Lecture 17: 3D Coordinate Systems

References: Course Pack p.121-123, 131-146.

3D Cartesian Coordinates

We can describe all space using coordinates (*x, y, z*), each variable ranging from -∞ to +∞.

1. PDEs in 3D Cartesian Coordinates

Consider the wave equation. In one dimensional space we had $\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2\Psi(x,t)}{\partial t^2}$.

This can be generalised to 2D (see Course Pack p.111-117) and 3D.

In 3D the wave equation becomes $\frac{\partial^2\Psi(x,y,z,t)}{\partial x^2} + \frac{\partial^2\Psi(x,y,z,t)}{\partial y^2} + \frac{\partial^2\Psi(x,y,z,t)}{\partial z^2} = \frac{1}{c^2}\frac{\partial^2\Psi(x,y,z,t)}{\partial t^2}$,

which may be written in shorthand as $\nabla^2\Psi(x,y,z,t) = \frac{1}{c^2}\frac{\partial^2\Psi(x,y,z,t)}{\partial t^2}$.

Let us look for a solution of the form $\Psi(x,y,z,t) = X(x)Y(y)Z(z)T(t)$, i.e. we try to separate the variables, as done in 1D. Differentiating gives

$\frac{\partial^2\Psi(x,y,z,t)}{\partial x^2} = Y(y)Z(z)T(t)\frac{d^2X(x)}{dx^2}$, and similarly $\frac{\partial^2\Psi(x,y,z,t)}{\partial y^2} = X(x)Z(z)T(t)\frac{d^2Y(y)}{dy^2}$,

$\frac{\partial^2\Psi(x,y,z,t)}{\partial z^2} = X(x)Y(y)T(t)\frac{d^2Z(z)}{dz^2}$, $\quad \frac{\partial^2\Psi(x,y,z,t)}{\partial t^2} = X(x)Y(y)Z(z)\frac{d^2T(t)}{dt^2}$.

Substituting these into the PDE then dividing through by $\Psi(x,y,z,t) = X(x)Y(y)Z(z)T(t)$, we get

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} + \frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2} + \frac{1}{Z(z)}\frac{d^2Z(z)}{dz^2} = \frac{1}{c^2T(t)}\frac{d^2T(t)}{dt^2}. \quad (*)$$

Each term in this expression is a function of only *one* variable. In order for the equation to hold for all *x, y, z* and *t*, each term must equal a constant. We want a *wave* solution to the wave equation, i.e. harmonic terms, so we choose each term to equal a *negative* constant. We let

$$\frac{1}{T(t)}\frac{d^2T(t)}{dt^2} = -\omega^2, \quad \frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = -{k_x}^2, \quad \frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2} = -{k_y}^2, \quad \frac{1}{Z(z)}\frac{d^2Z(z)}{dz^2} = -{k_z}^2.$$

Comparing with equation (*) we see that the constants, ω, k_x, k_y, k_z are related by $\frac{\omega^2}{c^2} = k_x^2 + k_y^2 + k_z^2 = k^2$.

Each of the ODEs above has the normal harmonic solutions, which we can write in terms of sines and cosines below. (The bracketed layout simply means that each variable can be represented either by sine or cosine depending on the boundary conditions and must not be confused with matrices).

$$X(x) \sim \begin{Bmatrix}\sin k_x x\\ \cos k_x x\end{Bmatrix}, \quad Y(y) \sim \begin{Bmatrix}\sin k_y y\\ \cos k_y y\end{Bmatrix}, \quad Z(z) \sim \begin{Bmatrix}\sin k_z z\\ \cos k_z z\end{Bmatrix}, \quad T(t) \sim \begin{Bmatrix}\sin \omega t\\ \cos \omega t\end{Bmatrix}.$$

Giving special solutions of the form $\Psi(x,y,z,t) = A\begin{Bmatrix}\sin k_x x\\ \cos k_x x\end{Bmatrix}\begin{Bmatrix}\sin k_y y\\ \cos k_y y\end{Bmatrix}\begin{Bmatrix}\sin k_z z\\ \cos k_z z\end{Bmatrix}\begin{Bmatrix}\sin \omega t\\ \cos \omega t\end{Bmatrix}$.

Or sometimes it is more convenient to use complex exponentials,

$$X(x) \approx e^{\pm ik_x x}, \quad Y(y) \approx e^{\pm ik_y y}, \quad Z(z) \approx e^{\pm ik_z z}, \quad T(t) \approx e^{\pm i\omega t}$$

Then we get special solutions such as

$$\Psi(x,y,z,t) = A\exp(i\omega t - ik_x x - ik_y y - ik_z z) = A\exp(i\omega t - i\mathbf{k.r}) \quad \text{where } \boldsymbol{k} = k_x\mathbf{i} + k_y\mathbf{j} + k_z\mathbf{k}.$$

As we might have expected, the solutions are plane waves with wavevector ***k*** (which is also the direction of travel of the wave) and frequency ω = c*k*.

A general solution can then be written as a sum over special solutions, and applying boundary conditions will determine which terms contribute and the allowed values of k_x, etc.

For example, suppose we have a box with dimensions L_1, L_2, L_3 in the x, y, z directions respectively and know that Ψ must vanish at the walls. Then the special solutions will be:

$$\Psi(x,y,z,t) = A\sin k_x x \sin k_y y \sin k_z z \sin \omega t \quad \text{where } k_x = \frac{n_1\pi}{L_1},\ k_y = \frac{n_2\pi}{L_2},\ k_z = \frac{n_3\pi}{L_3}.$$

So each special solution, or 'mode' will be characterized by *three* integers, n_1, n_2, n_3.

And this mode will have angular frequency $\omega^2 = c^2(k_x{}^2 + k_z{}^2 + k_z{}^2) = \pi^2 c^2\left(\frac{n_1{}^2}{L_1{}^2} + \frac{n_2{}^2}{L_2{}^2} + \frac{n_3{}^2}{L_3{}^2}\right)$.

An important question which arises in various areas of physics is the question of how many different modes (i.e. unique combinations of integers n_1, n_2, n_3) exist in a given frequency range, or in the frequency interval ω to $\omega + d\omega$? The answer is central to the derivation of Planck's Law for blackbody radiation, the Debye theory of heat capacities of solids, and various other situations.

2. Integrals in 3D Cartesian Coordinates

We have dV = dx dy dz, and must perform a triple integral over x, y and z. Normally we will only choose to work in Cartesian coordinates if the region over which we are to integrate is cuboid or comprises all space. Integrating over spherical regions, for example, is very nasty in Cartesian coordinates!

Example

Find the 3D Fourier transform, $F(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \iiint_{\text{all space}} f(\mathbf{r}) e^{-i\mathbf{k}.\mathbf{r}} dV$, *of* $f(x,y,z) = \begin{cases} 1, & |x| < a, |y| < b, |z| < c \\ 0 & \textit{otherwise} \end{cases}$.

The integral is just the product of three 1D integrals, and is thus easily evaluated:

$$F(k_x,k_y,k_z) = \frac{\mathbf{1}}{(\mathbf{2}\pi)^{3/2}} \int_{-a}^{a} e^{-ik_x x}dx \int_{-b}^{b} e^{-ik_y y}dy \int_{-c}^{c} e^{-ik_z z}dz = \frac{\mathbf{1}}{(\mathbf{2}\pi)^{3/2}} \left(\frac{e^{ik_x a} - e^{-ik_x a}}{ik_x}\right)\left(\frac{e^{ik_y b} - e^{-ik_y b}}{ik_y}\right)\left(\frac{e^{ik_z c} - e^{-ik_z c}}{ik_z}\right)$$

This is therefore a product of three *sinc* functions, i.e. $\left(\frac{e^{ik_x a} - e^{-ik_x a}}{ik_x}\right) = \frac{\mathbf{2}i\sin(k_x a)}{ik_x} = \mathbf{2}a\ \mathbf{sinc}(k_x a)$.

So doing this for all three components we get:

$$F(k_x,k_y,k_z) = \frac{\mathbf{8}}{(\mathbf{2}\pi)^{3/2}} \frac{\sin(k_x a)}{k_x} \frac{\sin(k_y b)}{k_y} \frac{\sin(k_z c)}{k_z} = \frac{\mathbf{8}abc}{(\mathbf{2}\pi)^{3/2}} \mathbf{sinc}(k_x a)\mathbf{sinc}(k_y b)\mathbf{sinc}(k_z c)$$

Integrals of this sort are encountered in condensed matter physics in crystals with rectangular lattices.

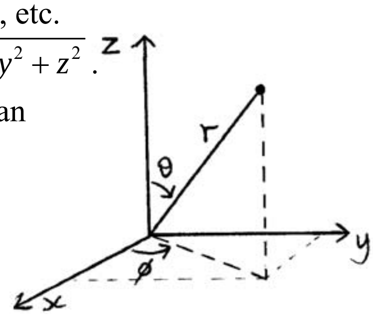
<u>3D Spherical Polar Coordinates</u>

1. Spherical Polar Coordinates: Revision

Spherical polars are the coordinate system of choice in almost all 3D problems. This is because most 3D objects are shaped more like spheres than cubes, e.g. atoms, nuclei, planets, etc.

And many potentials (Coulomb, gravitational, etc.) depend on $|\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$.

Physicists define r, θ, ϕ as shown in the figure. They are related to Cartesian coordinates by $x = r\sin\theta\cos\phi$, $\quad y = r\sin\theta\sin\phi$, $\quad z = r\cos\theta$.



2. 3D Integrals in Spherical Polars

The volume element is $dV = r^2\sin\theta\, dr d\theta d\phi$ (given on data sheet).

To cover over all space, we take $0 \le r < \infty$, $\quad 0 \le \theta < \pi$, $\quad 0 \le \phi < 2\pi$.

Exercise 1 *Show by integration in spherical coordinates that a sphere of radius R has volume $4\pi R^3/3$.*

We have $$V = \iiint_{sphere} r^2 \sin\theta \, dr \, d\theta \, d\phi = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \int_0^R r^2 dr = [\phi]_0^{2\pi} [-\cos\theta]_0^{\pi} \left[\frac{r^3}{3}\right]_0^R = \frac{4\pi R^3}{3} .$$

Exercise 2 *Find the Fourier transform of a screened Coulomb potential,* $U(r) = \dfrac{e^{-\lambda r}}{4\pi\varepsilon_0 r}$.

[This exercise is relevant to determining the scattering of electrons by a nucleus. The screening comes from the electrons bound in the atom. You will meet integrals like this in the Y3 nuclear physics module.]

As in lecture 17 we have the 3D Fourier transform $F(\mathbf{k}) = \dfrac{1}{(2\pi)^{3/2}} \iiint_{all\ space} f(\mathbf{r}) e^{-i\mathbf{k}.\mathbf{r}} dV$.

In this case $f(\mathbf{r}) = U(r)$ is a function only of the magnitude of r and not its direction and so has perfect radial symmetry. Again the volume element is $dV = r^2 \sin\theta dr d\theta d\phi$ (given on data sheet).

We therefore have $F(\mathbf{k}) = \dfrac{1}{(2\pi)^{3/2}} \iiint_{all\ space} U(r) e^{-i\mathbf{k}.\mathbf{r}} r^2 \sin\theta \, dr \, d\theta \, d\phi$.

There is a standard 'trick' which is to chose the direction of $\mathbf{k}$ to be parallel to the polar (z) axis for the integral. Then $\mathbf{k}.\mathbf{r}$ becomes $kr\cos\theta$. Now clearly the whole integral is a function only of the magnitude of $\mathbf{k}$, not its direction, i.e. $F(\mathbf{k})$ becomes $F(k)$:

$$F(k) = \frac{1}{(2\pi)^{3/2}} \iiint_{all\ space} \frac{e^{-\lambda r}}{4\pi\varepsilon_0 r} e^{-ikr\cos\theta} r^2 \sin\theta \, dr \, d\theta \, d\phi = \frac{1}{(2\pi)^{3/2}} \frac{1}{4\pi\varepsilon_0} \int_0^{2\pi} d\phi \int_0^{\infty} dr \, re^{-\lambda r} \int_0^{\pi} d\theta \, e^{-ikr\cos\theta} \sin\theta$$

The integral over ϕ is trivial: it just gives a factor of 2π.
But note that the factor $e^{-ikr\cos\theta}$ involves r and θ. Which integral should we do next? The presence of the $\sin\theta$ together with the $e^{-ikr\cos\theta}$ makes integration by substitution over θ the obvious choice:

i.e. let $A = ikr\cos\theta$ *so* $dA = -ikr\sin\theta \, d\theta$ Rewrite $\int \sin\theta \, e^{-ikr\cos\theta} d\theta = \int -\sin\theta \, e^{-A} \dfrac{dA}{ikr\sin\theta}$

So $$\int_0^{\pi} \sin\theta \, e^{-ikr\cos\theta} d\theta = \frac{1}{ikr}\left[e^{-ikr\cos\theta}\right]_0^{\pi} = \frac{1}{ikr}\left(e^{ikr} - e^{-ikr}\right) = \frac{1}{ikr} 2i\sin kr = \frac{2\sin kr}{kr} = 2\,\mathrm{sinc}(kr)$$

We are then left with the integral over r:

$$F(k) = \frac{1}{(2\pi)^{3/2}} \frac{1}{4\pi\varepsilon_0} 2\pi \int_0^{\infty} dr \, re^{-\lambda r} \frac{2\sin kr}{kr} = \frac{1}{(2\pi)^{3/2}} \frac{1}{\varepsilon_0 k} \int_0^{\infty} (\sin kr) \, e^{-\lambda r} \, dr .$$

This type of integral was met earlier in the tutorial question exercises on Fourier transforms. The trick is to write the sine in terms of complex exponentials:

$$\int_0^{\infty} (\sin kr) \, e^{-\lambda r} \, dr = \frac{1}{2i} \int_0^{\infty} \left[e^{ikr} - e^{-ikr}\right] e^{-\lambda r} dr = \frac{1}{2i} \int_0^{\infty} \left[e^{-r(\lambda - ik)} - e^{-r(\lambda + ik)}\right] dr = \frac{1}{2i}\left[\frac{1}{\lambda - ik} - \frac{1}{\lambda + ik}\right] = \frac{k}{\lambda^2 + k^2}$$

This gives the final result: $$F(k) = \frac{1}{(2\pi)^{3/2}} \frac{1}{\varepsilon_0(\lambda^2 + k^2)}$$