Fundamentals

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Content (week 2)

- Solid angles
- Legendre polynomials and spherical harmonics
- Mathematical basis:
  - Functions and distributions
  - Probability densities
  - Change of variables
  - Dirac Delta distributions
  - Probability tables

Solid angles

The direction of a moving particle is represented by its solid angle, so that

$$\boldsymbol{V}_{\rm n} = V_{\rm n}\,\boldsymbol{\Omega}$$

where $V_{\rm n} = |\boldsymbol{V}_{\rm n}|$ and $|\boldsymbol{\Omega}| = 1$.
X: principal axis
ψ: colatitude or polar angle ($0 \le \psi \le \pi$)
ϕ: azimuth ($0 \le \phi \le 2\pi$)
$\mu = \cos\psi\,,\ \eta\,,\ \xi$: direction cosines

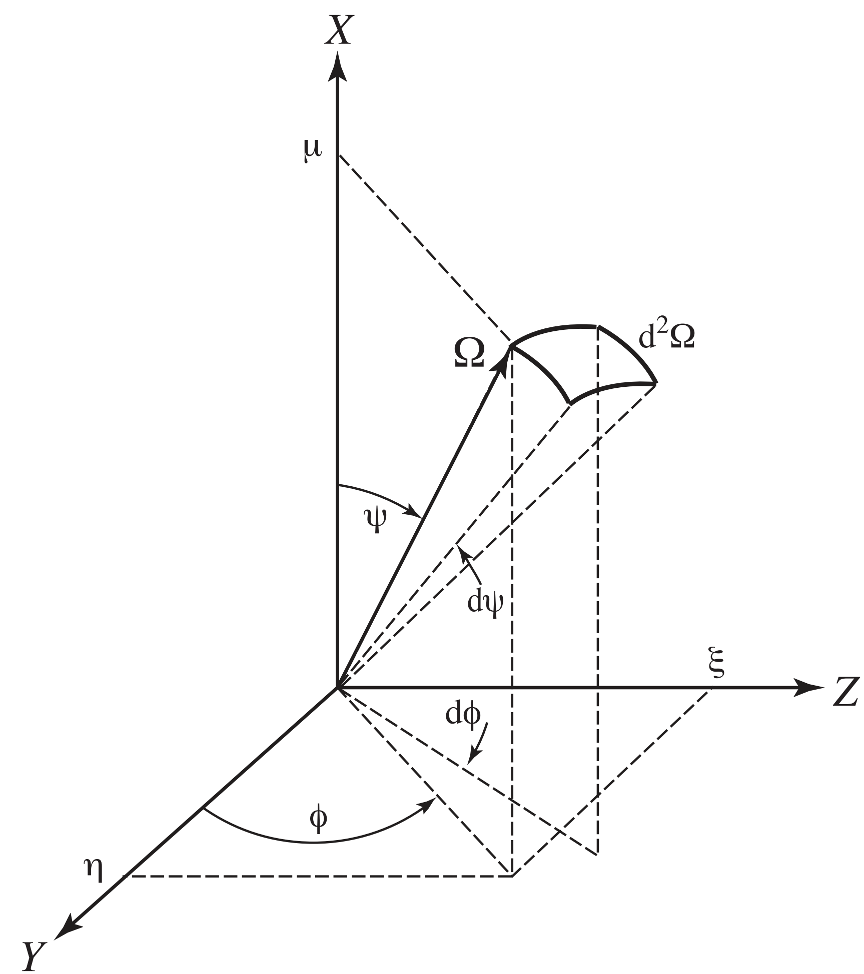
$$\boldsymbol{\Omega} = \mu\,\boldsymbol{i} + \eta\,\boldsymbol{j} + \xi\,\boldsymbol{k}$$

where

$$\eta = \sqrt{1-\mu^2}\cos\phi \quad \text{and} \quad \xi = \sqrt{1-\mu^2}\sin\phi \ .$$

The differential solid angle is the differential unit surface over the sphere of radius 1:

$$d^2\Omega = (1\,d\psi)(1\ \sin\psi\,d\phi) = \sin\psi\,d\psi\,d\phi \ .$$



Legendre polynomials

Some quantities $f(\mu)$ are distributions of the direction cosine μ but not of the azimuth. They can be developed in term of Legendre polynomials:

$$f(\mu) = \sum_{\ell=0}^{L} \frac{2\ell+1}{2} f_\ell \, P_\ell(\mu)$$

Legendre polynomials obey the following orthonormal relations:

$$\int_{-1}^{1} d\mu \; P_\ell(\mu) \, P_{\ell'}(\mu) = \frac{2}{2\ell+1} \, \delta_{\ell,\ell'}$$

so that the ℓ–th order coefficient of the distribution is obtained using

$$f_\ell = \int_{-1}^{1} d\mu \, P_\ell(\mu) \, f(\mu) \quad .$$

Legendre polynomials

The Legendre polynomials are defined by the relations

$$P_0(\mu) = 1 \; , \quad P_1(\mu) = \mu$$

and

$$P_{\ell+1}(\mu) = \frac{1}{\ell+1} \left[(2\ell+1)\mu \, P_\ell(\mu) - \ell \, P_{\ell-1}(\mu) \right] \quad \text{if } \ell \geq 1.$$

Real spherical harmonics

Some quantities $f(\boldsymbol{\Omega})$ are distributions of the solid angle $\boldsymbol{\Omega}$. They can be developed in term of real spherical harmonics:

$$f(\boldsymbol{\Omega}) = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi} \sum_{m=-\ell}^{\ell} f_\ell^m \, R_\ell^m(\boldsymbol{\Omega})$$

where $R_\ell^m(\boldsymbol{\Omega})$ is a real spherical harmonics component, a distribution of the solid angle $\boldsymbol{\Omega}$. The first component μ of the solid angle is the cosine of the polar angle and ϕ represents the azimuthal angle. These components are expressed in term of the associated Legendre functions $P_\ell^{|m|}(\mu)$ using

$$R_\ell^m(\boldsymbol{\Omega}) = \sqrt{(2-\delta_{m,0}) \, \frac{(\ell-|m|)!}{(\ell+|m|)!}} \; P_\ell^{|m|}(\mu) \, \mathcal{T}_m(\phi)$$

where $P_\ell^m(\mu)$ is defined in terme of the ℓ–th order Legendre polynomial $P_\ell(\mu)$ as

$$P_\ell^m(\mu) = (1-\mu^2)^{m/2} \, \frac{d^m}{d\mu^m} \, P_\ell(\mu) \quad , \quad m \geq 0$$

Real spherical harmonics 2

and where

$$\mathcal{T}_m(\phi) = \begin{cases} \cos m\phi \,, & \text{if } m \geq 0; \\ \sin |m|\phi \,, & \text{otherwise.} \end{cases}$$

Note that we have used the Ferrer definition of the associated Legendre functions $P_\ell^m(\mu)$, in which the factor $(-1)^m$ is absent.
Real spherical harmonics obey the following orthonormal relations:

$$\int_{4\pi} d^2\Omega \; R_\ell^m(\mathbf{\Omega}) \, R_{\ell'}^{m'}(\mathbf{\Omega}) = \frac{4\pi}{2\ell+1} \, \delta_{\ell,\ell'} \, \delta_{m,m'}$$

The components of the distribution are written

$$f_\ell^m = \int_{4\pi} d^2\Omega \; R_\ell^m(\mathbf{\Omega}) \, f(\mathbf{\Omega}) \quad .$$

In the previous relations, we have introduced the integral over 4π to represent an integration over all possible directions. This integral is defined as

$$\int_{4\pi} d^2\Omega \, f(\mathbf{\Omega}) \equiv \int_{-1}^{1} d\mu \int_0^{2\pi} d\phi \, f(\mu, \phi) \quad .$$

Real spherical harmonics 3

The real spherical harmonics satisfy the addition theorem which can be written in term of two different solid angles $\mathbf{\Omega}$ and $\mathbf{\Omega}'$ as

$$P_\ell(\mathbf{\Omega}\cdot\mathbf{\Omega}') = \sum_{m=-\ell}^{\ell} R_\ell^m(\mathbf{\Omega})\, R_\ell^m(\mathbf{\Omega}') \ ; \ \ \ell \geq 0 \ .$$

The real spherical harmonics can be written as polynomials in direction cosines as follows:

$$R_0^0 = 1 \ ,$$

$$R_1^{-1} = \xi \ , \quad R_1^0 = \mu \ , \quad R_1^1 = \eta \ ,$$

$$R_2^{-2} = \sqrt{3}\,\eta\xi \ , \quad R_2^{-1} = \sqrt{3}\,\mu\xi \ , \quad R_2^0 = \frac{1}{2}\left(3\mu^2 - 1\right) \ ,$$

$$R_2^1 = \sqrt{3}\,\mu\eta \ , \quad R_2^2 = \frac{\sqrt{3}}{2}\left(\eta^2 - \xi^2\right) \ , \ \text{etc.}$$

Functions and distributions

Many important quantities in reactor physics are probability densities or number densities with respect to space, solid angle and/or energy.
A distribution is an abstract quantity that gain physical significance only when combined with an order–n differential and associated with a support, i.e., a definition domain.

Definition

A probability density $P(x)$ is a distribution of the random variable x defined in such a way that the average of a function $f(x)$ is given by relation

$$\langle f(x) \rangle = \int_{\mathcal{D}} dx\, f(x)\, P(x)$$

so that its normalization is

$$\langle 1 \rangle = \int_{\mathcal{D}} dx\, P(x) = 1.$$

Functions and distributions 2

Let's take, as example, the probability density $P_{\rm f}(\mathbf{\Omega})$ representing the angular distribution of secondary fission neutrons. This quantity is only meaningful with

- an order–2 differential $d^2\Omega = \sin\psi \, d\psi \, d\phi$ where $\psi = \cos^{-1}\mu$ is the polar angle of the secondary neutron with respect to the principal axis and ϕ is the azimuthal angle. This differential is a scalar quantity. We should therefore avoid the notation $d\mathbf{\Omega}$.
- the support $0 \le \psi \le \pi$ and $0 \le \phi \le 2\pi$.

In this case, $P_{\rm f}(\mathbf{\Omega})\, d^2\Omega$ is the probability for the direction of the secondary neutron to be equal to $\mathbf{\Omega}$ within a $d^2\Omega$ interval.

If we assume isotropic emission for this neutron, then $P_{\rm f}(\mathbf{\Omega})$ will be equal to a constant:

$$P_{\rm f}(\mathbf{\Omega}) \equiv P_{\rm f}(\mu, \phi) = c \quad .$$

The value of this constant can be obtained from the knowledge that any probability density is normalized to one:

$$\int_{-1}^{1} d\mu \int_{0}^{2\pi} d\phi \, P_{\rm f}(\mu, \phi) = (2)(2\pi)c = 1$$

so that

$$P_{\rm f}(\mathbf{\Omega}) = \frac{1}{4\pi} \quad .$$

Functions and distributions

Distributions behave differently than functions. They are characterized by the following properties:

1. A distribution $D(x)$ is positive ($D(x) \geq 0$).
2. The product of a function $f(x)$ by a distribution $D(x)$ is a distribution of x. In this case, $f(x)D(x)$ is a distribution of x.
3. The product of two distributions of x has no mathematical meaning.
4. If $D_2(x,y)$ is a distribution of x and y, then a distribution of x only is obtained using the following reduction formula:

$$D_1(x) = \int_{S_y} dy\, D_2(x,y)$$

where S_y is the support of y.

Functions and distributions

5. Let's give a distribution $D_{\mathrm{a}}(x)$ over support $\{S_x : x_1 \leq x \leq x_2\}$. It is possible to obtain $D_{\mathrm{b}}(y)$ with $y = f(x)$, where $f(x)$ is a strictly increasing or decreasing function of x over S_x. In this case,

$$D_b(y) = D_a(x)\left|\frac{dx}{dy}\right|$$

which can be explicitly written as

$$D_b(y) = \begin{cases} D_a(x)\,\dfrac{dx}{dy}\ ; \quad S_y : f(x_1) \leq y \leq f(x_2), & \text{if } \dfrac{dy}{dx} > 0; \\ -D_a(x)\,\dfrac{dx}{dy}\ ; \quad S_y : f(x_2) \leq y \leq f(x_1), & \text{if } \dfrac{dy}{dx} < 0. \end{cases}$$

Change of variables

Let's compute the probability density $P_{\mathrm{f}}(\psi)$ relative to the polar angle, for an isotropic distribution in LAB. A distribution reduction is first performed, leading to an expression for $P_{\mathrm{f}}(\mu) = P_{\mathrm{f}}(\cos\psi)$. We obtain

$$P_{\mathrm{f}}(\cos\psi) = \int_0^{2\pi} d\phi \; P_{\mathrm{f}}(\cos\psi, \phi) = \frac{1}{4\pi} \int_0^{2\pi} d\phi = \frac{1}{2} \; ; \quad \text{with} \quad -1 \le \cos\psi \le 1 \quad .$$

Next, a change of variable is performed, as

$$P_{\mathrm{f}}(\psi)\, d\psi = P_{\mathrm{f}}(\cos\psi)\; |d(\cos\psi)|$$

so that

$$P_{\mathrm{f}}(\psi) = \frac{\sin\psi}{2}$$

with

$$\int_0^{\pi} d\psi \; P_{\mathrm{f}}(\psi) = 1 \quad .$$

Change of variables

Note that we have keep the same symbol to identify $P_{\rm f}(\mathbf{\Omega})$, $P_{\rm f}(\cos\psi)$ and $P_{\rm f}(\psi)$ even through they are different mathematical quantities. This shortcut is called generic symbolism and will be used through this book. The exact meaning of $P_{\rm f}$ is found by looking at its arguments.

Let us now compute back the probability density $P_{\rm f}(\mu) = P_{\rm f}(\cos\psi)$ with respect of the principal direction cosine μ. We perform a change of variable toward $\mu = f(\psi) = \cos\psi$, so that

$$\frac{d}{d\psi} f(\psi) = -\sin\psi < 0\,; \quad \text{with} \quad 0 \le \psi \le \pi$$

and

$$P_{\rm f}(\mu) = -P_{\rm f}(\psi)\,\frac{d\psi}{df(\psi)} = -\left[\frac{\sin\psi}{2}\right]\left[\frac{1}{-\sin\psi}\right] = \frac{1}{2}\,; \quad \text{with} \quad -1 \le \mu \le 1 \quad .$$

Dirac delta distributions

The Dirac delta distribution is a probability density that can be view as the mathematical expression of certainty. If a variable x, defined over support S_x, is always equal to x_0 with $x_0 \in S_x$, then the corresponding probability density is written $\delta(x - x_0)$. We can write

$$\int_{S_x} dx\, f(x)\, \delta(x - x_0) = f(x_0)$$

where $f(x)$ is any function of x defined over the support. The Dirac delta distribution is normalized to one, as any probability density, so that $\int_{S_x} dx\, \delta(x - x_0) = 1$.

A change of variable can be performed in the usual way. If $y = f(x)$ and

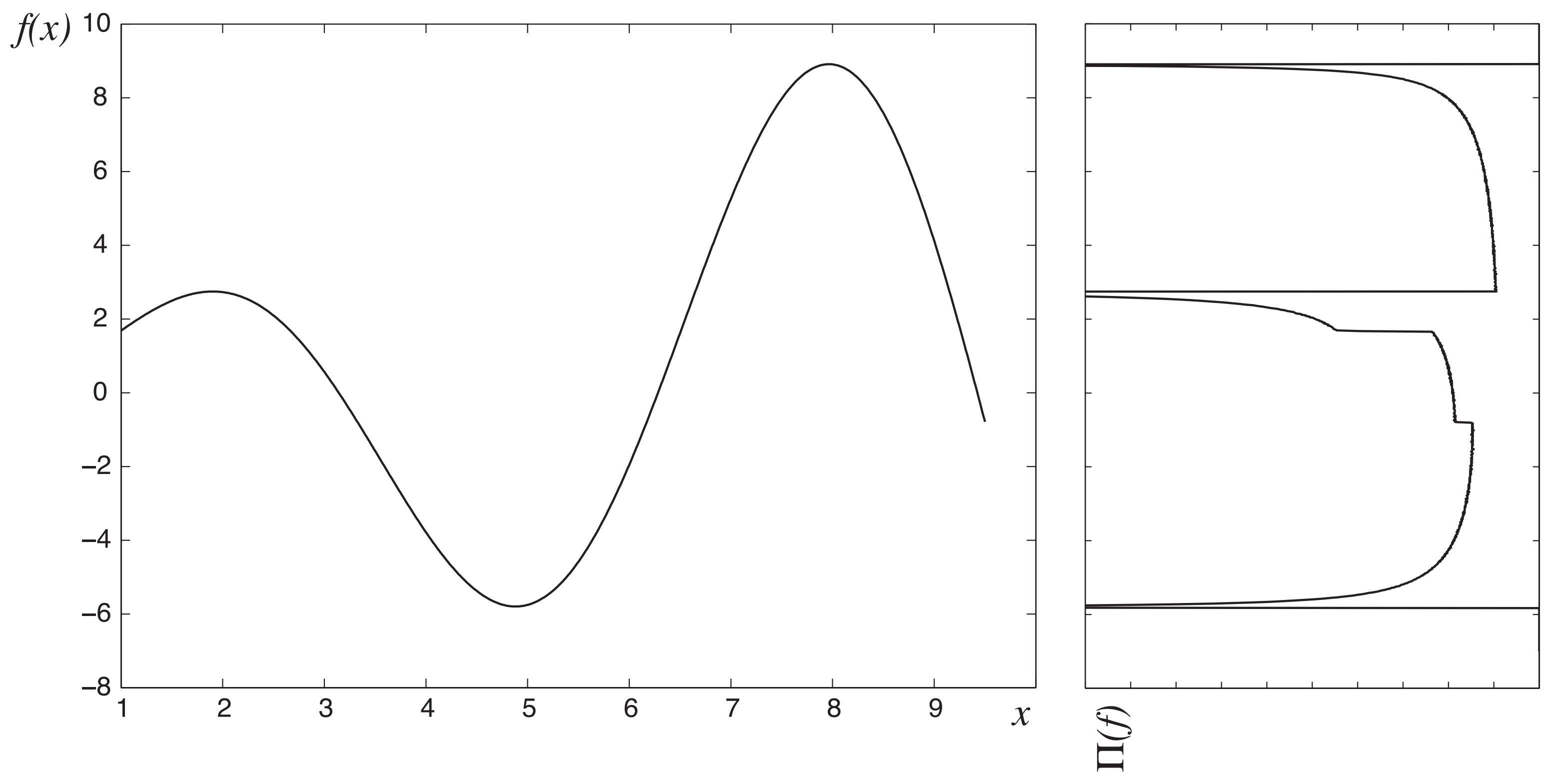
$$\delta(y) = \delta(x) \left| \frac{dx}{dy} \right|$$

so that in the particular case where $y = \lambda x$, the delta distribution reduces to

$$\delta(\lambda x) = \frac{\delta(x)}{|\lambda|} \quad .$$

Probability tables

Probability tables corresponding to a function $f(x)$ with $x_1 \leq x \leq x_2$ can be defined from the probability density $\Pi(f)$. $\Pi(f)df$ is the probability for function $f(x)$, to have a value between f and $f + df$ inside domain $x_1 \leq x \leq x_2$. An illustration of this probability density is shown in the following figure:



Probability tables

To obtain the $f(x)$ curve:

```
>> x1=1 ; x2=9.5 ;
>> dx=(x2-x1)/999 ;
>> x=x1:dx:x2 ;
>> y=(x+1).*sin(x) ;
>> plot(x,y)
```

To obtain the $\Pi(f)$ curve:

```
>> fmin=-7 ;  fmax=10. ;
>> db=(fmax-fmin)/999 ;
>> b=fmin:db:fmax ;
>> c=zeros(1,1000) ;
>> for i=1:100000
  xi=x1+(x2-x1)*(i-1)/99999 ;
  yi=(xi+1)*sin(xi) ;
  f=(yi-fmin)/(fmax-fmin) ; k=1+fix(f*999) ;
  c(k)=c(k)+1 ;
end
>> plot(b,c)
```

Probability tables 3

The probability density $\Pi(f)$ is normalized to unity:

$$\int_{\min(f)}^{\max(f)} df\, \Pi(f) = 1 \quad .$$

The probability density $\Pi(f)$ is next transformed into an equivalent probability density $\Pi'(f)$ defined as a weighted sum of K Dirac delta distributions:

$$\Pi'(f) = \sum_{k=1}^{K} \delta(f - f_k)\, \omega_k$$

where

$$\sum_{k=1}^{K} \omega_k = 1 \quad .$$

The discrete values ω_k and $f_k \in S_f$ are the weights and base points, respectively. The support of function $f(x)$ is $\{S_f : \min(f) \le f \le \max(f)\}$. The set of values $\{\omega_k,\ f_k,;\ k = 1, K\}$ is an order K probability table.

Probability tables

Using this approach, any Riemann integral with a f–dependent integrand and defined over domain $x_1 \leq x \leq x_2$, can be replaced by an equivalent Lebesgue integral defined over support S_f. We can write

$$\frac{1}{x_2 - x_1} \int_{x_1}^{x_2} dx \, g\left[f(x)\right] = \int_{\min(f)}^{\max(f)} df \, \Pi(f) \, g(f)$$

and

$$\int_{\min(f)}^{\max(f)} df \, \Pi'(f) \, g(f) = \sum_{k=1}^{K} \omega_k \, g(f_k) \quad .$$