

Mathematics Methods and Thermodynamics

Mathematics - Functions, Transformations and Deltas

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CLASS OVERVIEW

- ▶ Integral Ranges
- ▶ Kronecker Delta
- ▶ Orthogonality
- ▶ Recursion Relations
- ▶ Dirac Delta
- ▶ Fourier Transform

REVIEW

- ▶ Last week we discussed special ODE
- ▶ These are useful ODE solved in a general way with special functions
- ▶ Some of the more useful functions that come from these special ODEs for chemistry are:
 - ▶ Laguerre Polynomial
 - ▶ Legendre Polynomial
 - ▶ Hermite Polynomial
- ▶ Fourier Series is a method of approximating any function into an expansion of trigonometric functions
- ▶ Fourier series is different from Fourier transform in that it is discrete while Fourier transform is continuous

INTEGRAL RANGE

- ▶ One of the questions from the previous week asked for you to transform the integral range from \int_0^3 to $\int_{-\pi}^{\pi}$
- ▶ But how is this actually done?

INTEGRAL RANGE

- First lets consider what happens when you change the coordinate via $x = u + 1$

$$\int_{x=0}^{x=10} F(x) = \int_{u+1=0}^{u+1=10} F(u+1)$$

$$\int_{u=-1}^{u=9} F(u+1)$$

INTEGRAL RANGE

- ▶ When you write the integrals in this form \int_x it becomes much easier to see how it transforms more generally if you have some function that transform x to u lets call this $u(x)$ then the integral range transform as

$$\int_a^b F(x) dx = \int_{u(a)}^{u(b)} F(u(x)) du$$

INTEGRAL RANGE

- ▶ In the case where we are trying to transform to known limits, for example transforming to \int_c^d , we need to find an appropriate function that will convert x to u ($X(u)$) if we lay out the question as follows we can see how we might find such a function

$$\int_{x=a}^{x=b} F(x) dx = \int_{X(c)=a}^{X(d)=b} F(X(u)) du$$

INTEGRAL RANGE

- ▶ For this unknown function we have two known points

$$X(c) = a$$

$$X(d) = b$$

- ▶ So for this function when we put in the new lower limit we get the old lower limit and similarly for the upper limit

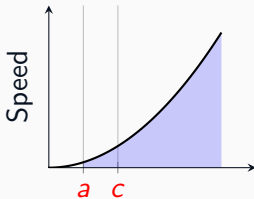
INTEGRAL RANGE

- ▶ What type of function should $X(u)$ be?
- ▶ Ideally it would have 2 unknowns (that can be solved with our two knowns) and not warp our function i.e. linear

INTEGRAL RANGE

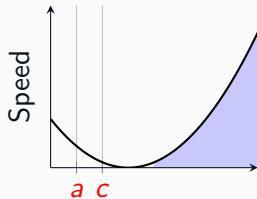
- ▶ If for a moment we ignore our upper limit you should know how to translate a function by some amount along the axis Δx

$$F(x) \rightarrow F(x - \Delta x)$$



Time

$f(x)$



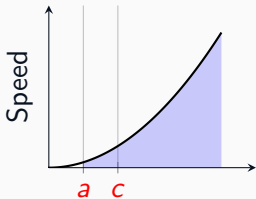
Time

$f(x - \Delta x)$

INTEGRAL RANGE

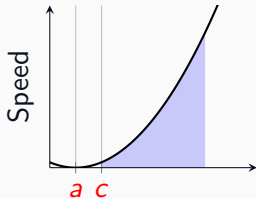
- ▶ If for a moment we ignore our upper limit you should know how to translate a function by some amount along the axis Δx

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Time

$f(x)$

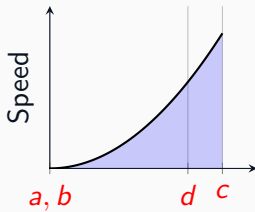


Time

$f(x - (b - a))$

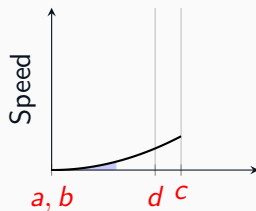
INTEGRAL RANGE

- ▶ To also set the upper limit we must scale the coordinate



Time

$$f(x)$$

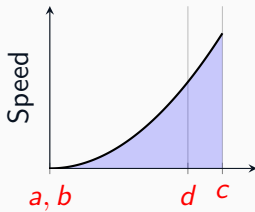


Time

$$f\left(\frac{1}{2}x\right)$$

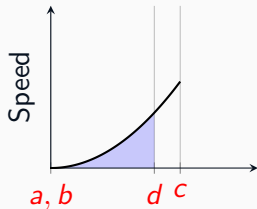
INTEGRAL RANGE

- To also set the upper limit we must scale the coordinate



Time

$$f(x)$$



Time

$$f\left(\frac{d-c}{b-a}x\right)$$

INTEGRAL RANGE

- ▶ The general form of $X(u)$ must therefore contain an addition and a multiplication.
- ▶ Generally we can write this as

$$X(u) = Au + B$$

INTEGRAL RANGE

- ▶ Now that we have a general form we can go about using our knowns to solve our unknowns

$$X(c) = Au + B = a$$

$$X(d) = Au + B = b$$

- ▶ Solving first equation for A

$$A = \frac{a - B}{c}$$

- ▶ Substituting into the second equation then solving for B

$$B = \frac{bc - ad}{c - d}$$

INTEGRAL RANGE

- ▶ Finally substituting B into A

$$A = \frac{a - b}{c - d}$$

INTEGRAL RANGE

- ▶ One last thing to remember is that since we are applying a coordinate transformation then we need to use the same rules we do for integration by substitution. As in we need to apply the change in size of an infinitely small chunk of dx to du

$$\int_a^b F(x) dx = \int_c^d F(Au + B) \frac{dAu + B}{du} du$$

Where

$$A = \frac{a - b}{c - d}$$

$$B = \frac{bc - ad}{c - d}$$

$$\frac{dAu + B}{du} = A = \frac{a - b}{c - d}$$

KRONECKER DELTA

- ▶ Last week we came across the Kronecker Delta
- ▶ This is given the definition

$$\delta_{n,m} = \begin{cases} 1 & \text{If } n = m \\ 0 & \text{else} \end{cases}$$

- ▶ It is the mathematical form of an on off switch and is often used in orthogonality relationships
- ▶ The Kronecker Delta only works with integers. Meaning it is discrete

KRONECKER DELTA

- ▶ How would these Kronecker Delta's behave?

$$\sum_{i=0}^5 i\delta_{i,3} = 3$$

$$\sum_{i=0}^5 i\delta_{i,7} = 0$$

$$\sum_{i=0}^5 \sum_{j=0}^5 jx^i \delta_{i,3} = \sum_{j=0}^5 jx^3$$

ORTHOGONALITY

- ▶ A lot of the polynomials from ODEs have a property called orthogonality
- ▶ This property can be useful to avoid integration under certain conditions
- ▶ The general form for orthogonality for some indexed function like a ODE function $F_n(x)$ is

$$\int_a^b G(x) F_n(x) F_m(x) dx = k\delta_{n,m}$$

- ▶ Where $G(x)$ is some function (sometimes called the weighting function) that makes $F_n(x)$ orthogonal. This is sometimes just $G(x) = 1$. It depends upon what $F_n(x)$ is. For example with Laguerres it is $G(x) = e^{-x}$.

ORTHOGONALITY

- ▶ Here are the orthogonality relationships for the three ODEs we mentioned last week

Generalised Laguerre

$$\int_0^{\infty} x^{\alpha} e^{-x} L_n^{\alpha}(x) L_m^{\alpha}(x) dx = \frac{\Gamma(n + \alpha + 1)}{n!} \delta_{n,m}$$

Laguerre

$$\int_0^{\infty} e^{-x} L_n L_m = \delta_{n,m}$$

ORTHOGONALITY

- ▶ Here are the orthogonality relationships for the three ODEs we mentioned last week

Legendre

$$\int_{-1}^1 P_n(x) P_m(x) dx = \frac{2}{2n+1} \delta_{n,m}$$

Hermite

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = \sqrt{\pi} 2^n n! \delta_{n,m}$$

USING ORTHOGONALITY

- ▶ Orthogonality can be quite useful consider the following

$$\int_0^{\infty} \sum_{i=0}^{10} \sum_{j=0}^{10} C_{i,j} e^{-x} L_i(x) L_j(x) dx = \sum_{i=0}^{10} C_{i,i}$$

- ▶ This sort of expression can turn up quite often in places where we use approximate functions

RECURSION RELATIONS

- ▶ In addition to orthogonality these polynomials also typically have recursion relations
- ▶ These are relations that link a polynomial of one degree to another degree
- ▶ For Example with Laguerre polynomials we have the recursion relations

$$xL_n(x) = -(n+1)L_{n+1}(x) + (2n+1)L_n(x) - nL_{n-1}(x)$$

$$xL'_n(x) = nL_n(x) - nL_{n-1}(x)$$

$$xL''_n(x) = (x-1)L'_n(x) - nL_n(x)$$

THE DIRAC DELTA

- ▶ We saw that the Kronecker delta is discrete and is a picking function for a discrete sum

$$\sum_{i=0}^{20} C_i F_i(x) \delta_{i,3} = C_3 F_3(x)$$

- ▶ What about the continuous case?
- ▶ What is a continuous sum?
- ▶ An integral is the continuous alternative of a discrete sum

THE DIRAC DELTA

- ▶ The Dirac delta is the continuous version of the Kronecker delta

$$\int_{-10}^{10} F(x)\delta(x) dx = F(0)$$

- ▶ For the Dirac delta $\delta(G(x))$ the function is picked where the value from the function is equal to zero
- ▶ This means it could “pick” more than one value if there is more than one root for $G(x)$, in this case the answer is the sum of the values

THE DIRAC DELTA

- ▶ The Dirac delta has the definition that it is 0 everywhere except at the origin
- ▶ At the origin its value is *undefined*
- ▶ However at the origin its *area* is defined as 1
- ▶ As a result the Dirac delta has no meaning in contexts without an area so without an integral the results are *undefined*

THE DIRAC DELTA

- ▶ Given this information have a go at the bonus question from a previous worksheet

$$\int_0^2 (\sin(x) x^3 e^{-x} + \ln(x) x^2) \delta(x-1) dx$$

$$(\sin(1) 1^3 e^{-1} + \ln(1) 1^2)$$

$$(\sin(1) e^{-1} + \ln(1))$$

FOURIER SERIES

- ▶ Last week we discussed the real coefficients Fourier series
- ▶ This series allows us to approximate a function as a series of sinusoid functions

$$f(x) = f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos(nx) + \sum_{n=1}^{\infty} b_n \sin(nx)$$

- ▶ Where we can calculate the coefficients as the following

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx$$

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) dx$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(nx) dx$$

FOURIER SERIES

- ▶ We can extend Fourier series to complex coefficients using the relationship

$$e^{\pm ix} = \cos(x) \pm i \sin(x)$$

Which is Euler's identity

- ▶ We extend Fourier series to the complex coefficient domain by using the following function

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{-inx}$$

COMPLEX NUMBERS

- ▶ Complex numbers are an integral part to the Fourier transform
- ▶ We can describe a complex number in two parts

$$z = x + iy$$

- ▶ Where x is the real part, y is the imaginary part and i is the imaginary number $i = \sqrt{-1}$. This is square or standard notation

COMPLEX NUMBERS

- ▶ Addition is done by adding each part

$$z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2)$$

- ▶ Multiplication is done like bracket expansion

$$z_1 z_2 = (x_1 + iy_1)(x_2 + iy_2)$$

$$z_1 z_2 = x_1 x_2 + ix_1 y_2 + iy_1 x_2 + i^2 y_1 y_2$$

$$z_1 z_2 = x_1 x_2 + ix_1 y_2 + iy_1 x_2 - y_1 y_2$$

COMPLEX NUMBERS

- ▶ Division is best done using polar notation
- ▶ In polar notation a complex number is

$$z = |z| e^{i\theta}$$

$$|z| = \sqrt{zz^*} = \sqrt{(x + iy)(x - iy)}$$

$$|z| = \sqrt{zz^*} = \sqrt{x^2 + y^2}$$

$$x = |z| \cos(\theta)$$

$$y = |z| \sin(\theta)$$

$$\theta = \begin{cases} \arctan \frac{y}{x} & x > 0 \\ \arctan \frac{y}{x} + 180^\circ & x < 0 \end{cases}$$

COMPLEX NUMBERS

- ▶ Multiplication in polar notation is

$$z_1 z_2 = |z_1| |z_2| e^{i(\theta_1 + \theta_2)}$$

- ▶ Division in polar notation is

$$\frac{z_1}{z_2} = |z_1| |z_2| e^{i(\theta_1 - \theta_2)}$$

FOURIER SERIES

- ▶ For the Fourier series with complex coefficient

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{inx}$$

- ▶ To calculate the coefficients we evaluate the integral multiplied by the complex term, e^{-imx}

$$\int_{-\pi}^{\pi} f(x) e^{-imx} dx = \int_{-\pi}^{\pi} \left(\sum_{n=-\infty}^{\infty} A_n e^{inx} \right) e^{-imx} dx$$

FOURIER SERIES

$$\sum_{n=-\infty}^{\infty} A_n \int_{-\pi}^{\pi} e^{i(n-m)x} dx$$

$$\sum_{n=-\infty}^{\infty} A_n \int_{-\pi}^{\pi} (\cos((n-m)x) + i \sin((n-m)x)) dx$$

$$\sum_{m=-\infty}^{\infty} A_n 2\pi \delta_{n,m} = 2\pi A_m$$

FOURIER SERIES

► Therefore

$$\int_{-\pi}^{\pi} f(x) e^{-inx} dx = 2\pi A_n$$

$$A_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx} dx$$

FOURIER SERIES

- ▶ The Fourier series we have discussed is for a function in the range $-\pi$ to π
- ▶ If we have a periodic function that repeats around the origin with a period of L we can represent it via a coordinate transform as:

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\left(\frac{2\pi nx}{L}\right)}$$

$$A_n = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) e^{i\left(\frac{2\pi nx}{L}\right)} dx$$

- ▶ These equations are the basis for Fourier transform as $L \rightarrow \infty$

FOURIER TRANSFORM

- ▶ Now for the *Fourier Transform*
- ▶ This is an incredible useful transformation that breaks down a wave (or any well behaved function) into all of its component sinusoidal functions
- ▶ The Fourier Transform relies upon that any waveform is actually just a sum of simple sinusoidal functions of different frequencies

FOURIER TRANSFORM

- ▶ From the complex Fourier Series

$$f(x) = \sum_{n=-\infty}^{\infty} A_n e^{i\left(\frac{2\pi nx}{L}\right)}$$

- ▶ We extend to the Fourier transform which works for non periodic (as in not discrete, but instead continuous) by extending $L \rightarrow \infty$
- ▶ When we extend to infinity we replace the discrete parts continuous parts:
 - ▶ $A_n \rightarrow F(k)$
 - ▶ $\frac{n}{L} \rightarrow k$
 - ▶ $\sum_{-\infty}^{\infty} \rightarrow \int_{-\infty}^{\infty}$

FOURIER TRANSFORM

- ▶ The Fourier transform is therefore

$$f(x) = \mathcal{F}^{-1}[F(k)] = \int_{-\infty}^{\infty} F(k) e^{2\pi i k x} dk$$

- ▶ Where $F(k)$ can be found via

$$F(k) = \mathcal{F}[f(x)] = \int_{-\infty}^{\infty} f(x) e^{-2\pi i k x} dx$$

- ▶ The later equation is the Fourier transform $\mathcal{F}[f(x)]$, while the former is the inverse $\mathcal{F}^{-1}[F(k)]$

FOURIER TRANSFORM

- ▶ We usually represent the Fourier transform in the frequency ν and time domains t

$$F(\nu) = \mathcal{F}[f(t)] = \int_{-\infty}^{\infty} f(t) e^{-2\pi i \nu t} dt$$

$$f(t) = \mathcal{F}^{-1}[F(\nu)] = \int_{-\infty}^{\infty} F(\nu) e^{2\pi i \nu t} d\nu$$

- ▶ The Fourier transform of intensity vs time $f(t)$ becomes a function of intensity vs frequency $F(\nu)$

FOURIER TRANSFORM

- ▶ There are many relations of Fourier transform that are useful in different situations
- ▶ In terms of ODEs the most important relation is that Fourier transform of a derivative is given by

$$\mathcal{F} \left[\frac{d^n f(t)}{dt^n} \right] = (i2\pi\nu)^n F(\nu)$$

Here we see that additional derivatives in time become a multiplication in frequency

FOURIER TRANSFORM

- ▶ The Fourier transform is a linear transformation

$$\mathcal{F}[f(t) + g(t)] = \mathcal{F}[f(t)] + \mathcal{F}[g(t)]$$

- ▶ We can use these two properties on the following ODE

$$y''(t) - y(t) = -g(t)$$

- ▶ First take the Fourier transform of the equation

$$\mathcal{F}[y''(t)] - \mathcal{F}[y(t)] = -\mathcal{F}[g(t)]$$

$$(2\pi i\nu)^2 Y(\nu) - Y(\nu) = -G(\nu)$$

FOURIER TRANSFORM

- ▶ We can now solve for Y in the frequency domain easier than in the time domain

$$Y(\nu) = \frac{G(\nu)}{1 + 4\pi^2\nu^2}$$

- ▶ Then apply the inverse transform

$$y(t) = \mathcal{F}^{-1}[Y(\nu)] = \mathcal{F}^{-1}\left[\frac{G(\nu)}{1 + 4\pi^2\nu^2}\right]$$

- ▶ We now use the modulation property of Fourier transforms that states

$$\mathcal{F}[g(t)h(t)] = G(\nu) * H(\nu)$$

$a * b$ is a convolution no multiplication

FOURIER TRANSFORM

- ▶ This gives us

$$y(t) = \mathcal{F}^{-1} \left[\frac{1}{1 + 4\pi^2\nu^2} \right] * \mathcal{F}^{-1} [G(\nu)]$$

$$y(t) = \mathcal{F}^{-1} \left[\frac{1}{1 + 4\pi^2\nu^2} \right] * g(t)$$

$$y(t) = \frac{e^{-|t|}}{2} * g(t)$$

- ▶ Finally we apply a deconvolution

$$\frac{1}{2} \int_{-\infty}^{\infty} e^{-|t-\tau|} g(\tau) d\tau$$

FOURIER TRANSFORM

- ▶ To summarise, Fourier transform represents the function in a different way without losing information
- ▶ The Fourier transformation is defined as follows

$$F(\nu) = \mathcal{F}[f(t)] = \int_{-\infty}^{\infty} f(t) e^{-2\pi i \nu t} dt$$

$$f(t) = \mathcal{F}^{-1}[F(\nu)] = \int_{-\infty}^{\infty} F(\nu) e^{2\pi i \nu t} d\nu$$

- ▶ We usually represent the Fourier transform as a transformation from the time domain to the frequency domain
- ▶ We can use the Fourier transform to solve ODE under certain conditions

SUMMARY

- ▶ We covered how integral ranges transform with the coordinates and how you can obtain a specific integral range
- ▶ The Kronecker delta, which is a discrete picking function
- ▶ The orthogonality and recursion relations of special functions
- ▶ The Dirac delta which is a continuous picking function
- ▶ The Fourier transform and its application in ODEs