The wave packet also undergoes a deformation.

The Heisenberg's principle of uncertainty:

$$(\Delta x)(\Delta k) = \frac{1}{\sqrt{2}}\sqrt{1+\frac{t^2\hbar^2}{m^2}\sigma^4} > \frac{1}{\sqrt{2}}.$$

where $\Delta k = \sigma$.

((**Mathematica**))



Plot3D of $|\psi(x,t)|^2$ in the *x*-*t* plane.

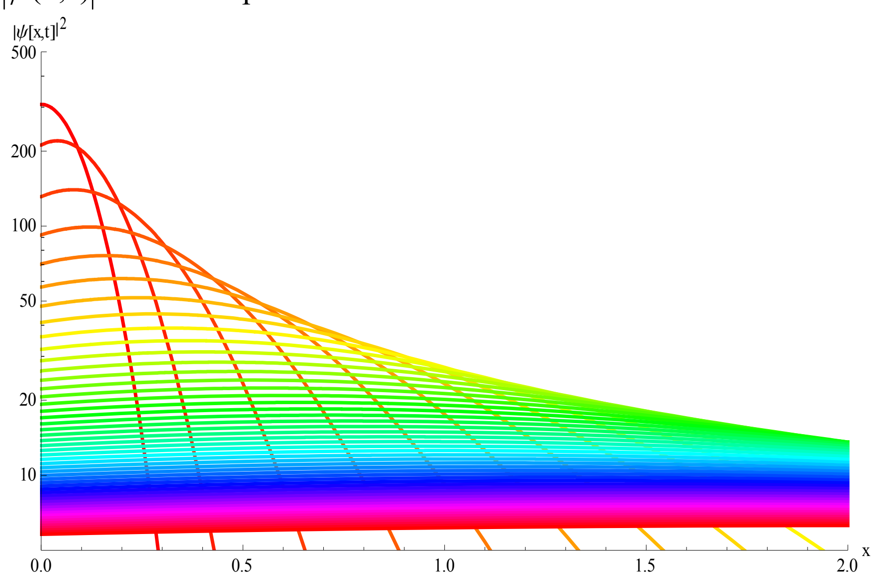


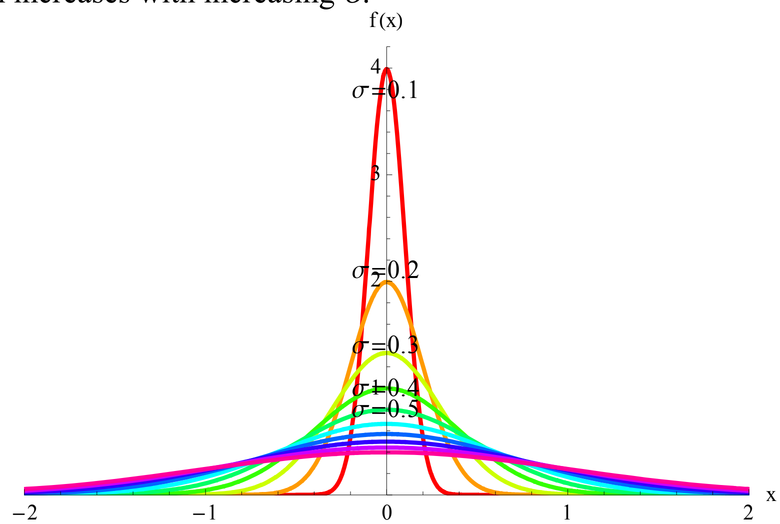
Fig. Spread of wave packet, , where σ = 7. m = 1. $\hbar = 1$. x_0 = 0. k_0 = 2. t is changed between 0 and 1. Δt = 0.02.

10.17 Fourier transform of Gaussian distribution function

The Gaussian distribution function is given by

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{x^2}{2\sigma^2}).$$

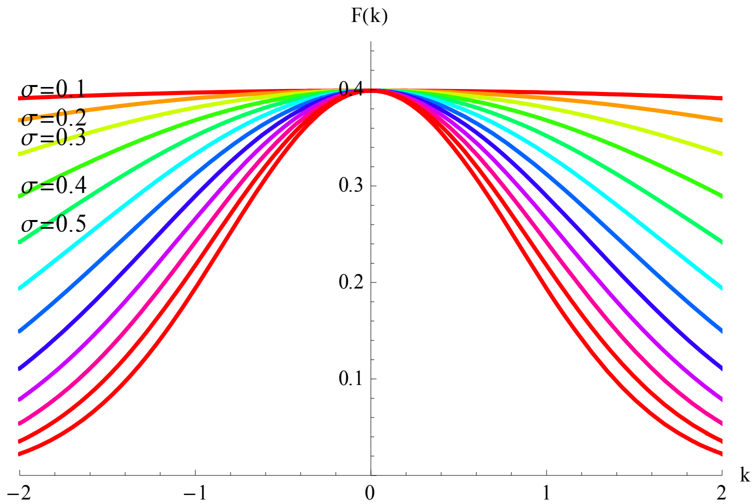
The line width increases with increasing σ.



The Fourier transform of $f(x)$ is given by

$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx} f(x)dx = \frac{1}{\sqrt{2\pi}}\exp(-\frac{1}{2}k^2\sigma^2)$$

The width of the line shape decreases with increasing σ.



10.18 Heisenberg's principle of uncertainty

Werner Heisenberg (5 December 1901– 1 February 1976) was a German theoretical physicist who made foundational contributions to quantum mechanics and is best known for asserting the uncertainty principle of quantum theory. In addition, he made important contributions to nuclear physics, quantum field theory, and particle physics. Heisenberg, along with Max Born and Pascual Jordan, set forth the matrix formulation of quantum mechanics in 1925. Heisenberg was awarded the 1932 Nobel Prize in Physics for the creation of quantum mechanics, and its application especially to the discovery of the allotropic forms of hydrogen.

http://en.wikipedia.org/wiki/Werner_Heisenberg

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(1)

$$\left\langle \hat{p}^n \right\rangle = \langle\psi|\hat{p}^n|\psi\rangle = \int_{-\infty}^{\infty}\langle\psi|p\rangle\langle p|\hat{p}^n|\psi\rangle dp = \int_{-\infty}^{\infty}\langle p|\psi\rangle^* p^n\langle p|\psi\rangle dp$$

(2)

$$\left\langle \hat{p}^n \right\rangle = \langle\psi|\hat{p}^n|\psi\rangle = \int_{-\infty}^{\infty}\langle\psi|x\rangle\langle x|\hat{p}^n|\psi\rangle dx = \int_{-\infty}^{\infty}\langle x|\psi\rangle^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\langle x|\psi\rangle dx$$

(3)

$$\left\langle \hat{x}^n \right\rangle = \langle\psi|\hat{x}^n|\psi\rangle = \int_{-\infty}^{\infty}\langle\psi|x\rangle\langle x|\hat{x}^n|\psi\rangle dx = \int_{-\infty}^{\infty}\langle x|\psi\rangle^* x^n\langle x|\psi\rangle dx$$

(4)

$$\left\langle \hat{x}^n \right\rangle = \langle\psi|\hat{x}^n|\psi\rangle = \int_{-\infty}^{\infty}\langle\psi|p\rangle\langle p|\hat{x}^n|\psi\rangle dp = \int_{-\infty}^{\infty}\langle p|\psi\rangle^*\left(i\hbar\frac{\partial}{\partial p}\right)^n\langle p|\psi\rangle dp$$

Derivation of Eq.(1) from Eq.(2)

We start with Eq.(1),

$$\left\langle \hat{p}^n \right\rangle = \int_{-\infty}^{\infty}\langle x|\psi\rangle^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\langle x|\psi\rangle dx$$

$$\begin{aligned}
\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\langle x|\psi\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n e^{ipx/\hbar}\langle p|\psi\rangle dp \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(\frac{\hbar}{i}\frac{i}{\hbar}p\right)^n e^{ipx/\hbar}\langle p|\psi\rangle dp \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} p^n e^{ipx/\hbar}\langle p|\psi\rangle dp
\end{aligned}$$

Then we have

$$\begin{aligned}
\left\langle \hat{p}^n \right\rangle &= \int_{-\infty}^{\infty} dx\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ip'x/\hbar}\langle p'|\psi\rangle^* dp'\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} p^n e^{ipx/\hbar}\langle p|\psi\rangle dp \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\int_{-\infty}^{\infty} dp'\int_{-\infty}^{\infty} dx e^{i(p-p')x/\hbar}\langle p'|\psi\rangle^* p^n\langle p|\psi\rangle
\end{aligned}$$

Since

$$\int_{-\infty}^{\infty} dx e^{i(p-p')x/\hbar} = 2\pi\delta[\frac{1}{\hbar}(p-p')] = 2\pi\hbar\delta(p-p'),$$

we have Eq.(1)

$$\langle \hat{p}^n \rangle = \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \langle p'|\psi\rangle^* p^n \langle p|\psi\rangle \delta(p-p') = \int_{-\infty}^{\infty} dp \langle p|\psi\rangle^* p^n \langle p|\psi\rangle$$

Derivation of Eq.(3) from Eq.(4)

$$\langle \hat{x}^n \rangle = \int_{-\infty}^{\infty} \langle p|\psi\rangle^* \left(i\hbar \frac{\partial}{\partial p} \right)^n \langle p|\psi\rangle dp$$

Here

$$\left(i\hbar \frac{\partial}{\partial p} \right)^n \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \left(i\hbar \frac{\partial}{\partial p} \right)^n e^{-ipx/\hbar} \langle x|\psi\rangle dx$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \left(-i\hbar \frac{i}{\hbar} x \right)^n e^{-ipx/\hbar} \langle x|\psi\rangle dx$$
$$== \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} x^n e^{-ipx/\hbar} \langle x|\psi\rangle dx$$

Then

$$\langle \hat{x}^n \rangle = \int_{-\infty}^{\infty} dp \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx'/\hbar} \langle x'|\psi\rangle^* dx' \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} x^n e^{-ipx/\hbar} \langle x|\psi\rangle dx$$
$$== \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \langle x'|\psi\rangle^* x^n \langle x|\psi\rangle \int_{-\infty}^{\infty} dp e^{ip(x'-x)/\hbar}$$

Since

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

then we have

$$\langle \hat{x}^n \rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \langle x'|\psi\rangle^* x^n \langle x|\psi\rangle \delta(x-x') = \int_{-\infty}^{\infty} dx \langle x|\psi\rangle^* x^n \langle x|\psi\rangle$$

((Example)) Calculation of *Δx Δp* for the Gaussian distribution

(1) Given that

$$\psi(x) = \left(\frac{\pi}{\alpha}\right)^{-1/4} e^{-\frac{\alpha x^2}{2}}$$

calculate

(a) $\langle \hat{x}^n \rangle$

(b) $\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$.

(2) Calculate the momentum space wave function for system described by the wave function

$$\psi(x) = \left(\frac{\pi}{\alpha}\right)^{-1/4} e^{-\frac{\alpha x^2}{2}}$$

calculate

(a) $\langle \hat{p}^n \rangle$

(b) $\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$

(c) $\Delta x \Delta p$

((**Mathematica**))

```
Clear["Global`*"];

ψ[x_] = (π/α)^(-1/4) Exp[-α x^2/2];

xbar[n_] = ∫_{-∞}^{∞} ψ[x] x^n ψ[x] ⅆx // Simplify[#, {α > 0, n > 0}] &;

Δx = Sqrt[xbar[2] - xbar[1]^2] // Simplify[#, {α > 0}] &
```

$$\frac{1}{\sqrt{2}\sqrt{\alpha}}$$

```
Φ[p_] = 1/Sqrt[2 π ℏ] ∫_{-∞}^{∞} Exp[-ⅈ p x/ℏ] ψ[x] ⅆx // Simplify[#, {α > 0}] &
```

$$\frac{e^{-\frac{p^2}{2\alpha\hbar^2}}}{\pi^{1/4}\alpha^{1/4}\sqrt{\hbar}}$$

```
pbar[n_] = ∫_{-∞}^{∞} Φ[p] p^n Φ[p] ⅆp //
   Simplify[#, {α > 0, n > 0, ℏ > 0}] &;

Δp = Sqrt[pbar[2] - pbar[1]^2] // Simplify[#, {α > 0, ℏ > 0}] &
```

$$\frac{\sqrt{\alpha}\,\hbar}{\sqrt{2}}$$

```
Δx Δp
```

$$\frac{\hbar}{2}$$

10.19 Simple harmonics; momentum space

$$\xi = \beta x\,,\; p = \hbar k\,,\; \kappa = \frac{k}{\beta} = \frac{p}{\hbar\beta}$$

where ξ and κ are the dimensionless quantities.

$$|x\rangle = \sqrt{\beta}|\xi\rangle\,,\ |k\rangle = \sqrt{\hbar}|p\rangle\,,\ |\kappa\rangle = \sqrt{\beta}|k\rangle$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}\,,\ \langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{\frac{ipx}{\hbar}}$$

$$\langle x|p\rangle = \sqrt{\frac{\beta}{\hbar}}\langle \xi|k\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}$$

$$\langle \xi|k\rangle = \frac{1}{\sqrt{2\pi\beta}}e^{ikx}\,,\ \langle \xi|\kappa\rangle = \frac{1}{\sqrt{2\pi}}e^{i\kappa\xi}$$

Then we have the Fourier transform

$$\varphi_n(\kappa) = \langle \kappa|n\rangle = \int \langle \kappa|\xi\rangle\langle \xi|n\rangle d\xi = \int \frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\langle \xi|n\rangle d\xi$$

So $\langle \kappa|n\rangle$ is the Fourier transform of $\langle \xi|n\rangle$. Note that

$$\langle \kappa|n\rangle = \sqrt{\beta}\langle k|n\rangle,\ \langle \xi|n\rangle = \frac{1}{\sqrt{\beta}}\langle x|n\rangle$$

Fourier transform of $\langle \xi|0\rangle$;

$$\langle \xi|0\rangle = \pi^{-\frac{1}{4}}e^{-\frac{\xi^2}{2}}$$

is given by

$$\langle x|0\rangle = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\langle \xi|0\rangle d\xi = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\pi^{-\frac{1}{4}}e^{-\frac{\xi^2}{2}}d\xi$$

Note that

$$-\frac{1}{2}\xi^2 - i\kappa\xi = -\frac{1}{2}(\xi + i\kappa)^2 - -\frac{1}{2}\kappa^2$$

we have

$$\langle\kappa|0\rangle = \frac{\pi^{-\frac{1}{4}}e^{-\frac{\kappa^2}{2}}}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(\xi+i\kappa)^2}d\xi = \pi^{-\frac{1}{4}}e^{-\frac{\kappa^2}{2}}$$

In general we have the following relations.

$$\varphi_n(\kappa) = (-i)^n\varphi_n(\xi)|_{\xi=\kappa}$$

$$|\varphi_n(\kappa)|^2 = |\varphi_n(\xi)|^2|_{\xi=\kappa}$$

((Proof))

We show that $\varphi_n(\kappa)$ satisfies the same differential equation for $\varphi_n(\xi)$.

$$\varphi_n(\kappa) = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\varphi_n(\xi)d\xi$$

with

$$\varphi_n(\xi) = (\sqrt{\pi}2^n n!)^{-\frac{1}{2}}e^{-\frac{\xi^2}{2}}H_n(\xi)$$

$$\frac{d^2\varphi_n(\kappa)}{d\kappa^2} = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}(-\xi^2)e^{-i\kappa\xi}\varphi_n(\xi)d\xi$$

Here $\varphi_n(\xi)$ satisfies the differential equation.

$$(\frac{d^2}{d\xi^2} - \xi^2 + 2n + 1)\varphi_n(\xi) = 0$$

Taking the Fourier transform of this equation,

$$\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\frac{d^2\varphi_n(\xi)}{d\xi^2}d\xi = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}(-i\kappa)^2 e^{-i\kappa\xi}\varphi_n(\xi)d\xi$$

$$\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}(2n+1-\xi^2)\varphi_n(\xi)d\xi = (2n+1)\varphi_n(\kappa) + \frac{d^2\varphi_n(\kappa)}{d\kappa^2}$$

or

$$(\frac{d^2}{d\kappa^2} - \kappa^2 + 2n + 1)\varphi_n(\kappa) = 0$$

$\varphi_n(\kappa)$ satisfies the same differential equation as $\varphi_n(\xi)$.

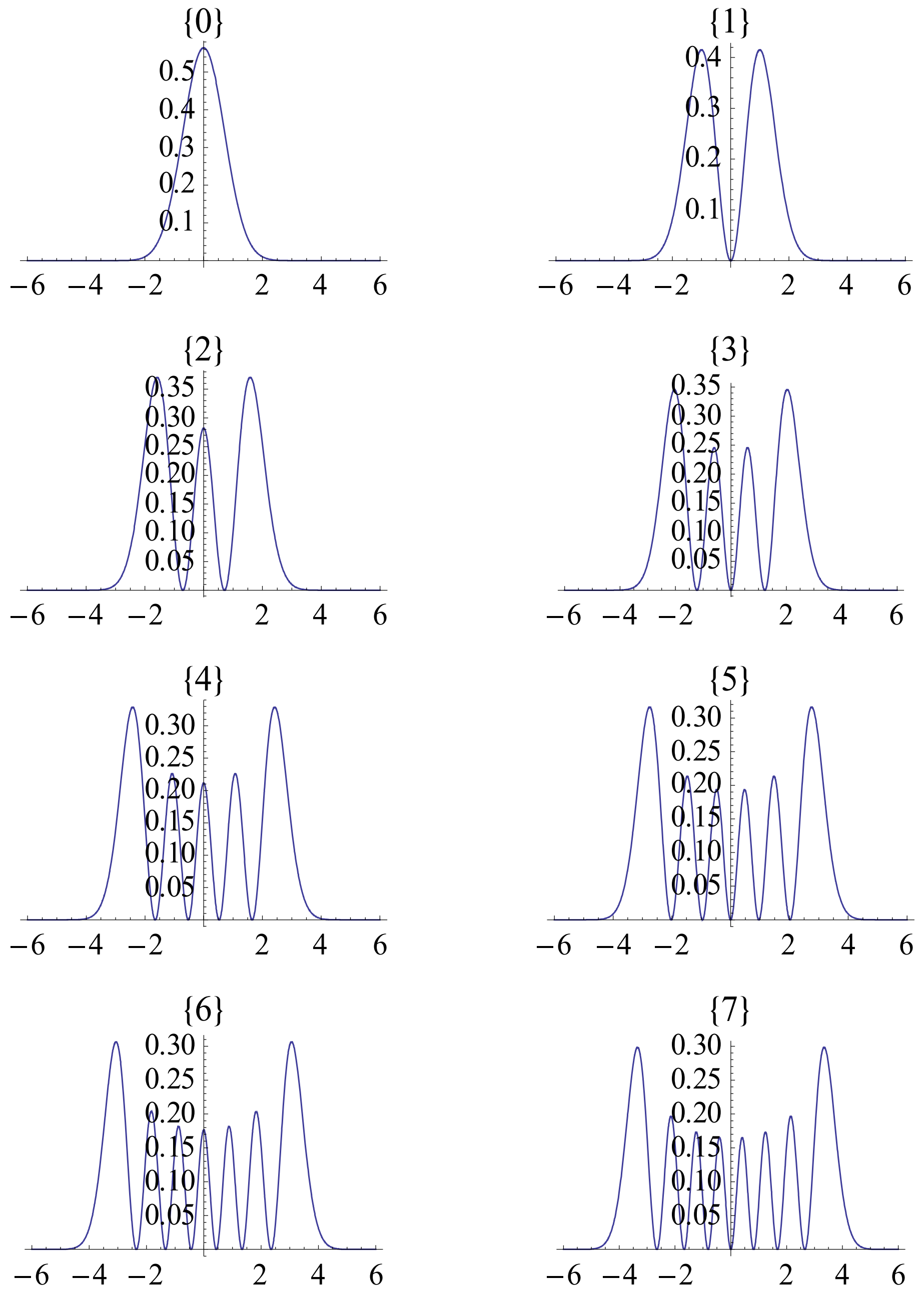
((Mathematica))

```
ψ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n!)^(-1/2) Exp[-ξ^2/2] HermiteH[n, ξ]

Φ[n_, κ_] := FourierTransform[ψ[n, ξ], ξ, κ]

Table[Φ[n, κ], {n, 0, 5}]
```

$$\left\{\frac{e^{-\frac{\kappa^2}{2}}}{\pi^{1/4}},\ \frac{i\sqrt{2}\,e^{-\frac{\kappa^2}{2}}\,\kappa}{\pi^{1/4}},\ \frac{e^{-\frac{\kappa^2}{2}}\left(2-4\kappa^2\right)}{2\sqrt{2}\,\pi^{1/4}},\ -\frac{i\,e^{-\frac{\kappa^2}{2}}\,\kappa\left(-3+2\kappa^2\right)}{\sqrt{3}\,\pi^{1/4}},\ \frac{e^{-\frac{\kappa^2}{2}}\left(3-12\kappa^2+4\kappa^4\right)}{2\sqrt{6}\,\pi^{1/4}},\ \frac{i\,e^{-\frac{\kappa^2}{2}}\,\kappa\left(15-20\kappa^2+4\kappa^4\right)}{2\sqrt{15}\,\pi^{1/4}}\right\}$$

```
Table[Φ[n, κ]* Φ[n, κ], {n, 0, 5}]
```

$$\left\{\frac{e^{-\kappa^2}}{\sqrt{\pi}},\ \frac{2\,e^{-\kappa^2}\,\kappa^2}{\sqrt{\pi}},\ \frac{e^{-\kappa^2}\left(2-4\kappa^2\right)^2}{8\sqrt{\pi}},\ \frac{e^{-\kappa^2}\,\kappa^2\left(-3+2\kappa^2\right)^2}{3\sqrt{\pi}},\ \frac{e^{-\kappa^2}\left(3-12\kappa^2+4\kappa^4\right)^2}{24\sqrt{\pi}},\ \frac{e^{-\kappa^2}\,\kappa^2\left(15-20\kappa^2+4\kappa^4\right)^2}{60\sqrt{\pi}}\right\}$$


{0}
0.5
0.4
0.3
0.2
0.1
−6 −4 −2 2 4 6
{1}
0.4
0.3
0.2
0.1
−6 −4 −2 2 4 6
{2}
0.35
0.30
0.25
0.20
0.15
0.10
0.05
−6 −4 −2 2 4 6
{3}
0.35
0.30
0.25
0.20
0.15
0.10
0.05
−6 −4 −2 2 4 6
{4}
0.30
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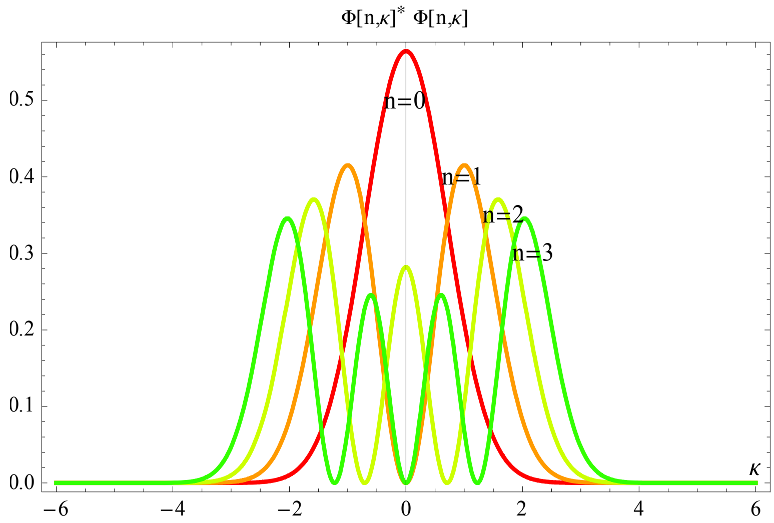

APPENDIX Mathematica

1. Type I Fourier transform

FourierTransform[f[t], t, ω]; Fourier transform of $f(t)$
InverseFourierTransform[F[ω], ω, t] Inverse Fourier transform of $F(\omega)$

2. Type II Fourier transform

FourierTransform[f [x], x, k, FourierParameters→{0,-1}];
Fourier transform of $f(x)$

InverseFourierTransform[$F(k)$, k, x, FourierParameters→{0,-1}];
Inverse Fourier transform of $F(k)$

3. DiracComb[x]:
to represent the Dirac comb function giving a delta function at every integer point.

4. Convolve[f, g, x, y];
to gives the convolution of two functions f and g;