16.3 7^{th}
12.8 6^{th}

Addition Theorem Spherical Harmonics

The spherical harmonics $Y_\ell^m(\vartheta,\varphi)$ describe angular momentum where ℓ represents the magnitude and m its projection on an **axis** (z-axis). A rotation of the coordinate system does **not** change the magnitude but will generate an expansion of the original function in m-components in the rotated system, i.e. $Y_\ell^m(\mathbb{R}\Omega) = \sum_{m'} D^\ell_{mm'}(\mathbb{R})Y_\ell^{m'}(\Omega)$ where

$\Omega \equiv (\vartheta,\varphi)$ and $\mathbb{R}\Omega = (\vartheta',\varphi')$ in the rotated system (earlier (ϑ,φ))

Since we have $2\ell+1$ m-values the rotational matrix $\mathbb{D}^\ell(\mathbb{R})$ will be $(2\ell+1)\times(2\ell+1)$ and since it gives a transformation between orthonormal sets $\mathbb{D}^\ell(\mathbb{R})$ will be unitary, that is

$$\mathbb{D}^\ell(\mathbb{R})^* = \left(\mathbb{D}^\ell(\mathbb{R})^{-1}\right)^T$$

The quantity $A = \sum_m Y_\ell^m(\Omega_1)^* Y_\ell^m(\Omega_2)$, with Ω_1 and Ω_2 being two different directions and with the summation over all allowed m-values, is <u>rotationally invariant.</u>

$$\mathbb{R}A = \sum_m \left(\sum_\mu D^\ell_{\mu m}(\mathbb{R})Y_\ell^\mu(\Omega_1)\right)^*\left(\sum_\nu D^\ell_{\nu m}(\mathbb{R})Y_\ell^\nu(\Omega_2)\right)$$

Reorder the summation:

$$\mathbb{R}A = \sum_{\mu,\nu} Y_\ell^\mu(\Omega_1)^* Y_\ell^\nu(\Omega_2)\sum_m D^\ell_{\mu m}(\mathbb{R})^* D^\ell_{\nu m}(\mathbb{R}) =$$

$$= \sum_{\mu,\nu} Y_\ell^\mu(\Omega_1)^* Y_\ell^\nu(\Omega_2)\sum_m \left[\mathbb{D}^\ell(\mathbb{R})^{-1}\right]_{m\mu}\left[\mathbb{D}^\ell(\mathbb{R})\right]_{\nu m} =$$

$$= \sum_{\mu,\nu} \delta_{\mu\nu} Y_\ell^\mu(\Omega_1)^* Y_\ell^\nu(\Omega_2) = \sum_\mu Y_\ell^\mu(\Omega_1)^* Y_\ell^\mu(\Omega_2) = A$$

Since A is rotationally invariant we can facilitate evaluating it by choosing a rotation that places Ω_1

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in the polar direction so that $\vartheta_1 = 0$. ϑ of Ω_2 will then be the angle x between the Ω_1 and Ω_2 directions.

We now have $Y_\ell^m(\Omega_1) = Y_\ell^m(0,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}}\,\delta_{m0}$ since in the polar direction all Y_ℓ^m with $m \neq 0$ must be zero since the φ-angle becomes undefined. Furthermore, $P_n(1) = 1$.

Thus, $A = \sum_m Y_\ell^m(0,\varphi_1)^* Y_\ell^m(x,\varphi_2) = \sum_m \sqrt{\frac{2\ell+1}{4\pi}}\,\delta_{m0}\, Y_\ell^m(x,\varphi_2) =$

$$= \sqrt{\frac{2\ell+1}{4\pi}}\; \underbrace{Y_\ell^0(x,\varphi_2)}_{\sqrt{\frac{2\ell+1}{4\pi}}\,P_\ell(\cos x)} = \frac{2\ell+1}{4\pi}\,P_\ell(\cos x)$$

$$\therefore \quad \boxed{P_\ell(\cos x) = \frac{4\pi}{2\ell+1}\sum_m Y_\ell^m(\Omega_1)^* Y_\ell^m(\Omega_2)}$$

Integral transforms

These are given as a function relation of the type

$$g(x) = \int_a^b f(t)\,K(x,t)\,dt$$ where a, b and the kernel $K(x,t)$ are the same for every function pair g and f.

From the linearity of the integration we have

Linear: $\int_a^b \{c_1 f_1(t) + c_2 f_2(t)\}\,K(x,t)\,dt = c_1 g_1(x) + c_2 g_2(x)$

~~The~~ ~~main~~ important value of integral transforms lies in the fact that a differential equation in real space becomes an algebraic equation in transform space

The Fourier transform is defined as

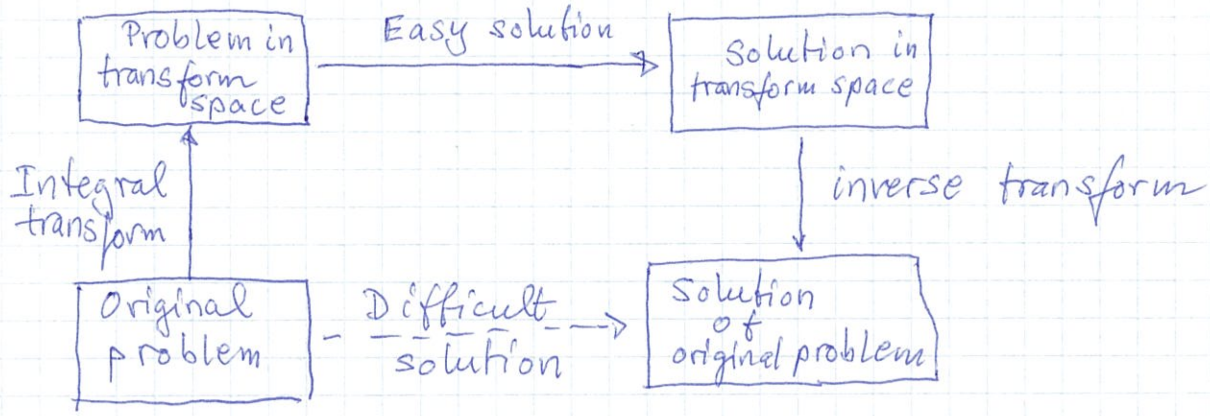
$$\boxed{g(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)\,e^{i\omega t}\,dt} \quad \text{where } f(t) \to 0 \text{ as } |t| \to \infty$$

The transformed derivative:

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{df(t)}{dt}\,e^{i\omega t}\,dt = \frac{1}{\sqrt{2\pi}}\underbrace{\Big[f(t)e^{i\omega t}\Big]_{-\infty}^{\infty}}_{=0} -$$

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

Illustration:



The practicality will depend on whether one can find the inverse transform $\mathcal{L}^{-1} g(\omega) = f(t)$ to bring the solution back to real space.

The Laplace transform: $\quad F(s) = \int_0^{\infty} e^{-st} f(t)\,dt$

The Hankel transform: $\quad g(\alpha) = \int_0^{\infty} f(t)\,t\,J_n(\alpha t)\,dt$

The Mellin transform: $\quad g(\alpha) = \int_0^{\infty} f(t)\,t^{\alpha-1}\,dt$

For $f(t) = e^{-t}$ $\quad g(\alpha) \equiv \Gamma(\alpha)$

Fourier cosine and sine transforms:

Since the interval is symmetrical with respect to the origin we can define

$f(t)$ even: $g_c(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\cos\omega t\, dt = \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(t)\cos\omega t\, dt$

$f(t)$ odd: $g_s(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\sin\omega t\, dt = \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(t)\sin\omega t\, dt$

Examples:

1. $f(t) = e^{-\alpha|t|}$, $\alpha > 0$ $\quad g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{0} e^{\alpha t + i\omega t} dt + \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{-\alpha t + i\omega t} dt =$

$$= \frac{1}{\sqrt{2\pi}} \left\{ \left[\frac{e^{\alpha t + i\omega t}}{\alpha + i\omega} \right]_{-\infty}^{0} + \left[\frac{e^{-\alpha t + i\omega t}}{-\alpha + i\omega} \right]_0^{\infty} \right\} =$$

$$= \frac{1}{\sqrt{2\pi}} \left\{ \frac{1}{\alpha + i\omega} - \frac{1}{-\alpha + i\omega} \right\} = \frac{1}{\sqrt{2\pi}} \frac{2\alpha}{\alpha^2 + \omega^2} \quad \text{(Real)}$$

If $f(t)$ is an even real-valued function then

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

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\cos\omega t\, dt + \frac{i}{\sqrt{2\pi}} \underbrace{\int_{-\infty}^{\infty} f(t)\sin\omega t\, dt}_{=0} =$$

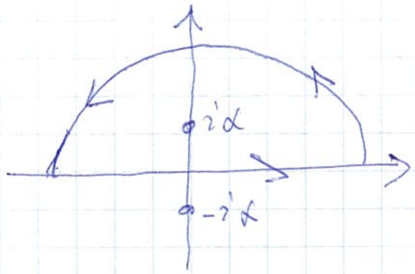
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\cos\omega t\, dt \quad \text{which is real.}$$

2. $f(t) = \frac{1}{\sqrt{2\pi}} \frac{2\alpha}{\alpha^2 + t^2}$, i.e. the transform from above

We have $g(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{2\alpha e^{i\omega t} dt}{(t - i\alpha)(t + i\alpha)}$. Use contour integration

poles at $\pm i\alpha$

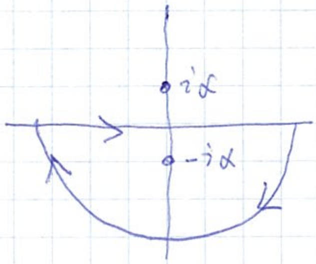
For $\omega > 0$ use Jordan's lemma to close in the upper half-plane:



The pole at $i\alpha$ is contained and contributes the residue $\left.\frac{(t-i\alpha)2\alpha e^{i\omega t}}{(t-i\alpha)(t+i\alpha)}\right|_{t=i\alpha} = \frac{1}{i}e^{-\alpha\omega}$

$\therefore$ $\omega > 0$: $g(\omega) = \frac{1}{2\pi}(2\pi i)\frac{1}{i}e^{-\alpha\omega} =$

$= e^{-\alpha\omega}$



$\omega < 0$: Close in the lower half-plane.

The pole at $-i\alpha$ is contained and contributes the residue $\left.\frac{(t+i\alpha)2\alpha e^{i\omega t}}{(t-i\alpha)(t+i\alpha)}\right|_{t=-i\alpha} = \frac{1}{-i}e^{\alpha\omega}$

We find $g(\omega) = (-2\pi i)\frac{1}{2\pi}\cdot\left(\frac{1}{-i}e^{\alpha\omega}\right)$ with the extra minus-sign from traversing clock-wise

$\therefore$ $\omega < 0$: $g(\omega) = e^{\alpha\omega}$

For $\omega = 0$ the integral becomes

$$g(0) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{2\alpha\, dt}{t^2+\alpha^2} = \frac{1}{2\pi}\cdot\frac{2}{\alpha^2}\int_{-\infty}^{\infty}\frac{\alpha\, dt}{\frac{t^2}{\alpha^2}+1} = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\frac{dt}{\alpha}}{\left(\frac{t}{\alpha}\right)^2+1} =$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{du}{u^2+1} = \frac{1}{\pi}\Big[\operatorname{atan}(u)\Big]_{-\infty}^{\infty} = \frac{1}{\pi}\left(\frac{\pi}{2}-\left(-\frac{\pi}{2}\right)\right) = 1$$

~~Alt~~ All together: $g(\omega) = e^{-\alpha|\omega|}$ i.e. the original untransformed function

3. $f(t) = e^{-at^2}$, $a > 0$ Gaussian function

$g(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-at^2}\cdot e^{i\omega t}\, dt$; complete the square as

$-at^2 + i\omega t = -a\left(t - \frac{i\omega}{2a}\right)^2 - \frac{\omega^2}{4a}$

$$\Rightarrow g(\omega) = \frac{1}{\sqrt{2\pi}}e^{-\frac{\omega^2}{4a}}\int_{-\infty}^{\infty} e^{-a\left(t-\frac{i\omega}{2a}\right)^2} dt = \left[\begin{array}{l} t - i\omega/2a = s \\ t = \infty \to s = \infty + \frac{i\omega}{2a} \\ t = -\infty \to s = -\infty + \frac{i\omega}{2a} \\ dt = ds \end{array}\right] =$$

$$= \frac{1}{\sqrt{2\pi}}e^{-\omega^2/4a}\int_{-\infty+\frac{i\omega}{2a}}^{\infty+\frac{i\omega}{2a}} e^{-as^2}\, ds$$

Do as contour integral by closing along the real axis

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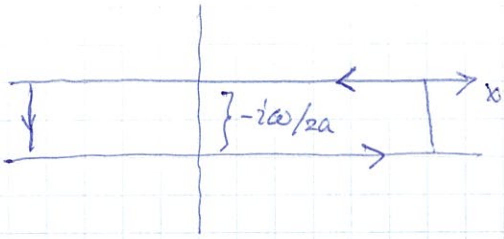


No poles are contained

so $\displaystyle\int_{-\infty+i\omega/2a}^{\infty+i\omega/2a} e^{-as^2}ds = \int_{-\infty}^{\infty} e^{-as^2}ds = \sqrt{\frac{\pi}{a}}$

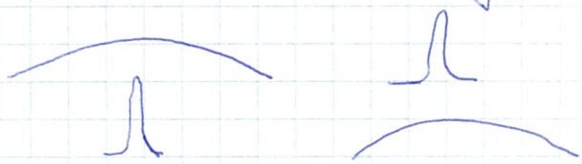
And $g(\omega) = \frac{1}{\sqrt{2\pi}} e^{-\omega^2/4a} \cdot \sqrt{\frac{\pi}{a}} = \frac{1}{\sqrt{2a}} e^{-\omega^2/4a}$ New Gaussian

Note inverse relation between real space and transform space:

a small a Large

real space $f(t) = e^{-at^2}$

transform space $g(\omega) = e^{-\frac{\omega^2}{4a}}$



x ——— Fourier integral ——— x

Inverse transform

A δ-sequence which converges to a representation of the Dirac δ-function is $\delta_n(t) = \frac{1}{2\pi}\int_{-n}^{n} e^{i\omega t}d\omega$

we have $f(x) = \lim_{n\to\infty}\int_{-\infty}^{\infty} f(t)\,\delta_n(t-x)\,dt = \lim_{n\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)\left[\int_{-n}^{n} e^{i\omega(t-x)}d\omega\right]dt$

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

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-i\omega x}\cdot \underbrace{\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)\,e^{i\omega t}dt\right\}}_{g(\omega)} d\omega \Rightarrow$$

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

$f(x)$ expanded in terms of plane waves with frequency $\omega = 2\pi\nu$ and amplitude $g(\omega)$

Specifically

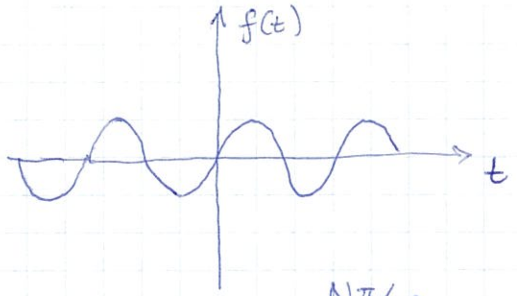
$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\omega)\,e^{-i\omega t}\,d\omega$$

$g(\omega)$ is frequency decomposition of the signal $f(t)$

Finite wave train

The sinusoidal $f(t) = \sin\omega_0 t$ with unique, well-defined frequency ω_0 gets clipped so that only a finite number N of oscillations remain

$$f(t) = \begin{cases} \sin\omega_0 t, & |t| < \frac{N\pi}{\omega_0} \\ 0, & |t| > \frac{N\pi}{\omega_0} \end{cases}$$



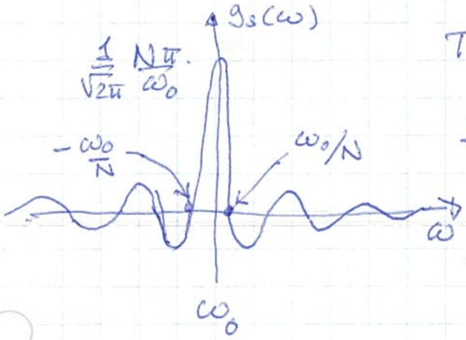
The function is odd

$$g_s(\omega) = \sqrt{\frac{2}{\pi}} \int_0^{N\pi/\omega_0} \sin\omega_0 t \sin\omega t \, dt =$$

$$= \sqrt{\frac{2}{\pi}} \int_0^{N\pi/\omega_0} \frac{1}{2}\left\{\cos[(\omega_0-\omega)t] - \cos[(\omega_0+\omega)t]\right\} dt =$$

$$= \sqrt{\frac{2}{\pi}} \left\{ \frac{\sin\left[(\omega_0-\omega)\frac{N\pi}{\omega_0}\right]}{2(\omega_0-\omega)} - \frac{\sin\left[(\omega_0+\omega)\frac{N\pi}{\omega_0}\right]}{2(\omega_0+\omega)} \right\}$$

For $\omega_0 \gg 1$ and $\omega \approx \omega_0$ the first term dominates



$$g_s(\omega) \doteq \frac{1}{\sqrt{2\pi}} \frac{\sin\left[(\omega_0-\omega)\frac{N\pi}{\omega_0}\right]}{\omega_0-\omega}$$

The zeros will be at

$$\frac{\omega_0-\omega}{\omega_0} = \frac{\Delta\omega}{\omega_0} = \pm\frac{n}{N}, \quad n = 1, 2, \dots N$$

The amplitude at the maximum $(\omega = \omega_0)$

$$\lim_{\omega\to\omega_0} \frac{1}{\sqrt{2\pi}} \frac{\sin\left[(\omega_0-\omega)\frac{N\pi}{\omega_0}\right]}{\omega_0-\omega} = \lim_{\omega\to\omega_0} \frac{1}{\sqrt{2\pi}} \frac{N\pi}{\omega_0} \cdot \frac{\sin\left[(\omega_0-\omega)\frac{N\pi}{\omega_0}\right]}{(\omega_0-\omega)\frac{N\pi}{\omega_0}}$$

$$= \lim_{x\to 0} \frac{1}{\sqrt{2\pi}} \frac{N\pi}{\omega_0} \frac{\sin x}{x} = \frac{1}{\sqrt{2\pi}} \cdot \frac{N\pi}{\omega_0}$$

The width of the first maximum $\Delta\omega = \omega_0\left(\frac{1}{N} - \left(-\frac{1}{N}\right)\right) =$

$$= \frac{2\omega_0}{N}$$

Take the half width as measure of the spread in frequency $\quad \Delta\omega = \frac{\omega_0}{N}$ $\Rightarrow$ the fewer cycles (N smaller) the larger the spread and the longer the ~~pulse~~ wave train the smaller the spread (N larger)

Transforms in 3-D space

In 3-D we have the transform $g(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\underline{r}) e^{i\underline{k}\cdot\underline{r}} d^3\underline{r}$

and the Fourier integral $$f(\underline{r}) = \frac{1}{(2\pi)^{3/2}} \int g(\underline{k}) e^{-i\underline{k}\cdot\underline{r}} d^3\underline{k}$$

Specific examples:

Denote $[\ldots]^T$ as the Fourier transform of the contained object.

1. The Yukawa potential $\frac{e^{-\alpha r}}{r}$

$$\left[\frac{e^{-\alpha r}}{r}\right]^T_{(\underline{k})} = \frac{1}{(2\pi)^{3/2}} \int \frac{e^{-\alpha r}}{r} e^{i\underline{k}\cdot\underline{r}} d^3\underline{r}$$; Use the spherical wave expansion of $e^{i\underline{k}\underline{r}}$

$$e^{i\underline{k}\cdot\underline{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y_l^m(\Omega_k)^* Y_l^m(\Omega_r)$$ so that

$$\left[\frac{e^{-\alpha r}}{r}\right]^T_{(\underline{k})} = \frac{4\pi}{(2\pi)^{3/2}} \int_0^\infty r^2 dr \int d\Omega_r \sum_{lm} i^l \frac{e^{-\alpha r}}{r} j_l(kr) Y_l^m(\Omega_k)^* Y_l^m(\Omega_r) =$$

$$= \frac{4\pi}{(2\pi)^{3/2}} \int_0^\infty r\, dr \int d\Omega_r \sum_{lm} i^l e^{-\alpha r} j_l(kr) Y_l^m(\Omega_k)^* Y_l^m(\Omega_r)$$

Due to the spherical symmetry of $\frac{e^{-\alpha r}}{r}$ all terms except $l = m = 0$ vanish in the integration over Ω_r:

$$\left[\frac{e^{-\alpha r}}{r}\right]^T_{(\underline{k})} = \frac{4\pi}{(2\pi)^{3/2}} \sum_{lm} i^l Y_l^m(\Omega_k)^* \int_0^\infty r e^{-\alpha r} j_l(kr) dr \underbrace{\int Y_l^m(\Omega_r) d\Omega_r}_{\delta_{l0}\cdot\delta_{m0}\cdot\sqrt{4\pi}} =$$

$$= \frac{4\pi}{(2\pi)^{3/2}} \int_0^\infty r e^{-\alpha r} \frac{\sin kr}{kr} dr =$$ where we used $Y_0^0(\Omega_k)^* = \frac{1}{\sqrt{4\pi}}$

$$= \frac{4\pi}{(2\pi)^{3/2}} \cdot \frac{1}{k} \int_0^\infty e^{-\alpha r} \sin kr\, dr ;$$ and $j_0(kr) = \frac{\sin kr}{kr}$

The integral $\int_0^\infty e^{-\alpha r}\sin kr\,dr = \underbrace{\left[-\frac{1}{\alpha}e^{-\alpha r}\sin kr\right]}_{=0} + \frac{k}{\alpha}\int_0^\infty e^{-\alpha r}\cos kr\,dr =$ 10

$$= \left[-\frac{k}{\alpha^2}e^{-\alpha r}\cos kr\right]_0^\infty - \frac{k^2}{\alpha^2}\int_0^\infty e^{-\alpha r}\sin kr\,dr \;;$$

$$\therefore \left(1+\frac{k^2}{\alpha^2}\right)\int_0^\infty e^{-\alpha r}\sin kr\,dr = \frac{k}{\alpha^2}$$

$$\int_0^\infty e^{-\alpha r}\sin kr\,dr = \frac{k}{\alpha^2+k^2} \Rightarrow$$

$$\Rightarrow \left[\frac{e^{-\alpha r}}{r}\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}}\cdot\frac{4\pi}{\alpha^2+k^2}$$

2. <u>Coulomb potential</u> Let $\alpha \to 0$ in the Yukawa potential

$$\lim_{\alpha\to 0}\left[\frac{e^{-\alpha r}}{r}\right]^T(\underline{k}) = \left[\frac{1}{r}\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}}\cdot\frac{4\pi}{k^2}$$

3. With $\left[\frac{1}{r}\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}}\cdot\frac{4\pi}{k^2} = \sqrt{\frac{2}{\pi}}\cdot\frac{1}{k^2}$ we have

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

The left-hand side is real so $\sqrt{\frac{\pi}{2}}\cdot\frac{1}{r} = \left\{\frac{1}{(2\pi)^{3/2}}\int\frac{1}{k^2}e^{-i\underline{k}\cdot\underline{r}}d^3\underline{k}\right\}^* =$

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

Interchange $\underline{k}$ and $\underline{r}$ which gives $\left[\frac{1}{r^2}\right]^T(\underline{k}) = \sqrt{\frac{\pi}{2}}\cdot\frac{1}{k}$

4. Hydrogenic 1s orbital $\sim e^{-Zr}$ in $\underline{k}$-space (momentum)

$$e^{-Zr} = -\frac{\partial}{\partial Z}\frac{e^{-Zr}}{r} \quad \text{so that}$$

$$\left[e^{-Zr}\right]^T(\underline{k}) = -\frac{\partial}{\partial Z}\left[\frac{e^{-Zr}}{r}\right]^T(\underline{k}) = -\frac{\partial}{\partial Z}\left\{\frac{1}{(2\pi)^{3/2}}\frac{4\pi}{Z^2+k^2}\right\} =$$

$$= \frac{1}{(2\pi)^{3/2}}\cdot\frac{8\pi Z}{(Z^2+k^2)^2}$$

OK, since $\frac{\partial}{\partial Z}$ and integration over other variables commute

5. Arbitrary function whose angular dependence is a spherical harmonic. Use spherical polar coordinates and the spherical wave expansion

$$\left[f(r)Y_\ell^m(\Omega_r)\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}}\int_0^\infty f(r)r^2dr\int d\Omega_r\, Y_\ell^m(\Omega_r)e^{i\underline{k}\cdot\underline{r}} =$$

$$= \frac{4\pi}{(2\pi)^{3/2}}\int_0^\infty f(r)r^2dr\int d\Omega_r\, Y_\ell^m(\Omega_r)\times\sum_{\ell',m'} i^{\ell'} j_{\ell'}(kr)Y_{\ell'}^{m'*}(\Omega_k)Y_{\ell'}^{m'}(\Omega_r)$$

The orthonormality of the Y_ℓ^m leaves only the Y_ℓ^{m} term contributing and

$$\left[f(r)Y_\ell^m(\Omega_r)\right]^T(\underline{k}) = \frac{4\pi\, i^\ell}{(2\pi)^{3/2}}\underbrace{Y_\ell^m(\Omega_k)}_{\text{spherical harmonic with same } \ell \text{ and } m}\underbrace{\int_0^\infty f(r)j_\ell(kr)r^2dr}_{\text{Hankel transform}}$$

6. Fourier transform of 3-D Gaussian.

Use spherical wave expansion ($\ell=m=0$ above) and $f(r)=f(r)\sqrt{4\pi}\,Y_0^0(\Omega_r)$

$$\left[e^{-ar^2}\right]^T(\underline{k}) = \frac{4\pi}{(2\pi)^{3/2}}\int_0^\infty e^{-ar^2}j_0(kr)r^2dr$$

$$\int_0^\infty e^{-ar^2}j_0(kr)r^2dr = \int_0^\infty e^{-ar^2}\frac{\sin kr}{kr}r^2dr = \frac{1}{k}\int_0^\infty re^{-ar^2}\sin kr\,dr =$$

$$= \frac{1}{k}\Big[\underbrace{-\frac{1}{2a}e^{-ar^2}\sin kr}_{=0}\Big]_0^\infty + \frac{1}{2a}\int_0^\infty e^{-ar^2}\cos kr\,dr;$$

The integrand is symmetric so we extend over the full "r-axis"

$$\int_0^\infty e^{-ar^2}\cos kr\,dr = \frac{1}{2}\int_{-\infty}^\infty e^{-ar^2}\cos kr\,dr = \frac{1}{2}\int_{-\infty}^\infty e^{-ar^2}\cdot e^{ikr}dr =$$

$$= \sqrt{2\pi}\cdot\frac{1}{2}\cdot\frac{1}{\sqrt{2a}}\exp\left(-\frac{k^2}{4a}\right)$$ from the transform of a Gaussian

Going from $\cos kr$ to e^{ikr} involved adding the odd function $i\sin kr$ which gives zero contribution over the symmetric interval. Thus $\left[e^{-ar^2}\right]^T(\underline{k}) = \frac{\sqrt{2\pi}}{2\sqrt{2a}}\cdot\frac{4\pi}{(2\pi)^{3/2}}\cdot\frac{1}{2a}e^{-k^2/4a}$

and $\quad \left[e^{-ar^2}\right]^T(\underline{k}) = \frac{1}{(2a)^{3/2}} \cdot e^{-k^2/4a}$

x —— Properties of Fourier transforms —— x

Write $g(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\underline{r})\, e^{i\underline{k}\cdot\underline{r}} d^3r \equiv \left[f(\underline{r})\right]^T(\underline{k})$

<u>Translation:</u> $\left[f(\underline{r}-\underline{R})\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\underline{r}-\underline{R})\, e^{i\underline{k}\cdot\underline{r}} d^3r = \begin{bmatrix} \underline{r}-\underline{R} = \underline{u} \\ \underline{r} = \underline{u}+\underline{R} \\ d^3r = d^3u \end{bmatrix} =$

$$= \frac{1}{(2\pi)^{3/2}} \int f(\underline{u})\, e^{i\underline{k}(\underline{u}+\underline{R})} d^3u =$$

$$= e^{i\underline{k}\underline{R}} \cdot \frac{1}{(2\pi)^{3/2}} \int f(\underline{u})\, e^{i\underline{k}\underline{u}} d^3u = e^{i\underline{k}\underline{R}}\, g(\underline{k})$$

<u>Scale:</u> $\left[f(\alpha\underline{r})\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\alpha\underline{r})\, e^{i\underline{k}\cdot\underline{r}} d^3r = \begin{bmatrix} \alpha\underline{r} = \underline{u} \\ \underline{r} = \underline{u}/\alpha \\ d^3r = \frac{1}{\alpha^3} d^3u \end{bmatrix} =$

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

$$= \frac{1}{\alpha^3}\, g(\underline{k}/\alpha)$$

<u>Sign change:</u> $\left[f(-\underline{r})\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int f(-\underline{r})\, e^{i\underline{k}\cdot\underline{r}} d^3r = \begin{bmatrix} -\underline{r} = \underline{u} \\ d^3r = d^3u \end{bmatrix} =$

$$= \frac{1}{(2\pi)^{3/2}} \int f(\underline{u})\, e^{-i\underline{k}\cdot\underline{u}} d^3u = g(-\underline{k})$$

<u>Complex conjugation:</u> $\left[f^*(\underline{r})\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int f^*(\underline{r})\, e^{i\underline{k}\cdot\underline{r}} d^3r = \begin{bmatrix} -\underline{r} = \underline{u} \\ d^3r = d^3u \end{bmatrix} =$

$$= \frac{1}{(2\pi)^{3/2}} \int f^*(\underline{u})\, e^{-i\underline{k}\cdot\underline{u}} d^3u = \left\{\frac{1}{(2\pi)^{3/2}} \int f(\underline{u})\, e^{i\underline{k}\cdot\underline{u}} d^3u\right\}^*$$

$$= g(\underline{k})^*$$

Gradient: Assume the integral exists

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

The gradient: $\nabla f(\underline{r}) = \frac{1}{(2\pi)^{3/2}} \int g(\underline{k}) \left[\nabla_r e^{-i\underline{k}\underline{r}} \right] d^3r =$

$$= \frac{1}{(2\pi)^{3/2}} \int g(\underline{k}) \left(-i\underline{k} e^{-i\underline{k}\cdot\underline{r}} \right) d^3r =$$

$$= \frac{1}{(2\pi)^{3/2}} \int \left[(-i\underline{k}) g(\underline{k}) \right] e^{-i\underline{k}\cdot\underline{r}} d^3r$$

$$\therefore \left[\nabla f(\underline{r}) \right]^T(\underline{k}) = -i\underline{k}\, g(\underline{k})$$

Laplace operator: $\left[\nabla (\nabla f(\underline{r})) \right]^T(\underline{k}) = (-i\underline{k})^2 g(\underline{k})$

Higher derivatives (1-D): $\left[\frac{d^n}{dt^n} f(t) \right]^T(\omega) = (-i\omega)^n g(\omega)$

× ———— Reducing a PDE to an ODE ———— ×

Vibrations ~~of~~ of an infinitely long string

The amplitude $y(x,t)$ satisfies the wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2} \quad \text{with } v \text{ the phase velocity}$$

initial conditions $y(x,0) = f(x)$ and $\left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = 0$

and $f(x) \xrightarrow[|x|\to\infty]{} 0$

Take Fourier transform in x to variable α

$$\int_{-\infty}^{\infty} \frac{\partial^2 y(x,t)}{\partial x^2} e^{i\alpha x} dx = \frac{1}{v^2} \int \frac{\partial^2 y(x,t)}{\partial t^2} e^{i\alpha x} dx =$$

$$= \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \int y(x,t) e^{i\alpha x} dx$$

set $Y(\alpha,t) = \frac{1}{\sqrt{2\pi}} \int y(x,t) e^{i\alpha x} dx$

then $(-i\alpha)^2 Y(\alpha,t) = \frac{1}{v^2}\frac{\partial^2 Y(\alpha,t)}{\partial t^2}$

[Integrate by parts and note that to be Fourier transformable $y(x,t) \xrightarrow[|x|\to\infty]{} 0$ and consequently its derivatives:

$$\int_{-\infty}^{\infty} \frac{\partial^2 y(x,t)}{\partial x^2} e^{i\alpha x} dx = \underbrace{\left[\frac{\partial y(x,t)}{\partial x} e^{i\alpha x}\right]_{-\infty}^{\infty}}_{=0} - i\alpha \int_{-\infty}^{\infty} \frac{\partial y(x,t)}{\partial x} e^{i\alpha x} dx =$$

$$= -i\alpha\left\{\underbrace{\left[y(x,t) e^{i\alpha x}\right]_{-\infty}^{\infty}}_{=0} - i\alpha \int_{-\infty}^{\infty} y(x,t) e^{i\alpha x} dx\right\} =$$

$$= (-i\alpha)^2 Y(\alpha,t)$$

This is now an ODE in t

Transform the initial conditions: $Y(\alpha,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{i\alpha x} dx = F(\alpha)$

$$\left.\frac{\partial Y(\alpha,t)}{\partial t}\right|_{t=0} = 0$$

Solve $\frac{\partial^2 Y(\alpha,t)}{\partial t^2} - (-i\alpha v)^2 Y(\alpha,t) = 0$

$$\Rightarrow Y(\alpha,t) = A(\alpha) e^{i\alpha v t} + B(\alpha) e^{-i\alpha v t}$$

$$\left.\frac{\partial Y(\alpha,t)}{\partial t}\right|_{t=0} = i\alpha v\left(A(\alpha) - B(\alpha)\right) = 0 \quad \Rightarrow B(\alpha) = A(\alpha)$$

$$Y(\alpha,0) = F(\alpha) = 2A(\alpha) \quad \Rightarrow A(\alpha) = \frac{1}{2} F(\alpha)$$

$$\therefore Y(\alpha,t) = F(\alpha) \frac{e^{i\alpha v t} + e^{-i\alpha v t}}{2}$$

Transform back: $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} Y(\alpha,t) e^{-i\alpha x} d\alpha = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\alpha) \frac{e^{i\alpha v t - i\alpha x} + e^{-i\alpha v t - i\alpha x}}{2} d\alpha$

$$\Rightarrow y(x,t) = \frac{1}{2}\left[f(x-vt) + f(x+vt)\right]$$

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

Half the amplitude travels toward $+x$ and the other half toward $-x$; both with velocity v

Coulomb Green's function

Green's fctn for the Poisson equation satisfies

$$\nabla_r^2 G(\underline{r},\underline{r}') = \delta(\underline{r}-\underline{r}')$$

Fourier transform both sides with respect to $\underline{r}$.

Denote $\left[G(\underline{r},\underline{r}')\right]^T(\underline{k}) \equiv g(\underline{k},\underline{r}')$

Left hand side becomes $-k^2 g(\underline{k},\underline{r}')$

Right hand side $\left[\delta(\underline{r}-\underline{r}')\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}} \int \delta(\underline{r}-\underline{r}') e^{i\underline{k}\underline{r}} d^3r = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}\underline{r}'}$

$$\text{so} \quad -k^2 g(\underline{k},\underline{r}') = \frac{1}{(2\pi)^{3/2}} e^{i\underline{k}\underline{r}'} \Rightarrow g(\underline{k},\underline{r}') = -\frac{1}{(2\pi)^{3/2}} \frac{e^{i\underline{k}\underline{r}'}}{k^2}$$

Take the inverse

$$G(\underline{r},\underline{r}') = -\frac{1}{(2\pi)^3} \int \frac{e^{i\underline{k}\circ\underline{r}'}}{k^2} e^{-i\underline{k}\underline{r}} d^3k =$$

$$= -\frac{1}{(2\pi)^3} \int \frac{d^3k}{k^2} e^{-i\underline{k}(\underline{r}-\underline{r}')}$$

proportional to the inverse transform of $1/k^2$ but with argument $\underline{r}-\underline{r}'$, we found earlier

$\sqrt{\frac{\pi}{2}} \frac{1}{|\underline{r}|} = \sqrt{\frac{\pi}{2}} \frac{1}{r} = \frac{1}{(2\pi)^{3/2}} \int \frac{1}{k^2} e^{-i\underline{k}\underline{r}} d^3r$ which gives

$$G(\underline{r},\underline{r}') = -\sqrt{\frac{\pi}{2}} \cdot \frac{1}{(2\pi)^{3/2}} \cdot \frac{1}{|\underline{r}-\underline{r}'|} = -\frac{1}{4\pi} \cdot \frac{1}{|\underline{r}-\underline{r}'|}$$

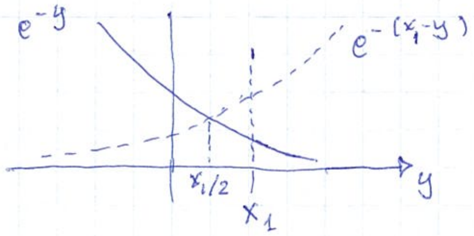
Fourier Convolution Theorem

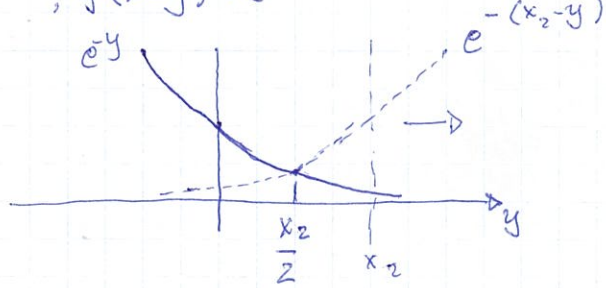
The convolution (Faltung, folding) of the two functions $f(x)$ and $g(x)$

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

in 3-D: $(f*g)(\underline{r}) \equiv \frac{1}{(2\pi)^{3/2}} \int g(\underline{r}') f(\underline{r}-\underline{r}')\, d^3r'$

Take as example $g(y) = e^{-y}$, $f(x-y) = e^{-(x-y)}$





Reflection around $\frac{x}{2}$

Consider the Fourier transform of the convolution

$$(f*g)^T(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy\, g(y) f(x-y) \right] e^{itx} =$$

set $e^{itx} = e^{ity} \cdot e^{it(x-y)}$

$$= \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy\, g(y) e^{ity} \right] \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, f(x-y) e^{it(x-y)} \right] =$$

$$= \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy\, g(y) e^{ity} \right] \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz\, f(z) e^{itz} \right] = G(t) \cdot F(t)$$

We can now write the convolution integral in terms of the inverse transform as

$$\int_{-\infty}^{\infty} g(y) f(x-y)\, dy = \sqrt{2\pi}\, (f*g)(x) = \sqrt{2\pi} \cdot \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (f*g)^T(t)\, e^{-ixt}\, dt =$$

$$= \int_{-\infty}^{\infty} G(t) F(t) e^{-ixt}\, dt$$

Two important observations:

1) The back transform of a product of transforms is the convolution of the functions

2) In real space the dependence is on two points (y and $x-y$)

while in transformed space the dependence is on t only, but an oscillating phase has been introduced.

Parseval relation

Specialize to $x=0$ giving $\int_{-\infty}^{\infty} f(-y)\,g(y)\,dy = \int_{-\infty}^{\infty} F(t)\,G(t)\,dt$

change $f(y)$ to $f^*(-y)$ $\Rightarrow f(-y) \to f^*(y)$

$$F(t) \to [f^*(-y)]^T = F^*(t)$$

$$\Rightarrow \boxed{\int_{-\infty}^{\infty} f^*(y)\,g(y)\,dy = \int_{-\infty}^{\infty} F^*(t)\,G(t)\,dt}$$ Parseval relation

Take $g=f$: $\int_{-\infty}^{\infty} |f(y)|^2 dy = \int_{-\infty}^{\infty} |F(t)|^2 dt$

Norm is conserved

Potential from charge distribution $\rho(\underline{r})$:

Coulomb's law or the Green's function for Poisson's equation gives

$$\psi(\underline{r}) = \frac{1}{4\pi}\int \frac{\rho(\underline{r}')\,d^3r'}{|\underline{r}-\underline{r}'|}$$ This is ~~of~~ the form of a convolution

Take $f(\underline{r}) = \frac{1}{r}$ giving $f(\underline{r}-\underline{r}') = \frac{1}{|\underline{r}-\underline{r}'|}$, $g(\underline{r}) = \rho(\underline{r})$

then $\psi(\underline{r}) = \frac{1}{4\pi}\int f^T(\underline{k})\,g^T(\underline{k})\,e^{-ikr}\,d^3k$

$f^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}}\cdot\frac{4\pi}{k^2}$ and $g^T(\underline{k}) = \rho^T(\underline{k})$

$$\Rightarrow \psi(\underline{r}) = \frac{1}{(2\pi)^{3/2}}\int \frac{\rho^T(\underline{k})}{k^2}\,e^{-i\underline{k}\cdot\underline{r}}\,d^3k$$

Only dependent on one point in $\underline{k}$-space

Two-center overlap integral

Two atomic orbitals $\varphi_a(\underline{r}-\underline{A})$ and $\varphi_b(\underline{r}-\underline{B})$ centered at $\underline{A}$ and $\underline{B}$, respectively. Their overlap is given by

$$S_{ab} = \int \varphi_a^*(\underline{r}-\underline{A})\, \varphi_b(\underline{r}-\underline{B})\, d^3r$$

Put the origin at $\underline{A}$: $\underline{r}' = \underline{r}-\underline{A}$ and $\underline{r}-\underline{B} = \underline{r}'-(\underline{B}-\underline{A}) \equiv \underline{r}'-\underline{R}$

$$S_{ab} = \int \varphi_a^*(\underline{r}')\, \varphi_b(\underline{r}'-\underline{R})\, d^3r$$

This is on the form of a convolution except for the sign in φ_b, but $[\varphi_b(-\underline{r})]^T(\underline{k}) = \varphi_b^T(-\underline{k})$

Thus, $S_{ab} = \int [\varphi_a^*]^T(\underline{k})\, \varphi_b^T(-\underline{k})\, e^{-i\underline{k}\underline{R}}\, d^3k$

Taking for the orbitals Slater Type Orbitals (STO) $\varphi = \varphi^* = e^{-\xi r}$ where ξ is a parameter describing the screening (effective charge felt by the electron) we have $\varphi^T = \frac{1}{(2\pi)^{3/2}} \cdot \frac{8\pi\xi}{(k^2+\xi^2)^2}$ and

$$S_{ab} = \frac{(8\pi\xi)^2}{(2\pi)^3} \int \frac{e^{-i\underline{k}\cdot\underline{R}}}{(k^2+\xi^2)^4}\, d^3k$$

Insert the spherical wave expansion and do the integration over Ω_k
The integrand $\frac{1}{(k^2+\xi^2)^4}$ does not have angular dependence so the only term to survive is $l=0$ where $Y_0^0 = \frac{1}{\sqrt{4\pi}}$

$$S_{ab} = \frac{(8\pi\xi)^2}{(2\pi)^3} \cdot 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l\, Y_l^m(\Omega_R) \int_0^\infty \frac{j_l(kR)k^2\, dk}{(k^2+\xi^2)^4} \int Y_l^{m*}(\Omega_k)\, d\Omega_k$$

$$\int Y_l^{m*}(\Omega_k)\, d\Omega_k = \int Y_l^{m*}(\Omega_k)\sqrt{4\pi}\, Y_0^0(\Omega_k)\, d\Omega_k = \sqrt{4\pi}\, \delta_{l0}\, \delta_{m0}$$

so $$S_{ab} = \frac{(8\pi\xi)^2}{(2\pi)^3} \cdot 4\pi \int_0^\infty \frac{j_0(kR)k^2}{(k^2+\xi^2)^4}\, dk$$

The integral is on the form of an integral representation of

$$k_n(x) = \frac{2^{n+2}(n+1)!}{\pi\, x^{n+1}} \int_0^\infty \frac{k^2 j_0(kx)}{(k^2+1)^{n+2}}\, dk$$

Exercise 14.7.10 A "well-known" integral representation for $K_\nu(x)$ has the form

$$K_\nu(x) = \frac{2^\nu \Gamma(\nu+\frac{1}{2})}{\sqrt{\pi}\, x^\nu} \int_0^\infty \frac{\cos xt}{(t^2+1)^{\nu+1/2}}\, dt$$

Derive the corresponding formula for the modified spherical $k_n(x)$

$$k_n(x) = \sqrt{\frac{2}{\pi x}}\, K_{n+1/2}(x) = \sqrt{\frac{2}{\pi x}}\, \frac{2^{n+\frac{1}{2}}\Gamma(n+1)}{\sqrt{\pi}\, x^{n+1/2}} \int_0^\infty \frac{\cos xt}{(t^2+1)^{n+1}}\, dt =$$

$$= \frac{2^{n+1}\, n!}{\pi\, x^{n+1}} \int_0^\infty \frac{\cos xt}{(t^2+1)^{n+1}}\, dt$$

Integrate by parts ; $\displaystyle\int_0^\infty \frac{\cos xt}{(t^2+1)^{n+1}}\, dt = \underbrace{\left[\frac{\sin xt}{x\,(t^2+1)^{n+1}}\right]_0^\infty}_{=0} - \frac{1}{x}\int_0^\infty \frac{\sin xt\cdot(-(n+1)\cdot 2t)}{(t^2+1)^{n+2}}$

$$= \frac{2(n+1)}{x}\int_0^\infty \frac{t\,\sin xt}{(t^2+1)^{n+2}}\, dt = 2(n+1)\int_0^\infty t^2\,\frac{\sin xt}{xt}\cdot\frac{dt}{(t^2+1)^{n+2}} =$$

$$= 2(n+1)\int_0^\infty \frac{t^2 j_0(xt)}{(t^2+1)^{n+2}}\, dt$$

and $$\boxed{k_n(x) = \frac{2^{n+2}(n+1)!}{\pi\, x^{n+1}}\int_0^\infty \frac{t^2 j_0(xt)\, dt}{(t^2+1)^{n+2}}}$$

x - - - - - - - - - - - x - - - - - - - x

In our case we have $\displaystyle S_{ab} = \frac{(8\pi\xi)^2}{(2\pi)^3}\cdot 4\pi \int_0^\infty \frac{j_0(kR)\,k^2 dk}{(k^2+\xi^2)^4}$

This can be seen as $k_2(\xi R)$:

$$\frac{1}{\xi^8}\int_0^\infty \frac{j_0(kR)\,k^2 dk}{\left(\left(\frac{k}{\xi}\right)^2+1\right)^4} = \frac{1}{\xi^5}\int_0^\infty \frac{j_0\left(\frac{k}{\xi}\cdot\xi R\right)\left(\frac{k}{\xi}\right)^2 d\left(\frac{k}{\xi}\right)}{\left(\left(\frac{k}{\xi}\right)^2+1\right)^4} \qquad \text{set } \frac{k}{\xi} = t,\ \xi R = x$$

$$= \frac{1}{\xi^5}\int_0^\infty \frac{t^2 j_0(xt)\, dt}{(t^2+1)^{2+2}} = \frac{1}{\xi^5}\, k_2(\xi R)\cdot \frac{\pi(\xi R)^3}{2^4\cdot 3!} \quad ; \quad k_2(x) = e^{-x}\left(\frac{1}{x}+\frac{3}{x^2}+\frac{3}{x^3}\right)$$

(14.196)

$$S_{ab} = \frac{8^2\pi^2\xi^2\cdot 4\pi}{8\pi^3}\cdot\frac{1}{\xi^5}\,\frac{\pi\,\xi^3 R^3}{2^5\cdot 3}\, k_2(\xi R) = \frac{\pi e^{-\xi R}}{3\xi^3}\left(\xi^2R^2 + 3\xi R + 3\right)$$

Multiple convolutions

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

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

set $t = z-y$ giving $x-y-t = x-z$ and $F(\omega) = f^T$, $G(\omega) = g^T$, $H(\omega) = h^T$

$$\Rightarrow [f*(g*h)](x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, f(y)\, g(z-y)\, h(x-z)$$

then $[f*g*h]^T(\omega) = F(\omega)G(\omega)H(\omega)$

order not relevant

Taking the inverse transform : $[f*g*h](x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega)G(\omega)H(\omega)e^{-i\omega x} d\omega$

so that $\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, f(y)\, g(z-y)\, h(x-z) = \sqrt{2\pi} \int_{-\infty}^{\infty} F(\omega)G(\omega)H(\omega)e^{-i\omega x} d\omega$

3-D: $[f*g*h](\underline{r}) = \frac{1}{(2\pi)^3} \int d^3r' \int d^3r''\, f(\underline{r}')\, g(\underline{r}''-\underline{r}')\, h(\underline{r}-\underline{r}'')$

$[f*g*h]^T(\underline{k}) = F(\underline{k})G(\underline{k})H(\underline{k})$

$$\int d^3r' \int d^3r''\, f(\underline{r}')\, g(\underline{r}''-\underline{r}')\, h(\underline{r}-\underline{r}'') = (2\pi)^{3/2} \int F(\underline{k})G(\underline{k})H(\underline{k})\, e^{-i\underline{k}\underline{r}}\, d^3k$$

6-D 3-D

Example: Electrostatic interaction between two charge distributions $\rho_1(\underline{r})$ and $\rho_2(\underline{r})$:

$$V = \int d^3r' \int d^3r'' \frac{\rho_1(\underline{r}')\,\rho_2(\underline{r}'')}{|\underline{r}''-\underline{r}'|}$$

This can be seen as a double convolution with the free argument $\underline{r}$ set to zero and a sign change in $h(-\underline{r}'')$ i.e. $\rho_2(\underline{r}'')$

So $V = (2\pi)^{3/2} \int d^3k \; \rho_1^T(\underline{k}) \cdot \left[\frac{1}{r}\right]^T(\underline{k}) \; \rho_2^T(-\underline{k}) =$ $\left(\left[\frac{1}{r}\right]^T = \frac{1}{(2\pi)^{3/2}} \cdot \frac{4\pi}{k^2} \right)$

$$= 4\pi \int \frac{d^3k}{k^2} \rho_1^T(\underline{k}) \, \rho_2^T(-\underline{k})$$

Transform of a product:

Since the transform and inverse are similar we can exploit it to find the transform of a product.
From the convolution theorem we have

$$\int_{-\infty}^{\infty} G(t)F(t)e^{-ixt}dt = \int_{-\infty}^{\infty} g(y)f(x-y)dy$$

change $x \to -x$, $y \to -y$ to make the left hand side assume the form of a transform and the right hand side retain the form of a convolution. We scale by $1/\sqrt{2\pi}$ to obtain the transform:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(-y)\,f(y-x)\,dy = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G(t)F(t)e^{ixt}dt = \left[G(t)F(t)\right]^T(x)$$

identify $[G(t)]^T(y) = g(-y)$ and $[F(t)]^T(x-y) = f(y-x)$

then $(F^T * G^T)(x) = \left[G(t)F(t)\right]^T(x)$

or equivalently $[fg]^T = F * G$ which requires f and g individually to have a Fourier transform.

Case: Assume the product fg transformable but f is not but has a MacLaurin expansion. From ~~the definition~~ differentiating the Fourier transform we have (20,3,5)

$$\frac{d^n}{dt^n} G(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) \frac{d^n}{dt^n} e^{ixt} dx = i^n \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^n g(x) e^{ixt} dx$$

so $\left[x^n g(x)\right]^T(t) = i^{-n} \frac{d^n}{dt^n} G(t)$

and we can write for the transform of the product

$$[fg]^T(t) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}[x^n g]^T = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} i^{-n} \frac{d^n}{dt^n} G(t) =$$

$$= \left\{ \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} i^{-n} \frac{d^n}{dt^n} \right\} G(t) = f\left(-i\frac{d}{dt}\right) G(t)$$

where $-i\frac{d}{dt}$ is the argument (corresponding to x)

Momentum Space

Position and momentum are conjugate variables which in Quantum Mechanics is expressed through the commutator relation $[x,p] = i\hbar$ ($\hbar = \frac{h}{2\pi}$ ← Planck's constant)

We can use either position (x) or momentum (p) as fundamental variable. In the x-representation x is a multiplicative operator $\hat{x}\psi(x) = x\psi(x)$ while $\hat{p}$ is a differential operator $\hat{p}\psi(x) = -i\hbar\frac{d\psi}{dx}$. The commutator

$$[\hat{x},\hat{p}]\psi(x) = \left(x\left(-i\hbar\frac{d}{dx}\right) - \left(-i\hbar\frac{d}{dx}\right)x\right)\psi = -i\hbar x\frac{d\psi}{dx} + i\hbar\frac{d}{dx}(x\psi) =$$

$$= i\hbar\psi$$

In the p-representation $\hat{p}$ is multiplicative $\hat{p}\varphi(p) = p\varphi(p)$ while $\hat{x}$ is a differential operator $\hat{x}\varphi(p) = i\hbar\frac{d\varphi(p)}{dp}$ and $[\hat{x},\hat{p}]\varphi(p) = \left\{ i\hbar\frac{d}{dp}(p\varphi(p)) - p\, i\hbar\frac{d}{dp}\varphi(p) \right) = i\hbar\varphi(p)$

For simplicity set $\hbar = 1$ and consider the Schrödinger equation $\hat{H}\psi \equiv \left[\frac{1}{2m}\hat{p}^2 + V(\hat{x})\right]\psi = E\psi$

x-representation: $-\frac{1}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$

p-representation: $\frac{p^2}{2m}\varphi(p) + V\left(i\frac{d}{dp}\right)\varphi(p) = E\varphi(p)$

Take the Fourier transform to go from the x-rep to the p-representation, i.e. momentum space. We have momentum eigenfunctions (x-rep) e^{ikx} so that

$$\hat{p}\, e^{ikx} = -i\frac{d}{dx}e^{ikx} = k e^{ikx} \quad (\hbar = 1)$$ and e^{ikx} act as basis in the Fourier decomposition. $(p = \hbar k)$

Transform the equation : $\psi \to g(\cancel{p})$, the second derivative $-\frac{d^2\psi}{dx^2}$ is transformed to $p^2 g(\cancel{p})$ and we get

$$\frac{p^2}{2m} g(\cancel{p}) + \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} V(x)\,\psi(x)\, e^{ikx}\, dx = E\, g(k)$$

if $V(x)$ has a Maclaurin expansion we have

$$\frac{p^2}{2m} g(k) + V\!\left(-i\frac{d}{dk}\right) g(k) = E\, g(k) \; ; \text{ identify } g^*(k) \longleftrightarrow \varphi(p)$$

Take complex conjugate (and scale by $\hbar=1$)

$$\Rightarrow \frac{p^2}{2m}\varphi(p) + V\!\left(i\frac{d}{dp}\right)\varphi(p) = E\,\varphi(p)$$

If $V(x)$ has a Fourier transform we can use the convolution theorem to transform into an integral equation

$$\frac{p^2}{2m}\varphi(p) + \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} V^T(p-p')\,\varphi(p')\,dp' = E\,\varphi(p)$$ (*)

For the hydrogen atom (Example 20.4.4)

$$-\frac{1}{2}\nabla^2\psi(\underline{r}) - \frac{1}{r}\psi(\underline{r}) = E\psi(\underline{r})$$ Atomic units $m = e = \hbar = 1$

Fourier transform $\psi(\underline{r}) \to \varphi(\underline{k})$

$$\frac{k^2}{2}\varphi(\underline{k}) - \frac{1}{(2\pi)^3}\int \frac{4\pi}{|\underline{k}-\underline{k}'|^2}\varphi(\underline{k}')\,d^3k' = E\,\varphi(\underline{k})$$

3-D analog of transform of product: $[fg]^T = \frac{1}{(\sqrt{2\pi})^3}\int f^T(\underline{k}-\underline{k}')\, g^T(\underline{k}')\, d^3k'$

and $\left[\frac{1}{r}\right]^T(\underline{k}) = \frac{1}{(2\pi)^{3/2}}\,\frac{4\pi}{|\underline{k}-\underline{k}'|^2}$

We will not solve the equation here but only demonstrate that the transformed hydrogen 1s state $\psi_{1s}(\underline{r}) \sim e^{-r}$ is a solution with the known energy $-\frac{1}{2}$ (in atomic units)

The transformed $\psi_{1s}(\underline{r}) \to \varphi(\underline{k}) = \dfrac{C}{(k^2+1)^2}$ (see earlier)

The constant C appears in all terms of the equation so it cancels out.

We now have: $\dfrac{1}{2}\dfrac{Ck^2}{(k^2+1)^2} - \dfrac{C}{2\pi^2}\displaystyle\int \dfrac{d^3k'}{|\underline{k}-\underline{k}'|^2(k'^2+1)^2} = E\,\dfrac{C}{(k^2+1)^2}$

The integral is on the form of a convolution, i.e. the transform of the product $\frac{1}{r}e^{-r} = \frac{e^{-r}}{r}$ which is the Yukawa potential with transform $\dfrac{4\pi}{k^2+1}$.

So $\dfrac{1}{2\pi^2}\displaystyle\int \dfrac{d^3k'}{|\underline{k}-\underline{k}'|^2(k^2+1)^2} = \dfrac{1}{2\pi^2}\int \sqrt{\dfrac{\pi}{2}}\,\dfrac{1}{r}\,\dfrac{(2\pi)^{3/2}}{8\pi}\,e^{-r}e^{i\underline{k}\underline{r}}\,d^3r$

$= \dfrac{1}{2\pi^2}\cdot\sqrt{\dfrac{\pi}{2}}\cdot\dfrac{(2\pi)^{3/2}}{8\pi}\displaystyle\int \dfrac{e^{-r}}{r}e^{i\underline{k}\underline{r}}\,d^3r = \dfrac{1}{2\pi^2}\cdot\dfrac{2\sqrt{2}\cdot\pi^2}{8\pi}\cdot\dfrac{4\pi}{k^2+1} = \dfrac{1}{2}\cdot\dfrac{1}{k^2+1}$

(factor $\dfrac{1}{(2\pi)^{3/2}}$ neglected on both sides)

Thus, $\dfrac{1}{2}\dfrac{k^2}{(k^2+1)^2} - \dfrac{1}{2}\dfrac{1}{k^2+1} = E\dfrac{1}{(k^2+1)^2}$

$\Rightarrow E = \frac{1}{2}(k^2 - k^2 - 1) = -\frac{1}{2}$ in atomic units (Hartree)

1 Hartree = 27.21138505 eV

$\Rightarrow E = 13.605$ eV

Laplace transforms

The Laplace transform $f(s)$ or $\mathcal{L}\{F(t)\}$ of a function $F(t)$ is given by

$$f(s) \equiv \mathcal{L}\{F(t)\} = \int_0^\infty e^{-st} F(t)\, dt \quad , F(t)=0 \text{ for } t<0$$

As for the Fourier transform there is no guarantee that the transform actually exists. However, if there exists a constant s_0 such that $|e^{-s_0 t}F(t)| \leq M$ for t sufficiently large $(M>0)$ then the transform exists as long as there is not a too strong divergence as $t \to 0$

$\mathcal{L}\{t^n\} = \int_0^\infty e^{-st} t^n dt$ exists for $n > -1$, but does not exist for $n \leq -1$.

Examples: $F(t) = 1$, $t>0$ (For the Laplace transform we require $F(t)=0$ for $t<0$)

$$\mathcal{L}\{1\} = \int_0^\infty e^{-st} dt = \frac{1}{s} \quad \text{for } s>0$$

$F(t) = e^{kt}$, $t>0$: $\mathcal{L}\{e^{kt}\} = \int_0^\infty e^{-st} \cdot e^{kt} dt = \int_0^\infty e^{-(s-k)t} dt =$

$$= \frac{1}{s-k} , \quad s>k$$

From this we deduce $\mathcal{L}\{\cosh(kt)\} = \mathcal{L}\{\frac{1}{2}(e^{kt} + e^{-kt})\} =$

(transform is linear) $= \frac{1}{2}\left[\mathcal{L}\{e^{kt}\} + \mathcal{L}\{e^{-kt}\}\right] = \frac{1}{2}\left(\frac{1}{s-k} + \frac{1}{s+k}\right) = \frac{s}{s^2-k^2}$

since $\cos(kt) = \cosh(ikt)$ we deduce

$$\mathcal{L}\{\cos(kt)\} = \frac{s}{s^2-(ik)^2} = \frac{s}{s^2+k^2}$$

The hyperbolic sine: $\mathcal{L}\{\sinh(kt)\} = \frac{1}{2}\left[\mathcal{L}\{e^{kt}\} - \mathcal{L}\{e^{-kt}\}\right] =$

$$= \frac{1}{2}\left(\frac{1}{s-k} - \frac{1}{s+k}\right) = \frac{k}{s^2-k^2}$$

and $\sin(kt) = -i\sinh(ikt) \Rightarrow \mathcal{L}\{\sin(kt)\} = \frac{-i\cdot(ik)}{s^2-(ik)^2} = \frac{k}{s^2+k^2}$

$F(t) = t^n$: $\quad \mathcal{L}\{t^n\} = \int_0^\infty e^{-st} t^n \, dt = \begin{bmatrix} st = u \\ t = \frac{u}{s} \\ dt = \frac{du}{s} \end{bmatrix} =$

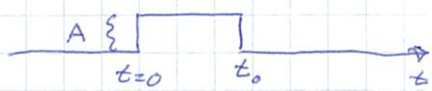
$$= \frac{1}{s^{n+1}} \int_0^\infty e^{-u} u^n \, du = \frac{\Gamma(n+1)}{s^{n+1}} = \frac{n!}{s^{n+1}}$$

Heaviside step function: $\quad u(t-k) = \begin{cases} 0, & t<k \\ 1, & t>k \end{cases}$

$$\mathcal{L}\{u(t-k)\} = \int_0^\infty e^{-st} u(t-k)\,dt = \int_k^\infty e^{-st}\,dt = \frac{1}{s}e^{-ks}$$

Square pulse: Step of A at $t=0$ and step down at $t=t_0$

$$F(t) = A\left[u(t) - u(t-t_0)\right]$$



$$\mathcal{L}\{F(t)\} = A\int_0^\infty e^{-st}\,dt - A\int_{t_0}^\infty e^{-st}\,dt = \frac{A}{s}\left(1 - e^{-st_0}\right)$$

Dirac δ-function: $\quad \mathcal{L}\{\delta(t-t_0)\} = \int_0^\infty e^{-st}\delta(t-t_0)\,dt = e^{-st_0}$

and $\mathcal{L}\{\delta(t)\} = \int_0^\infty e^{-st}\delta(t)\,dt = 1$

The inverse $\mathcal{L}^{-1}\{f(s)\} = F(t)$ is most simply found through identification or from tables, but in the general case by doing the Bromwich integral

$$F(t) = \frac{1}{2\pi i}\int_{\beta-i\infty}^{\beta+i\infty} e^{st} f(s)\,ds$$

Simplification through partial fraction expansion

Let $f(s) = \frac{g(s)}{h(s)}$ with $g(s), h(s)$ polynomials without common factor and $g(s)$ of lower degree than $h(s)$.

Then, if the factors of $h(s)$ are all linear and distinct ($h(s) = \prod_i (s-a_i)$ with $a_i \neq a_j$ for all i,j) we can write

$$f(s) = \frac{c_1}{s-a_1} + \frac{c_2}{s-a_2} + \dots + \frac{c_n}{s-a_n}$$

where a_i are roots of $h(s)$, i.e. $h(a_i) = 0$

If one root occurs m times then

$$f(s) = \frac{c_{1,m}}{(s-a_1)^m} + \frac{c_{1,m-1}}{(s-a_1)^{m-1}} + \dots + \frac{c_{1,1}}{s-a_1} + \sum_{i=2}^{n} \frac{c_i}{s-a_i}$$

For a quadratic factor in $h(s)$ the corresponding numerator depends linearly on s, i.e.

a factor $s^2+ps+q \longrightarrow \frac{as+b}{s^2+ps+q}$

Example: $f(s) = \frac{k^2}{s(s^2+k^2)} = \frac{c}{s} + \frac{as+b}{s^2+k^2} = \frac{cs^2+ck^2+as^2+bs}{s(s^2+k^2)}$

$$\Rightarrow \left.\begin{aligned} c+a &= 0 \\ b &= 0 \\ c &= 1 \end{aligned}\right\} \Rightarrow a = -1$$

and $f(s) = \frac{k^2}{s(s^2+k^2)} = \frac{1}{s} - \frac{s}{s^2+k^2}$

$$\mathcal{L}^{-1}\{f(s)\} = 1 - \cos(kt) \qquad (t \geq 0)$$

Example: Evaluate a definite integral using Laplace transforms. The integral $F(t) = \int_0^\infty \frac{\sin tx}{x}\,dx$ for general t

$t > 0$: Take the Laplace transform

$$f(s) = \mathcal{L}\left\{\int_0^\infty \frac{\sin tx}{x}\,dx\right\} = \int_0^\infty e^{-st} \int_0^\infty \frac{\sin tx}{x}\,dx\,dt =$$

$$= \begin{bmatrix} \text{interchange} \\ \text{the order} \\ \text{uniformly convergent} \end{bmatrix} = \int_0^\infty \frac{1}{x}\left\{\int_0^\infty e^{-st}\sin tx\,dt\right\}dx = \int_0^\infty \frac{1}{x}\cdot\frac{x}{s^2+x^2}dx =$$

$$= \int_0^\infty \frac{dx}{x^2+s^2} = \frac{1}{s}\left[\operatorname{atan}\left(\frac{x}{s}\right)\right]_0^\infty = \frac{\pi}{2s}$$

$$F(t) = \mathcal{L}^{-1}\left\{\frac{\pi}{2s}\right\} = \frac{\pi}{2}\mathcal{L}^{-1}\left\{\frac{1}{s}\right\} = \frac{\pi}{2}$$

$t<0$ $\quad F(t) = \int_0^\infty \frac{\sin(-xt)dx}{x} = -\int_0^\infty \frac{\sin xt}{x}dx = -\frac{\pi}{2}$

$F(0) = 0$ $\quad \Rightarrow F(t) = \begin{cases} \frac{\pi}{2}, & t>0 \\ 0, & t=0 \\ -\frac{\pi}{2}, & t<0 \end{cases}$ step function

Derivatives and initial values

$$\mathcal{L}\{F'(t)\} = \int_0^\infty e^{-st}\frac{dF}{dt}dt = \left[e^{-st}F(t)\right]_0^\infty - (-s)\int_0^\infty e^{-st}F(t)dt =$$

$$= -F(0+) + s\mathcal{L}\{F(t)\}$$ (transform only defined for $t \geq 0$)

$$\mathcal{L}\{F^{(2)}(t)\} = \int_0^\infty e^{-st}\frac{d^2F}{dt^2}dt = \left[e^{-st}\frac{dF}{dt}\right]_0^\infty + s\mathcal{L}\{F'(t)\} =$$

$$= -F'(0+) + s\{s\mathcal{L}\{F(t)\} - F(0+)\} =$$

$$= s^2\mathcal{L}\{F(t)\} - sF(0+) - F'(0)$$

$\therefore$ Initial conditions built into the transform

Finding a transform through transform of derivative

$\frac{d^2}{dt^2}\sin kt = -k^2\sin kt$; transform both sides

$$-k^2\mathcal{L}\{\sin kt\} = s^2\mathcal{L}\{\sin kt\} - s\sin(0) - \left.\frac{d}{dt}\sin kt\right|_{t=0} =$$

$$= s^2\mathcal{L}\{\sin kt\} - k$$

$$\Rightarrow \mathcal{L}\{\sin kt\} = \frac{k}{s^2+k^2}$$

Simple harmonic oscillator

$$m\frac{d^2X(t)}{dt^2} + kX(t) = 0 \quad , X(0) = X_0 \ , X'(0) = 0$$

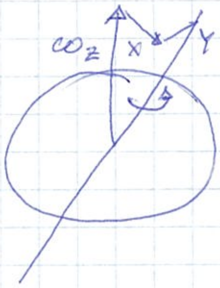
set $\mathcal{L}\{X(t)\} \equiv x(s)$; we find $ms^2x(s) - msX_0 + kx(s) = 0$

and $s^2x(s) - sX_0 + \omega_0^2 x(s) = 0 \quad , \omega_0^2 = \frac{k}{m}$

$$(s^2+\omega_0^2)\,x(s) = X_0\, s$$

$$x(s) = X_0 \frac{s}{s^2+\omega_0^2} \longrightarrow X(t) = X_0 \cos\omega_0 t$$

Coupled system of equations – Earth's nutation



$$\frac{dX}{dt} = -aY \qquad \frac{dY}{dt} = aX \qquad a = \frac{I_z - I_x}{I_z}\omega_z$$

Transform: $sx(s) - X_0 = -a\,y(s)$ (1)

$sy(s) - Y_0 = a\,x(s)$ (2)

scale (1) by s and (2) by a to eliminate $y(s)$:

$$s^2x(s) - sX_0 = -a^2x(s) - aY_0$$

$$\Rightarrow x(s) = X_0\frac{s}{s^2+a^2} - Y_0\frac{a}{s^2+a^2}$$

and $y(s) = \frac{Y_0}{s} + \frac{a}{s}\left\{X_0\frac{s}{s^2+a^2} - Y_0\frac{a}{s^2+a^2}\right\} =$

$$= \frac{Y_0}{s} + X_0\frac{a}{s^2+a^2} - \frac{Y_0}{s}\cdot\frac{a^2}{s^2+a^2} =$$

$$= X_0\frac{a}{s^2+a^2} + \frac{Y_0}{s}\left\{\frac{s^2+a^2-a^2}{s^2+a^2}\right\} =$$

$$= X_0\frac{a}{s^2+a^2} + Y_0\frac{s}{s^2+a^2}$$

$$\therefore \begin{cases} X(t) = X_0\cos(at) - Y_0\sin(at) \\ Y(t) = X_0\sin(at) + Y_0\cos(at) \end{cases}$$

set $Y_0 = 0 \Rightarrow$ circular orbit with radius X_0 traversed counterclockwise with angular velocity a

Ex. 15.9.3. (6^{th}) / 20.8.4 (7^{th}) Newton's second law for a particle of mass m that is subjected to an instantaneous momentum transfer at $t=0$ (impulse). Initially at rest at the origin

$$m\frac{d^2X}{dt^2} = P\delta(t) \quad \text{with } P \text{ constant}$$

Laplace transform $m s^2 x(s) - msX(0) - mX'(0) = P$

Initially at rest $\Rightarrow X(0) = X'(0) = 0 \quad \Rightarrow \quad x(s) = \frac{P}{m}\cdot\frac{1}{s^2}$

$\therefore X(t) = \frac{P}{m} t$, i.e. instantaneous transfer of constant momentum P

We have $\mathcal{L}\{t\} = \int_0^\infty t e^{-st} dt = \left[-\frac{1}{s} t e^{-st}\right]_0^\infty + \frac{1}{s}\int_0^\infty e^{-st} dt =$

$$= \left[-\frac{1}{s^2} e^{-st}\right]_0^\infty = \frac{1}{s^2}$$

x ——— Development of transforms ——— x

Substitute $s \to s-a$ in the definition of the transform

$$f(s) = \int_0^\infty e^{-st} F(t)\,dt \quad \text{i.e.} \quad f(s-a) = \int_0^\infty e^{-(s-a)t} F(t)\,dt =$$

$$= \int_0^\infty e^{-st}\{e^{at}F(t)\}dt \equiv$$

$$= \mathcal{L}\{e^{at}F(t)\}$$

This gives directly, e.g.,

$$\mathcal{L}\{e^{at}\sin kt\} = \frac{k}{(s-a)^2+k^2}, \quad \mathcal{L}\{e^{at}\cos kt\} = \frac{s-a}{(s-a)^2+k^2}, \quad s>a$$

Damped oscillator

Add a damping term to the harmonic oscillator

$$m X''(t) + b X'(t) + k X(t) = 0$$

Initial conditions $X(0) = X_0$, $X'(0) = 0$

Transform: $m\left[s^2 x(s) - s X_0\right] + b\left[s x(s) - X_0\right] + k x(s) = 0$

$$x(s)\left\{m s^2 + b s + k\right\} = X_0 (m s + b)$$

$$x(s) = X_0 \frac{m s + b}{m s^2 + b s + k} = X_0 \frac{s + b/m}{s^2 + \frac{b}{m} s + \frac{k}{m}}$$

complete the square: $s^2 + \frac{b}{m} s + \frac{k}{m} =$

$$= \left(s + \frac{b}{2m}\right)^2 + \frac{k}{m} - \frac{b^2}{4m^2}$$

restrict to small damping, i.e. $b^2 < 4km$ and set

$$\omega_1^2 = \frac{k}{m} - \frac{b^2}{4m^2}$$

Then $x(s) = X_0 \dfrac{s + b/m}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2} = X_0 \dfrac{s + b/2m}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2} + X_0 \dfrac{b/2m}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2}$

$$= X_0 \underbrace{\frac{s + b/2m}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2}}_{\mathcal{L}\left\{e^{-(b/2m)t} \cos \omega_1 t\right\}} + X_0 \cdot \frac{b}{2m\omega_1} \cdot \underbrace{\frac{\omega_1}{\left(s + \frac{b}{2m}\right)^2 + \omega_1^2}}_{\mathcal{L}\left\{e^{-(b/2m)t} \sin \omega_1 t\right\}}$$

$$\therefore \quad X(t) = X_0 e^{-(b/2m)t} \left\{\cos \omega_1 t + \frac{b}{2m\omega_1} \sin \omega_1 t\right\}$$

Translation

Multiply the transform by e^{-bs} with $b>0$

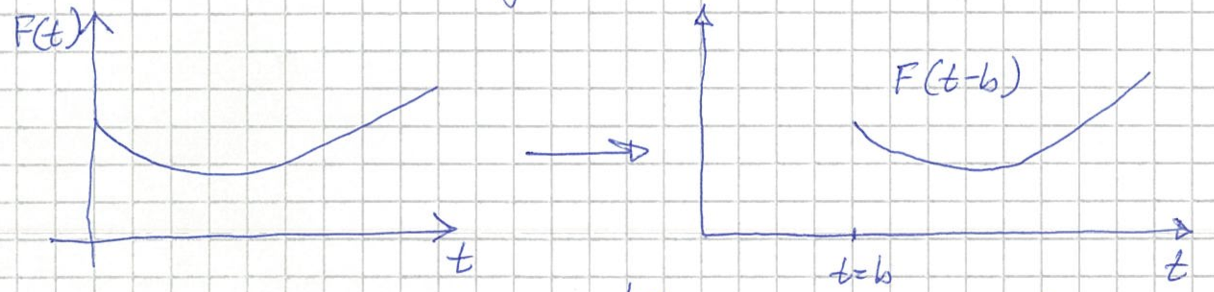
$$e^{-bs}f(s) = e^{-bs}\int_0^\infty e^{-st}F(t)dt = \int_0^\infty e^{-s(t+b)}F(t)dt$$

Put $t+b=\tau$ and $t=\tau-b$

$$e^{-bs}f(s) = \int_b^\infty e^{-s\tau}F(\tau-b)d\tau = \int_0^\infty e^{-s\tau}F(\tau-b)u(\tau-b)d\tau$$

where $u(\tau-b)$ is a Heaviside step function with step 1 at $\tau=b$

~~For~~ The function $F(t)$ was required to be zero for $t<0$ so that $F(\tau-b)=0$ for $0\leq\tau<b$ and the Heaviside function is not needed to allow changing the lower bound from b to 0.



$$\therefore\ e^{-bs}f(s) = \mathcal{L}\{F(t-b)\}$$

Derivative of transform

With $F(t)$ at least piecewise continuous and s chosen so that $e^{-st}F(t)$ converges exponentially for large t the integral $\int_0^\infty e^{-st}F(t)dt$ is uniformly convergent and can be differentiated with respect to s under the integral

$$f'(s) = \int_0^\infty(-t)e^{-st}F(t)dt = \mathcal{L}\{-tF(t)\}$$

In general: $f^{(n)}(s) = \mathcal{L}\{(-t)^nF(t)\}$ which allows to generate additional transforms

$$\mathcal{L}\{e^{kt}\} = \int_0^\infty e^{-st}e^{kt}dt = \frac{1}{s-k},\ s>k$$

and $\mathcal{L}\{te^{kt}\} = \frac{1}{(s-k)^2}$

$$\mathcal{L}\{t^2e^{kt}\} = -\frac{2}{(s-k)^3}$$

Laplace Convolution Theorem

Take two transforms $f_1(s) = \mathcal{L}\{F_1(t)\}$ and $f_2(s) = \mathcal{L}\{F_2(t)\}$

Multiply $f_1(s) f_2(s) = \int_0^\infty e^{-sx} F_1(x)\,dx \int_0^\infty e^{-sy} F(y)\,dy$

Introduce new variable $t = x+y$ and integrate ofer t and y
New limits $0 \le t \le \infty$ and $0 \le y \le t$. The transformation is linear with scale 1 so $dx\,dy = dt\,dy$ and

$$f_1(s) f_2(s) = \int_0^\infty e^{-st} dt \int_0^t F_1(t-y) F_2(y)\,dy =$$

$$= \mathcal{L}\left\{ \int_0^t F_1(t-y) F_2(y)\,dy \right\} = \mathcal{L}\{F_1 * F_2\}$$

Take inverse transform

$$\mathcal{L}^{-1}\{f_1(s) f_2(s)\} = \int_0^t F_1(t-y) F_2(y)\,dy$$

15.11.1 6th
20.9.1 7th

Driven oscillator with damping

$$m X''(t) + b X'(t) + k X(t) = F(t)$$

initial conditions $X(0) = X'(0) = 0$

Transformed equation $m s^2 x(s) + b s x(s) + k x(s) = f(s)$

solution in s-space: $x(s) = \frac{f(s)}{m} \frac{1}{(s+\frac{b}{2m})^2 + \omega_1^2}$, $\omega_1^2 = \frac{k}{m} - \frac{b^2}{4m^2}$

This is on the form of the convolution theorem and we directly find

$$X(t) = \frac{1}{m\omega_1} \int_0^t F(t-z)\, e^{-(b/2m)z} \sin \omega_1 z \, dz$$

$$\mathcal{L}\{\sin \omega_1 t\} = \frac{\omega_1}{s^2 + \omega_1^2} \qquad \mathcal{L}\{e^{-\frac{b}{2m}t} \sin \omega_1 t\} =$$

$$= \frac{\omega_1}{(s+\frac{b}{2m})^2 + \omega_1^2}$$

For an impulsive force $F(t) = P\delta(t)$

$$X(t) = \frac{P}{m\omega_1} e^{-\frac{b}{2m}t} \sin \omega_1 t$$

See also the case for $F(t) = F_0 \sin \omega t \rightarrow f(s) = \frac{F_0 \omega}{s^2 + \omega^2}$

Inverse Laplace transform - Bromwich integral

We seek $F(t) = \mathcal{L}^{-1}\{f(s)\}$ given that we know $f(s)$

We'll go via the Fourier transform but have the complication that for the transform to exist we must have $\lim_{\omega \to \infty} G(\omega) = 0$ and Dirichlet conditions apply (function given on the boundary, i.e. as $t \to \infty$)

The Laplace transform can be applied to functions that diverge exponentially. Take out an exponential factor $e^{\gamma t}$ from $F(t)$ so that $G(t)$ in $F(t) = e^{\gamma t} G(t)$ becomes Fourier transformable, i.e. if $F(t)$ diverges as $e^{\alpha t}$ then $\gamma > \alpha$ so that $G(t)$ converges.

With $G(t) = 0$ for $t < 0$ and satisfying suitable conditions so that the Fourier integral exists we have

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iut} du \int_0^{\infty} G(v) e^{iuv} dv \quad \left(G(t) = 0 \text{ for } t < 0 \right)$$

and $$F(t) = \frac{e^{\gamma t}}{2\pi} \int_{-\infty}^{\infty} e^{-iut} du \int_0^{\infty} \underbrace{F(v) e^{-\gamma v}}_{G(v)} e^{iuv} dv$$

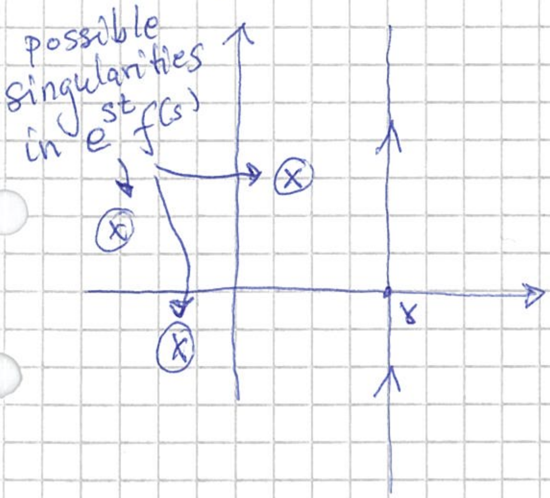
We want the integral over v as the Laplace transform and substitute $s = \gamma - iu$ which gives the integral over v as

$$\int_0^{\infty} F(v) e^{-sv} dv = f(s) \quad Re(s) \geq \gamma$$

Substitute into the expression for $F(t)$ with $du = -\frac{ds}{i}$ (γ constant) and $iu = \gamma - s$

$$F(t) = -\frac{e^{\gamma t}}{2\pi} \int_{\gamma + i\infty}^{\gamma - i\infty} e^{-(\gamma - s)t} f(s) \frac{ds}{i} = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} f(s) ds$$

This is the inverse transform with the path of integration rotated 90° in the complex plane and displaced to the right (using γ) so that all singularities in $f(s)$ lie to the left of the path of integration



The integral $\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} e^{st} f(s)\,ds$ is called Bromwich integral

For $t>0$ we can close the path of integration with a half circle in the left half plane and use the residue theorem

$$F(t) = 2\pi i \sum \{\text{residues included for } Re(s)<\gamma\}$$

Ex. 15.12.1 $\quad f(s) = \frac{a}{s^2-a^2} \Rightarrow e^{st} f(s) = \frac{a e^{st}}{s^2-a^2} = \frac{a e^{st}}{(s+a)(s-a)}$

singularities at $s=\pm a$

$$s=a: \quad Res(s=a) = \lim_{s\to a} \frac{(s-a)\,a e^{st}}{(s+a)(s-a)} = \frac{1}{2} e^{at}$$

$$s=-a: \quad Res(s=-a) = \lim_{s\to -a} \frac{(s+a)\,a e^{st}}{(s+a)(s-a)} = -\frac{1}{2} e^{-at}$$

and $F(t) = \frac{1}{2}\left(e^{at} - e^{-at}\right) = \sinh(at)$