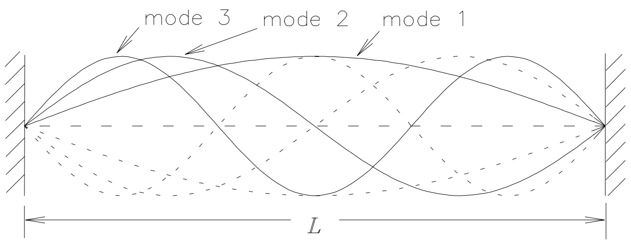
k-SPACE

The WAVENUMBER $k \equiv \dfrac{2\pi}{\lambda}$ of a wave has a special significance in both classical and quantum physics. Because waves are quantized (they can only occur in "packets" of energy $h\nu = \hbar\omega$ and momentum $h/\lambda = \hbar k$) we are often in the position of asking *what possible values* k can have, and *counting* the number of allowed k values. From this procedure arises the notion of "k-space" and the *density of states* in k-space, which may seem rather exotic on the first encounter but with which every physicist ultimately becomes intimately familiar.

The following arguments apply to *any* sort of wave (or *wavefunction*) that is *confined to a finite region* and constrained to have *nodes* at the *boundaries*.

1 Counting Modes in 1D



In a one dimensional "box" of length L, the "allowed" wavelengths are $\lambda_n = \dfrac{2L}{n}$ corresponding to wavenumbers $k_n = \dfrac{n\pi}{L}$. Thus the *smallest posssible wavenumber*, and the "distance" (in k-space) between successive allowed wavenumbers, is $\delta k = \dfrac{\pi}{L}$. There is $\delta N = 1$ allowed "state" per δk. Put another way, the "density" of allowed states *per unit wavenumber* is

$$\rho_k \equiv \frac{\delta N}{\delta k}$$

or, for this one-dimensional ($1D$) case,

$$\rho_{k_{1D}} = \frac{L}{\pi} \; .$$

Note that $n > 0 \Rightarrow k > 0$. We are drawing *standing waves*, $\cos kx = \frac{1}{2}\left(e^{ikx} + e^{-ikx}\right)$ (we choose $x = 0$ at the centre of the box, for symmetry), for which "negative" k values have no independent meaning.

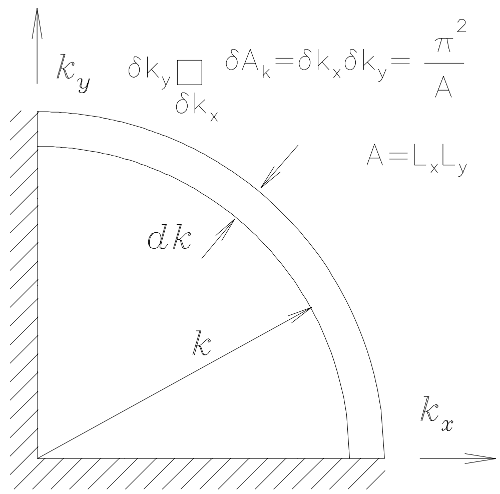
2 Counting Modes in 2D

In a rectangular box of width L_x and height L_y the modes which have nodes at all boundaries are products of sinusoidal functions of the form $\cos k_x x \cdot \cos k_y y$, where $k_x = n_x \dfrac{\pi}{L_x}$ and $k_y = n_y \dfrac{\pi}{L_y}$. Now the situation is a little more complicated, since $\vec{\boldsymbol{k}} = k_x \hat{\imath} + k_y \hat{\jmath}$ is a *vector*. In fact, we call it the **wavevector** instead of the wave*number*; the wave*number* $k \equiv |\vec{\boldsymbol{k}}|$ is then given by

$$k = \sqrt{k_x^2 + k_y^2} \; .$$

Why do we bother with the *magnitude* k instead of sticking to the intrinsically multidimensional *vector* $\vec{\boldsymbol{k}}$? Well, when we do **kinematics** we are often concerned with the *kinetic energy*, which is a *scalar* quantity depending only upon the *magnitude* of the momentum p (and upon the effective mass, if any) of the particle in question. Since we have discovered that *photons* (for example) are in some sense *particles* which have energy $\varepsilon = \hbar\omega$ and momentum $p = \hbar k$, we can conclude that $\varepsilon = \hbar ck$ (for massless particles only) and so, *if all we really care about is the energy ε of a given mode*, the only thing we need to know is its wave*number*, k.

But we still need to count up *how many* modes have (approximately) the *same* wavenumber k. This is where we have to return to the two-dimensional picture and begin talking in terms of **k-space**.



There is one allowed k_x for every $\delta k_x = \pi/L_x$ and one allowed k_y for every $\delta k_y = \pi/L_y$, so there is altogether $\delta N = 1$ allowed $\vec{\boldsymbol{k}}$ for every "*k-area*" element $\delta A_k = \delta k_x \cdot \delta k_y$ in two-dimensional k-space. (Yes, this is getting a little weird. Pay close attention!) Note that $\delta A_k = \pi^2/A$ where $A = L_x \cdot L_y$ is the actual physical area of the box in normal space. This element of k-space contains exactly $\delta N = 1$ allowed state, so once again we may define the *density of states* in k-space, $\rho_k \equiv \delta N/\delta A_k$ or, for this two-dimensional ($2D$) case,

$$\rho_{k_{2D}} = \frac{A}{\pi^2} \; .$$

Note that the density of states in k-space is proportional to the physical area of the region to which the waves are confined.

How many such states have (approximately) the *same wavenumber* k? This is a crucial question in many problems. To estimate the result we draw a *ring* in k-space with radius k and width dk. Recalling that only positive values of n_x and n_y are allowed (standing waves and all that), we only consider the upper right-hand quadrant of the circular ring; its "k-area" is thus $dA_k = \frac{1}{4} \cdot 2\pi\, k\, dk$. At a density of $\rho_{k_{2D}}$ states per unit k-area, this gives $\frac{\pi}{2}\rho_{k_{2D}}\, k\, dk = \frac{\pi}{2}\frac{A}{\pi^2}\, k\, dk$ or $\frac{A}{2\pi}\, k\, dk$ states in that ring quadrant. We can express this as a *density of wavenumber magnitudes* in terms of the distribution function

$$\mathcal{D}_{2D}(k)\, dk = \frac{A}{2\pi}\, k\, dk$$

which is defined as the number of allowed modes whose wavenumbers are within dk of a given k. Note that the number increases linearly with k, unlike in the $1D$ case where it is independent of k.

3 Counting Modes in 3D

In three dimensions, the extension is straightforward: $\vec{\boldsymbol{k}} = k_x\hat{\imath} + k_y\hat{\jmath} + k_z\hat{k}$ with $k_x = n_x\pi/L_x$, $n_x = 1, 2, 3, \cdots$ *etc.* Now there is $\delta N = 1$ allowed $\vec{\boldsymbol{k}}$ for each "*k-volume* element $\delta V_k = \delta k_x \cdot \delta k_y \cdot \delta k_y = \left(\frac{\pi}{L_x}\right) \cdot \left(\frac{\pi}{L_y}\right) \cdot \left(\frac{\pi}{L_z}\right) = \frac{\pi^3}{V}$, where $V = L_x {\cdot} L_y {\cdot} L_z$ is the actual physical volume of the three-dimensional box to which the waves are confined. This gives a density of modes in k-space of

$$\rho_{k_{3D}} = \frac{V}{\pi^3} \ .$$

The "volume" of k-space having wavenumbers within dk of $k = |\vec{\boldsymbol{k}}|$ is now the positive *octant* of a *spherical shell* of "radius" k and thickness dk: $dV_k = \frac{1}{8} \cdot 4\pi k^2\, dk$ and this shell contains $\rho_{k_{3D}} dV_k$ allowed modes, so the density of wavenumber magnitudes (distribution function) in $3D$ k-space is

$$\mathcal{D}_{3D}(k)\, dk = \frac{V}{2\pi^2}\, k^2\, dk \ .$$

Note that in this case the density increases as the *square* of the wavenumber. In fact, we can generalize: if d is the dimensionality of the region of confinement, then $\mathcal{D}_{dD}(k)\, dk \propto k^{d-1}\, dk$. In each case, the density of states in k-space is directly proportional to the size of the real-space region to which the waves are confined. More room, more possibilities.