

Physics 112

Single Particle Density of States

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(Dated: January 26, 2012)

In class, we went through the problem of counting states (of a single particle) in a box. We noted that a state is specified by a wavevector \vec{k} , and the fact that the particle is confined within a box of size $V = L \times L \times L$ implies that the allowed values of \vec{k} form a regular grid of points in k -space. We showed that the number of values of \vec{k} whose magnitude lie between k and $k + dk$ is $\tilde{\rho}(k) dk$ where

$$\tilde{\rho}(k) dk = \frac{V}{(2\pi)^3} 4\pi k^2 dk. \quad (1)$$

This result is general, and does not depend on the dispersion relation, i.e. the relation between the energy, ϵ , and the wavevector k (for example $\epsilon = \hbar ck$ for photons and $\epsilon = \hbar^2 k^2 / 2m$ for electrons).

However, since Boltzmann factors in statistical mechanics depend on energy rather than wavevector we need to convert Eq. (1) to give the density of states as a function of *energy* rather than k , i.e. we need the number of states per unit interval of energy, $\rho(\epsilon)$. This *does* require a knowledge of the dispersion relation. We now consider several cases.

1. Photons

Consider first electromagnetic radiation in a cavity (black body radiation) for which the quanta are called photons. Here, the dispersion relation is linear:

$$\epsilon = \hbar\omega = \hbar ck, \quad (2)$$

where c is the speed of light. Changing variables in Eq. (1) from k to ϵ gives the number of k -values whose energy is between ϵ and $\epsilon + d\epsilon$ to be

$$\frac{V}{(2\pi)^3} \frac{4\pi}{(\hbar c)^3} \epsilon^2 d\epsilon. \quad (3)$$

To get the density of states, we need to multiply Eq. (3) by 2 since there are two (transverse) polarization states of the photon, and write it as $\rho(\epsilon) d\epsilon$, so we see that the density of states, $\rho(\epsilon)$, is given by

$$\rho(\epsilon) = \frac{V}{\pi^2} \frac{1}{(\hbar c)^3} \epsilon^2. \quad (4)$$

Note that the density of states is proportional to ϵ^2 .

2. Lattice vibrations (“phonons”)

Sound wave propagate in a crystal lattice. Just as light waves are quantized into photons, sound waves are also quantized and the name given to a single quantum is the “phonon”. The dispersion relation at long wavelengths is

$$\epsilon = \hbar\omega = \hbar vk, \quad (5)$$

where v is the speed of sound. Unlike light, sound can be longitudinally polarized as well as transversely polarized, so there are three different polarizations (unlike 2 for light), 2

transverse and one longitudinal. Another difference between photons and phonons is that the speed of light is a constant, but the speed of sound depends on direction (and polarization). We will ignore this complication here, with the realization that in the final result, v will have to be replaced by an appropriate average over the direction of \vec{k} (and polarization). The density of states is therefore given by Eq. (4) multiplied by 3/2 and with c replaced v , i.e.

$$\rho(\epsilon) = \frac{3V}{2\pi^2} \frac{1}{(\hbar v)^3} \epsilon^2. \quad (6)$$

Whereas Eq. (4) is valid for all ϵ , Eq. (6) is only valid for small ϵ . The reason is that the dispersion relation is no longer linear once k becomes comparable to the inverse of the lattice spacing of the crystal. In addition, the total number of degrees of freedom is $3N$, where N is the number of atoms in the crystal, since each atom can vibrate in three possible directions. Hence we must have

$$\int_0^\infty \rho(\epsilon) d\epsilon = 3N. \quad (7)$$

A common approximation for the actual (quite complicated) density of phonon states in a crystal was first proposed by Debye. In it, one assumes that Eq. (6) is true up to an energy called the Debye energy $\epsilon_D \equiv \hbar\omega_D$, and zero for $\epsilon > \epsilon_D$. The Debye energy ϵ_D is chosen so that Eq. (7) is satisfied, i.e.

$$3N = \frac{3V}{2\pi^2} \frac{1}{(\hbar v)^3} \int_0^{\epsilon_D} \epsilon^2 d\epsilon,$$

which gives

$$\epsilon_D \equiv \hbar\omega_D \equiv k_B\theta_D = (6\pi^2 n)^{1/3} \hbar v, \quad (8)$$

where θ_D is called the Debye temperature and $n = N/V$ is the particle density. It is common to use Eq. (8) to rewrite Eq. (6) in terms of ϵ_D rather than v , so the Debye approximation to the density of states is:

$$\rho_D(\epsilon) = \begin{cases} 9N \frac{\epsilon^2}{\epsilon_D^3}, & (0 < \epsilon < \epsilon_D) \\ 0 & \text{otherwise.} \end{cases} \quad (9)$$

We see that in the Debye approximation, the density of states is characterized by a single material-dependent parameter $\epsilon_D \equiv k_B\theta_D$. Some examples of θ_D are

material	$\theta_D(K)$
Fe	470
Si	645
Pb	105
C	2230

Physically, $k_B\theta_D$ is the energy of a typical phonon in the crystal (and from quantum mechanics this is \hbar times the frequency of a typical lattice vibration). Note that θ_D is high for

carbon (diamond), which is a very hard material (i.e. has strong forces between atoms) and has light atoms, and so has high phonon frequencies. By contrast, θ_D is low for lead, which is soft (i.e. weak forces between atoms) and has heavy atoms. (Recall that for a classical simple harmonic oscillator, the frequency is given by $\omega = \sqrt{K/m}$, where K is the spring constant and m is the mass.)

3. Atoms or electrons

The energy is given by

$$\epsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

where $p = \hbar k$ is the momentum and m is the mass. The difference from the cases of photons or phonons is that the dispersion is quadratic (i.e. $\epsilon \propto k^2$) rather than linear ($\epsilon \propto k$).

In Eq. (1) we write $k^2 = 2m\epsilon/\hbar^2$ and $dk = md\epsilon/(\hbar^2 k) = \sqrt{m/(2\hbar^2\epsilon)} d\epsilon$. We also need to multiply by the multiplicity coming from the particle's spin s , which is $2s + 1$. Equation (1) therefore becomes

$$(2s + 1) \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} d\epsilon. \quad (10)$$

Writing this as $\rho(\epsilon) d\epsilon$ gives

$$\rho(\epsilon) = (2s + 1) \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2}. \quad (11)$$

For the very important case of spin-1/2 particles, such as electrons, we have $2s + 1 = 2$.

We see that the density of states is proportional to $\epsilon^{1/2}$. This differs from the ϵ^2 behavior found for photons and phonons because the dispersion relation is different ($\epsilon \propto k^2$ rather than k).

One last comment. We have worked out the density of states in three dimensions. The power of ϵ in Eqs. (4) and (11) depends on dimension, and in the homework you are asked to do an equivalent calculation for the case of two dimensions.