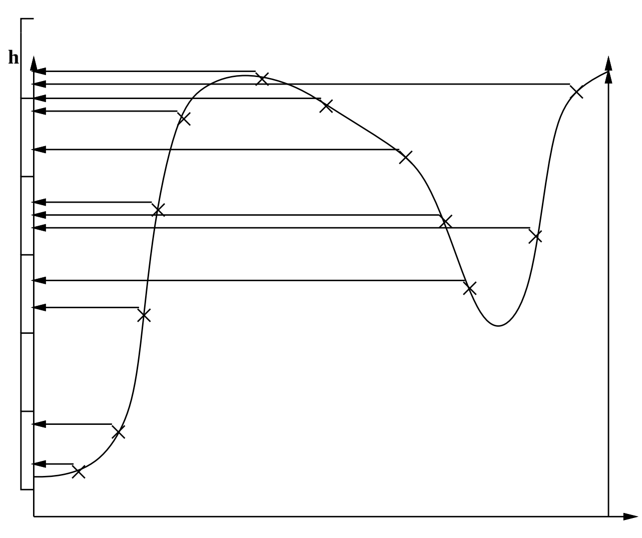
Physics 1: Density of States

The 'density of states' is a concept central to many areas of physics. We have a collection of things loosely described as 'states', which we label by i say, and each state has an associated value of a variable, f say. For some as yet unexplained reason, we want to concentrate only on the variable f and ignore the label i: ie We want only to know how many of the states have the value f and not the details as to which are the corresponding values of i. For example, in statistical physics, the probability of finding a state depends only on the energy of the state, and not on the details of the state. To calculate the energetics of a system we need only count the number of states of a given energy, ie we only require the *density of states.*

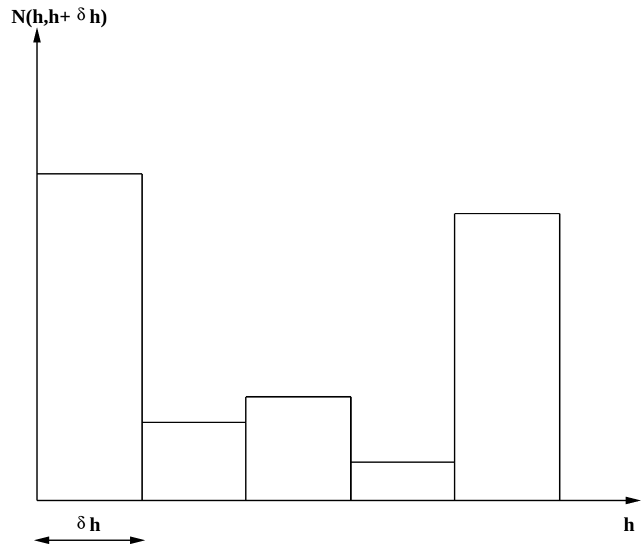
For a *discrete* situation this idea is simple: Consider a postman. Each house is a 'state' and on a particular day the number of letters delivered may be considered to be the variable f. The 'density of states' is then the number of houses with a fixed number of letters delivered. To find the average number of letters per house, we need only know the density of states, ρ_f say, in terms of which:

$$< f >= \frac{\sum_f f\rho_f}{\sum_f \rho_f}$$

For a *continuum* situation this idea is not so simple. Perhaps the simplest entry is via the continuum limit of a finite example. To be concrete, let us consider raindrops falling onto an irregular surface. For this problem the density of states corresponds to the number of raindrops that strike the surface at a particular height *per unit length of height*:



Although the discrete nature of the raindrops is a difficulty, one can use a 'pigeon hole' construction to assess the number of raindrops in a certain region and then take the continuum limit as the number of raindrops diverges:



where we have plotted the number of states found in the chosen interval. If the number of intervals is increased then the number of states in each interval decreases: What we want is the number of states *per unit length*, the *density of states.* If we have a smooth variation in numbers of states then the number of states per unit 'length' ought to become smooth and limit to a constant, as soon as the intervals become smaller than the structure of the surface, but before the number of states appears discrete. The density of states clearly becomes:

$$\rho(h)\delta h = N(h, h + \delta h)$$

in the limit that $\delta h \mapsto 0$, ie

$$\rho(h) = \frac{dN}{dh}$$

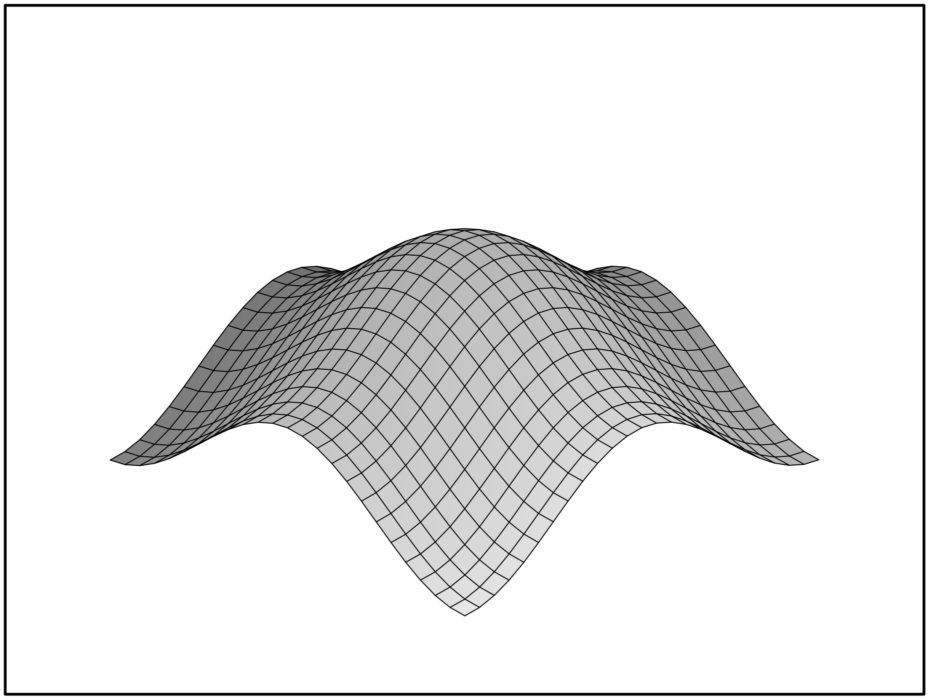
A second natural example of a density of states occurs in solid-state physics: The electronic *density of states*, or the number of states per unit of energy. When one considers electrons in metals, then from simple quantum mechanics we might expect an energy of the form:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})$$

in terms of kinetic energy and potential energy from the atoms. In the absence of potential, the electrons end up with energies:

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 \mid \mathbf{k} \mid^2}{2m}$$

in terms of the possible momenta $\hbar\mathbf{k}$. Although the existence of atoms modifies the shape of this 'energy dispersion', one would still expect to find that the momentum could be used as a label for the states and that each such momentum would have an associated energy. A particular example is that of the two-dimensional square lattice with nearest-neighbour 'interactions':



It is often useful to 'forget' about the particular momentum and 'remember' only the energy of the states, for which we need the *density of states* per unit energy. Electrons tend to 'fill up' the lowest energies of such a surface, up to a Fermi energy. This can be found using only the density of states, and does *not* depend on the details of the dispersion.

For the raindrops, it should also be clear that:

$$N(-\infty, h) = N_{total} \frac{1}{N_{total}} \sum_i \theta \left[h - h_i \right] \mapsto N_{total} \int_V \frac{dx}{V} \theta \left[h - h(x) \right]$$

where N_{total} is the total number of raindrops, the raindrops are presumed to fall anywhere in the volume V with equal likelihood, and where the θ function only contributes when the height is below h and so:

$$\rho(h) \mapsto N_{total} \int_V \frac{dx}{V} \delta \left[h - h(x) \right]$$

in terms of the Dirac δ-function, and a normalised density of states takes the generic form:

$$\rho(f) \mapsto \int_V \frac{d^d x}{V} \delta \left[f - f(x) \right]$$

where x is the continuum label for the state-space, *assumed* uniformly distributed.

The average of f depends only on the density of states:

$$< f >= \frac{1}{N_{total}} \sum_i f_i \mapsto \int_V \frac{dx}{V} f(x) = \int_V \frac{dx}{V} \int_{\mathbf{R}} df \delta \left[f - f(x) \right] f(x)$$

$$= \int_{\mathbf{R}} df f \int_V \frac{dx}{V} \delta \left[f - f(x) \right] = \int_{\mathbf{R}} df f \rho(f)$$