



# **FOURIER TRANSFORMS IN QUANTUM MECHANICS**

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**A SEMINAR BY JEEVAN M NANDEESH**



# THE FOURIER SERIES

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- The complex fourier series is given by:

$$F(x) = \sum_{r=-\infty}^{+\infty} a_r |\alpha\rangle$$

# THE FOURIER SERIES

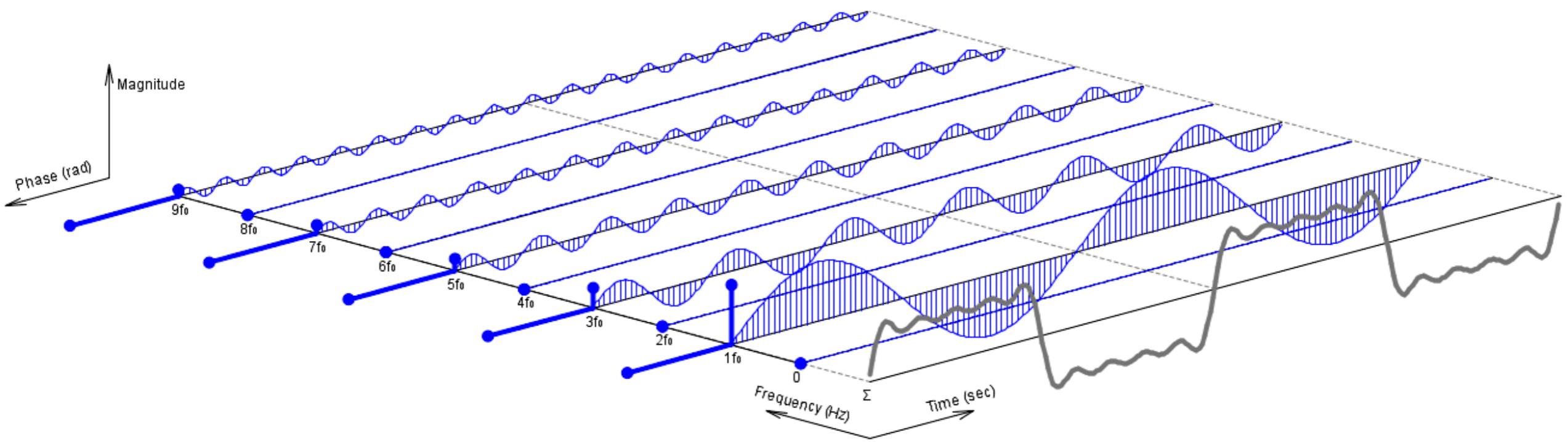
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- The complex fourier series is given by:

$$F(x) = \sum_{r=-\infty}^{+\infty} a_r e^{ir\omega t}$$

$$f(\chi) = \dots + \alpha_{-2} e^{-2i\omega\chi} + \alpha_{-1} e^{-i\omega\chi} + \alpha_0 + \alpha_1 e^{i\omega\chi} + \alpha_2 e^{2i\omega\chi} + \alpha_3 e^{3i\omega\chi} + \dots,$$

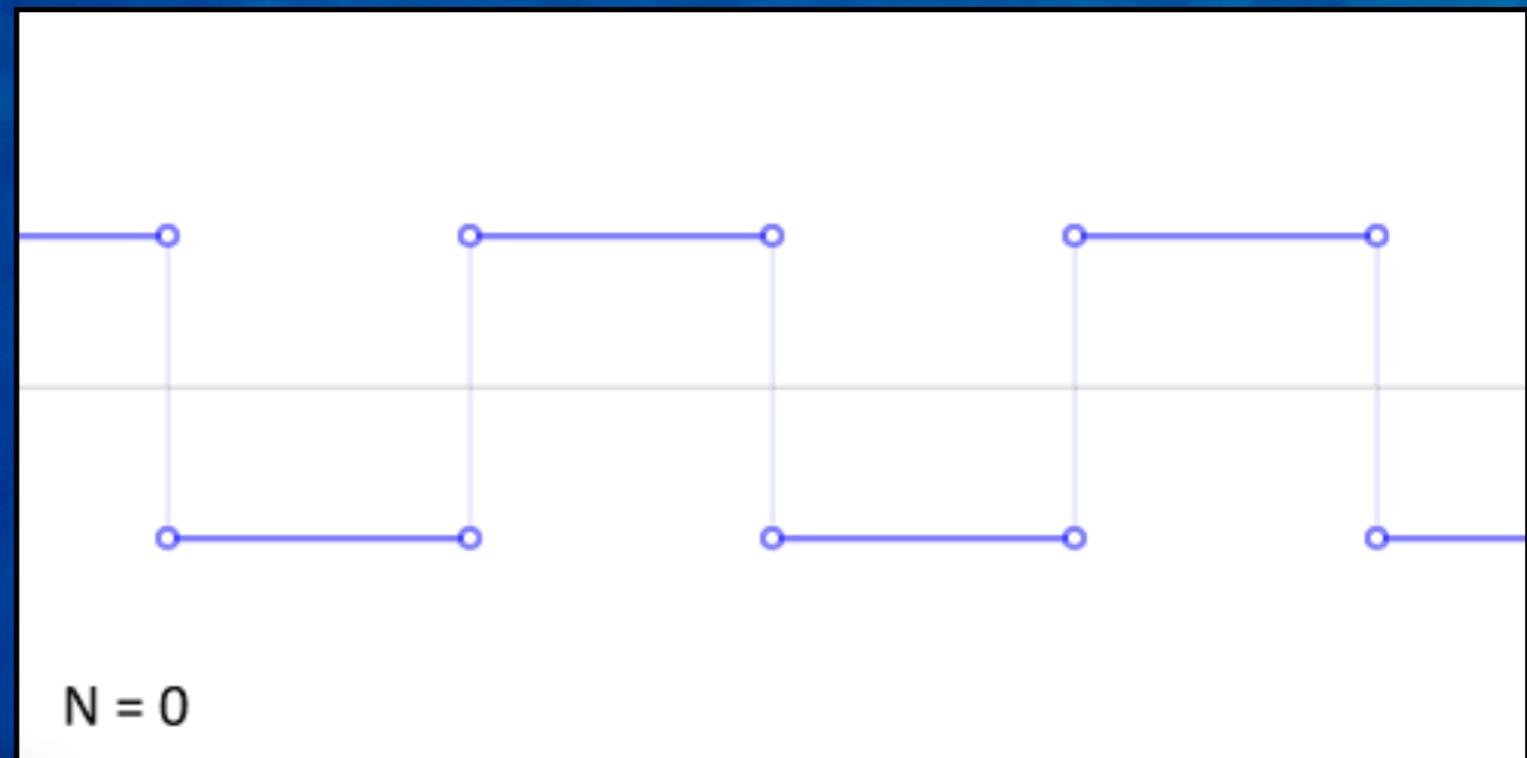
$$\begin{aligned} f(\chi) = & c + a_1 \cos \omega\chi + b_1 \sin \omega\chi + a_2 \cos 2\omega\chi + b_2 \sin 2\omega\chi + \\ & a_3 \cos 3\omega\chi + b_3 \sin 3\omega\chi + \dots, \end{aligned}$$



## FOURIER SERIES EXPANSION OF THE SQUARE WAVE FUNCTION

$$f(t) = \begin{cases} k & \text{if } 0 \leq t < a \\ -k & \text{if } a < t < 2a \end{cases}$$

$$f(x) = \frac{4}{\pi} \sum_{n=1,3,5,\dots}^{\infty} \frac{1}{n} \sin\left(\frac{n\pi x}{L}\right).$$



#Any function that is piecewise continuous in  
[-r,r] can be expressed as a linear combination  
of the orthogonal set of functions  $e^\lambda$  to be typed  
on the interval [-r,r]

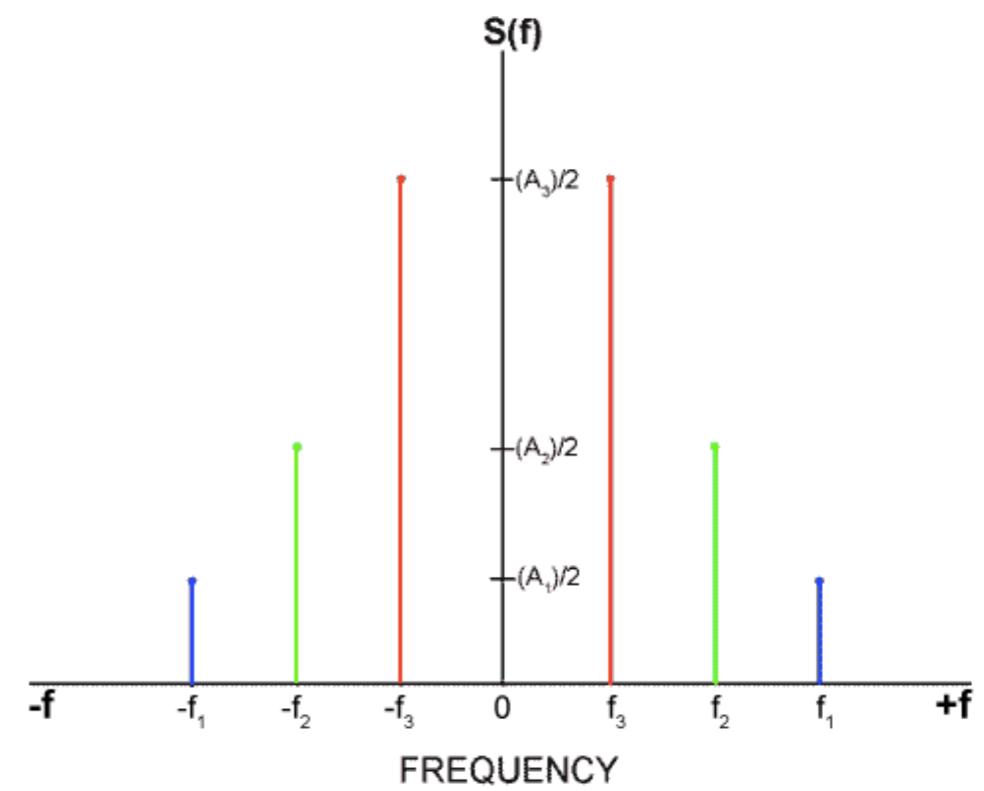
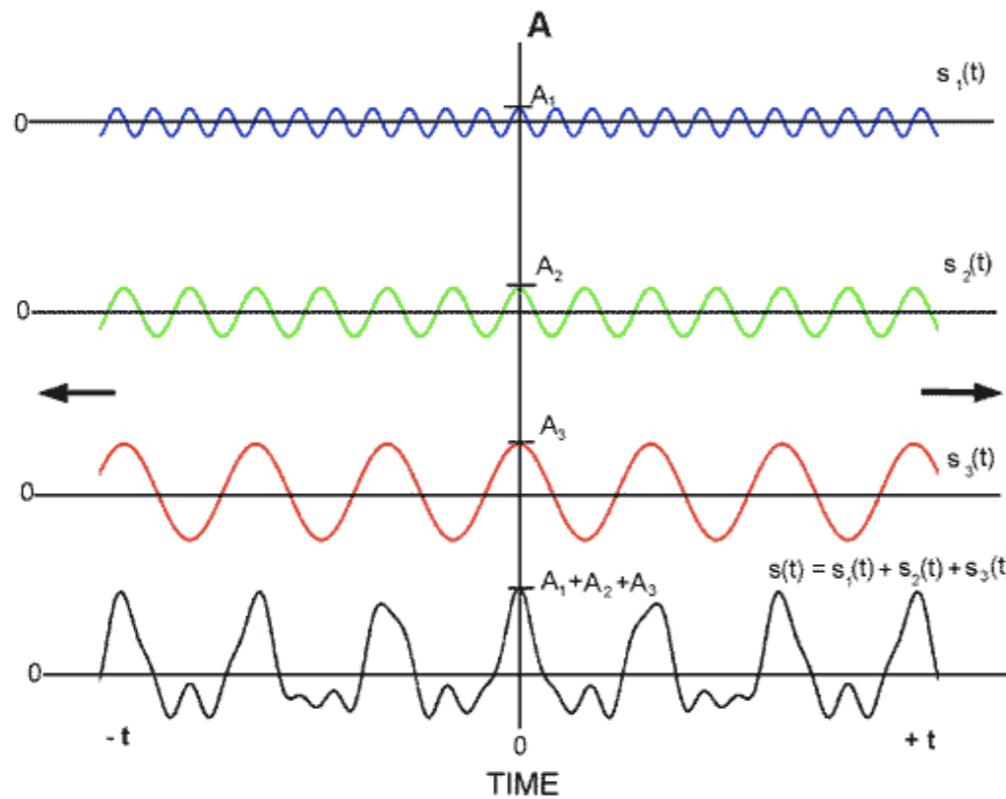
#This set of mutually orthogonal functions  
span an infinite dimensional Hilbert space (the  $L^2$   
Hilbert space)

# THE FOURIER TRANSFORM

- The Fourier transform of a function  $f(t)$  is given by:

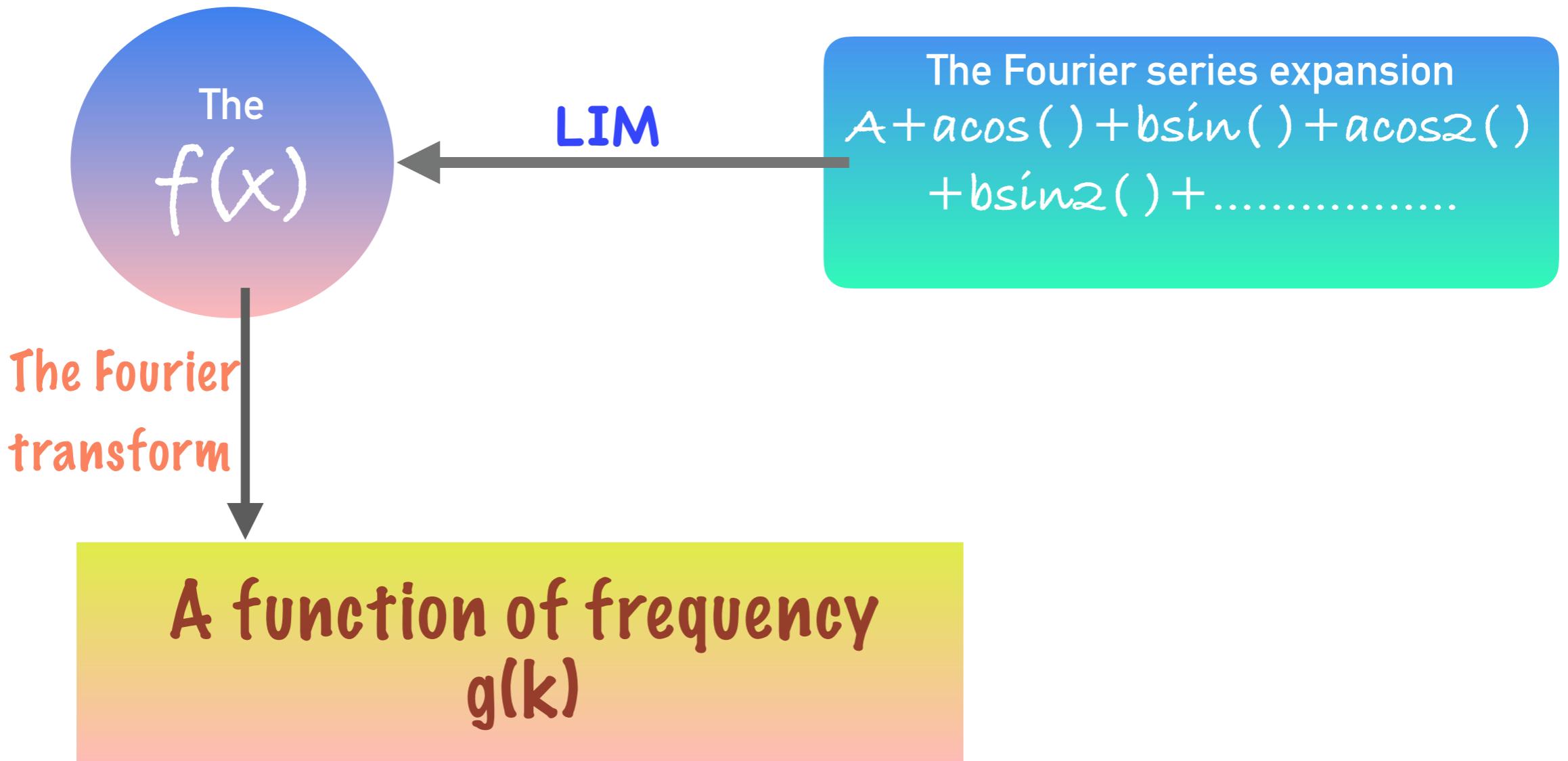
$$g(\omega) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt$$

- The transformation maps a function in the time ( $t$ ) domain to a function in the frequency ( $\omega$ ) domain.



# THE FOURIER TRANSFORM

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# FOURIER TRANSFORMS IN QUANTUM MECHANICS

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- SOME EXAMPLES:
- Transformation of a wave function from momentum space to ordinary space (and vice versa).
- Transformation of the Yukawa potential from momentum space to ordinary space (and vice versa)
- Transformation of the Dirac delta function.
- Transformation of the Exponential function.

	The position operator $x$	The infinitesimal translation operator	The momentum operator $p$
The operation	$x x'\rangle = x' \mathbf{x}'\rangle,$	$\mathcal{T}(dx') \mathbf{x}'\rangle =  \mathbf{x}' + dx'\rangle,$	$p p'\rangle = p' \mathbf{p}'\rangle$
Orthogonality	$\langle x'' x'\rangle = \delta(x'' - x').$		$\langle p' p''\rangle = \delta(p' - p'').$
Expansion of an arbitrary vector	$ \alpha\rangle = \int dx'  x'\rangle \langle x' \alpha\rangle,$		$ \alpha\rangle = \int dp'  p'\rangle \langle p' \alpha\rangle.$
The wave function	$\langle x' \alpha\rangle = \psi_\alpha(x').$		$\langle p' \alpha\rangle = \phi_\alpha(p').$
Probability	$\langle x' \alpha\rangle = \psi_\alpha(x').$		$\int dp' \langle \alpha p'\rangle \langle p' \alpha\rangle = \int dp'  \phi_\alpha(p') ^2 = 1.$

The commutation relations between the operators

$$[x_i, x_j] = 0, \quad [p_i, p_j] = 0, \quad [x_i, p_j] = i\hbar\delta_{ij}.$$

# A DERIVATION

- Consider the infinitesimal translation operator with the action

$$\mathcal{T}(d\mathbf{x}')|\mathbf{x}'\rangle = |\mathbf{x}' + d\mathbf{x}'\rangle$$

- This operator is given in terms of the operator 'p' as

$$\mathcal{T}(d\mathbf{x}') = 1 - i\mathbf{p} \cdot d\mathbf{x}'/\hbar,$$

- Let us operate on an arbitrary state which is expanded in terms of the eigenkets of the operator 'x'

$$\begin{aligned}\left(1 - \frac{i\mathbf{p}\Delta x'}{\hbar}\right)|\alpha\rangle &= \int dx' \mathcal{T}(\Delta x')|x'\rangle\langle x'|\alpha\rangle \\ &= \int dx' |x' + \Delta x'\rangle\langle x'|\alpha\rangle \\ &= \int dx' |x'\rangle\langle x' - \Delta x'|\alpha\rangle \\ &= \int dx' |x'\rangle \left( \langle x'|\alpha\rangle - \Delta x' \frac{\partial}{\partial x'} \langle x'|\alpha\rangle \right).\end{aligned}$$

- Comparing the LHS and RHS, we get,

# A DERIVATION

- we get the relation,

$$p|\alpha\rangle = \int dx' |x'\rangle \left( -i\hbar \frac{\partial}{\partial x'} \langle x'|\alpha\rangle \right)$$

- And, multiplying with the specified bra,

$$\langle x'|p|\alpha\rangle = -i\hbar \frac{\partial}{\partial x'} \langle x'|\alpha\rangle,$$

- Now, let us replace the arbitrary ket with an eigenket of the momentum operator 'p'

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

- but, WKT:

$$p|p'\rangle = p'|p'\rangle$$

- Therefore we can write:

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

- But the above equation represents a differential equation, whose solution is given by

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# A DERIVATION

- The solution is given by:

$$\langle x' | p' \rangle = N \exp\left(\frac{ip'x'}{\hbar}\right)$$

- Where  $N$  is the normalisation constant to be determined. From the calculations mentioned in slide [appendix 1], the normalisation constant is found to be:

$$N = \frac{1}{\sqrt{2\pi\hbar}}$$

- And we have the final expression:

$$\langle x' | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ip'x'}{\hbar}\right)$$

- This equation provides us with a relation between the eigenvectors of the position operator ‘ $x$ ’ and the eigenvectors of the momentum operator ‘ $p$ ’
- Using this relation, we can obtain a very interesting and insightful relation between the position space wave function  $\psi_\alpha(x')$  and the momentum space wave function....  $\phi_\alpha(p')$ .

# A DERIVATION

- Rewriting the position space wave function:

$$\langle x'|\alpha\rangle = \int dp' \langle x'|p'\rangle \langle p'|\alpha\rangle$$

- Rewriting the momentum space wave function:

$$\langle p'|\alpha\rangle = \int dx' \langle p'|x'\rangle \langle x'|\alpha\rangle$$

- Giving us the relations

$$\psi_\alpha(x') = \left[ \frac{1}{\sqrt{2\pi\hbar}} \right] \int dp' \exp\left( \frac{ip'x'}{\hbar} \right) \phi_\alpha(p')$$

$$\phi_\alpha(p') = \left[ \frac{1}{\sqrt{2\pi\hbar}} \right] \int dx' \exp\left( \frac{-ip'x'}{\hbar} \right) \psi_\alpha(x').$$

- These relations show that position space wave function and the momentum space wave function of our arbitrary state ( $\alpha$ ) are the fourier transforms of each other.

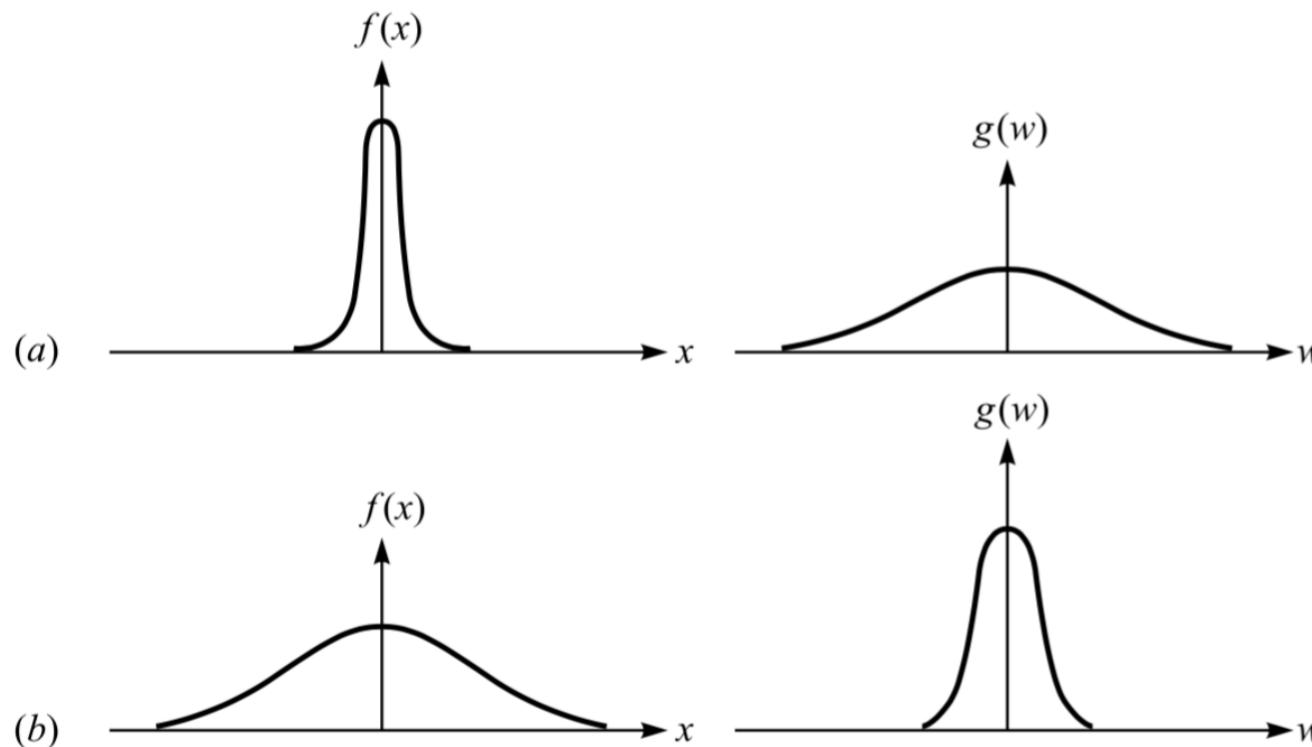
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# A DERIVATION

- We don't get any physical/mathematical inference out of the above equations unless we specify our wave functions. In that direction lets us set our position space wave function as the x-space wave function of a gaussian wave packet. The gaussian wave packet describes semi-localised particles such as electron/protons.

$$\langle x'|\alpha\rangle = \left[ \frac{1}{\pi^{1/4}\sqrt{d}} \right] \exp\left[ ikx' - \frac{x'^2}{2d^2} \right]$$

- Without going into the mathematics of the Fourier transformation of the above wave function into a function in momentum space, let us look at the below plots which explain a whole lot more:



1. Heisenberg's uncertainty principle occurs as a natural progression of these ideas. (ref. Modern quantum mechanics [2nd ed by JJ Sakurai]) p.57-58

# FOURIER TRANSFORM OF THE DIRAC DELTA FUNCTION

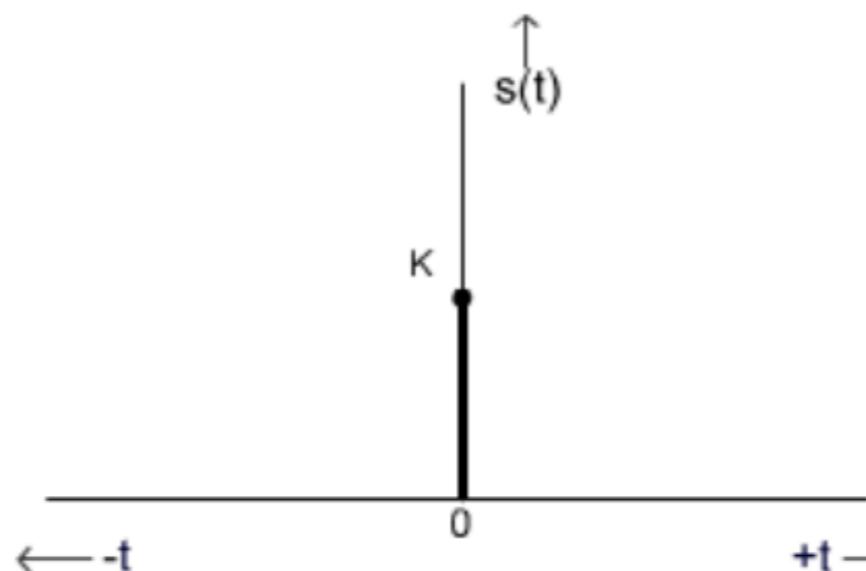
The delta function

$$\delta(t) = \begin{cases} 0 & t \neq 0 \\ \infty & t = 0 \end{cases}$$

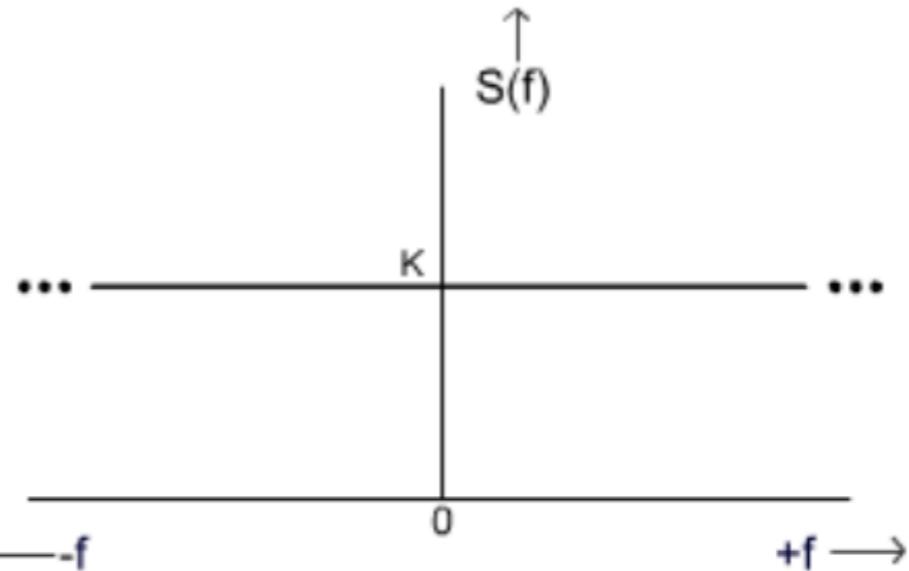
The Fourier transform

$$\tilde{f}(s) \equiv \int_{-\infty}^{\infty} dt \frac{e^{its}}{\sqrt{2\pi}} f(t).$$

TIME DOMAIN



FREQUENCY DOMAIN

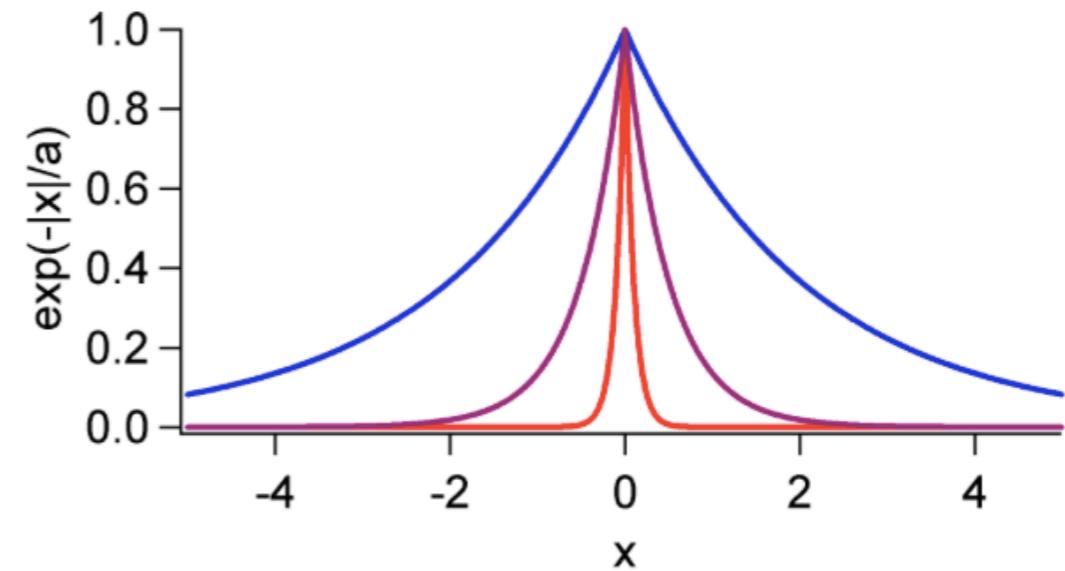


# FOURIER TRANSFORM OF THE EXPONENTIAL FUNCTION

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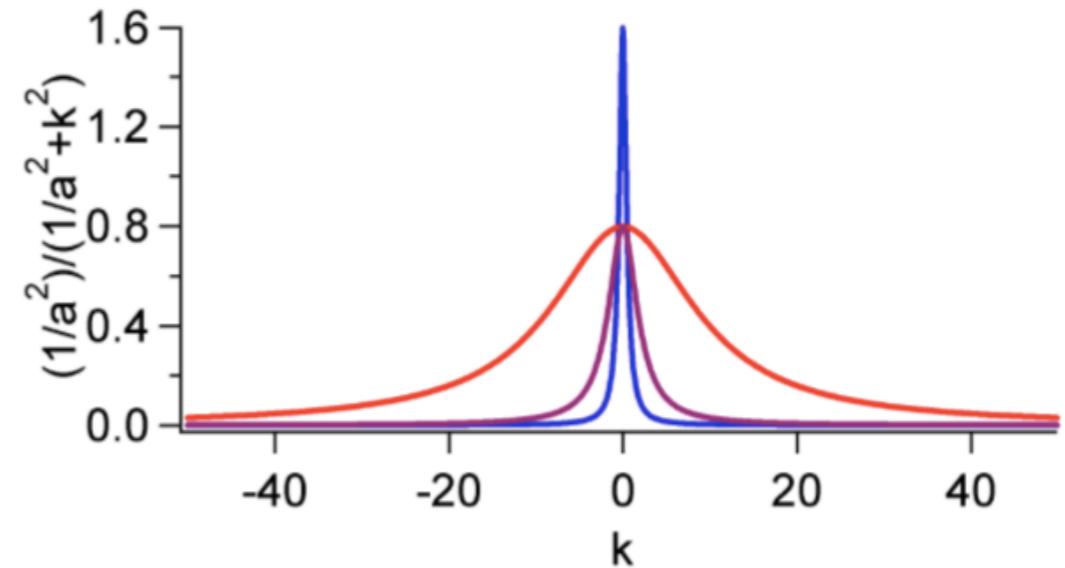
The Exponential function

$$G(x) = \exp\{-|x|/a\}$$



The Fourier transform

$$H(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-|x|/a} e^{-ikx} dx$$



# FOURIER TRANSFORM OF THE YUKAWA POTENTIAL FUNCTION

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The Yukawa potential function

$$V_{\text{Yukawa}}(r) = -g^2 \frac{e^{-kmr}}{r},$$

The Fourier transform

$$V(\mathbf{r}) = \frac{-g^2}{(2\pi)^3} \int e^{i\mathbf{k}\cdot\mathbf{r}} \frac{4\pi}{k^2 + m^2} d^3k$$

The Yukawa potential is the potential between two interacting particles, where the interaction is mediated by an exchange particle.

eg: The electromagnetic coulomb potential between two interacting electrons, the interaction being mediated by a photon of mass  $m=0$

# REFERENCES:

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1. Modern quantum mechanics (2nd ed.) by J.J. Sakurai and Jim Napolitano
2. Quantum Mechanics (2nd ed.) by Bransden and Joachain
3. Mathematical methods in physics by Tai L Chow

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<http://j.mp/fouriertransform>

| *thank you* |

# APPENDIX 1

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To get the normalization constant  $N$  let us first consider

$$\langle x' | x'' \rangle = \int dp' \langle x' | p' \rangle \langle p' | x'' \rangle. \quad (1.7.30)$$

The left-hand side is just  $\delta(x' - x'')$ ; the right-hand side can be evaluated using the explicit form of  $\langle x' | p' \rangle$ :

$$\begin{aligned} \delta(x' - x'') &= |N|^2 \int dp' \exp\left[\frac{ip'(x' - x'')}{\hbar}\right] \\ &= 2\pi\hbar|N|^2 \delta(x' - x''). \end{aligned} \quad (1.7.31)$$

Choosing  $N$  to be purely real and positive by convention, we finally have

$$\langle x' | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ip'x'}{\hbar}\right). \quad (1.7.32)$$