Physics 112
Single Particle Density of States

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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 $k$ whose magnitude lie between $k$ and $k + dk$ is

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

This result is general, and does not depend on the dispersion relation, i.e. the relation between the energy, $\epsilon$, and the wavevector $k$ (for example $\epsilon = \hbar c k$ 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 (blackbody radiation) for which the quanta are called photons. Here, the dispersion relation is linear:

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

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

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

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

Note that the density of states is proportional to $\epsilon^2$.

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

$$\epsilon = \hbar \omega = \hbar vk,$$ (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.

\[
\rho(\epsilon) = \frac{3V}{2\pi^2} \frac{1}{(\hbar v)^3} \epsilon^2.
\]

(6)

Whereas Eq. (4) is valid for all \( \epsilon \), Eq. (6) is only valid for small \( \epsilon \). 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

\[
\int_0^\infty \rho(\epsilon) \, d\epsilon = 3N.
\]

(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 \( \epsilon_D \) 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

\[
\epsilon_D = \hbar \omega_D = k_B \theta_D = (6\pi^2 n)^{1/3} \hbar v,
\]

(8)

where \( \theta_D \) 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 \( \epsilon_D \) rather than \( v \), so the Debye approximation to the density of states is:

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

(9)

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

<table>
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<tr>
<th>material</th>
<th>( \theta_D(K) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>470</td>
</tr>
<tr>
<td>Si</td>
<td>645</td>
</tr>
<tr>
<td>Pb</td>
<td>105</td>
</tr>
<tr>
<td>C</td>
<td>2230</td>
</tr>
</tbody>
</table>

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 \( \theta_D \) 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, $\theta_D$ 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 $dk = mde/(\hbar^2 k) = \sqrt{m/(2\hbar^2 \epsilon)} \, d\epsilon$. We also need to
multiply by the multiplicity coming from the particle’s spin $s$, which is $2s + 1$. Equation (1)
therefore becomes

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

(10)

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

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

(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 $\epsilon^2$ 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 $\epsilon$ 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.