The Density of States (DoS): Mode Counting vs. Phase Space

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In its practical usage, the density of states replaces the degeneracy (in the continuum limit) in the appropriate partition function.

The (usual definition of the) density of states (DoS) is the number of states in the range E to $E + dE$. Alternate definitions

may use, for example, ω to $\omega + d\omega$, where frequency is a more prudent parameter to use.

Define N as the total number of states or modes, and also define:

$$G := \frac{number\ of\ states}{unit\ volume} = \frac{N}{V} \tag{1}$$

and let g denote the DoS, defined as:

$$g = \frac{dG}{dE} = number\ of\ states\ in\ E\ to\ E + dE \tag{2}$$

Note that per unit volume refers to the spacing between intervals or points, and thus may be a length or area in lower dimensions.

There are, in general, two equivalent ways to calculating the density of state.

Method one involves counting modes (i.e., the number

of states). After deducing G, one substitute the dispersion relation to obtain $G = G(E)$, then one takes the derivative

with respect to E to get g, the DoS. Note that in this version, one has to divide G by the number of quadrants, since

only the energy values in the first quadrant are of matter.

Method two involves calculating the momentum integral in phase space. n is the dimension number.

$$G = \frac{1}{h^n} \int d^n p, \tag{3}$$

whence after finding G, one subs in the dispersion relation, then differentiate with respect to E to obtain g.

Both methods are easy. Both utilize the definitions

of G (total number of states per unit volume) and g above (number of states ver unit volume in a thin shell of energy).

1 Non-relativistic particle in a box:

The non-relativistic particle in a box has the following dispersion relation:

$$E = \frac{\hbar^2 k^2}{2m}, \tag{4}$$

where $p = \hbar k$, and k is the wave number. Solving for k in terms of E, one gets:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow \frac{dk}{dE} = \sqrt{\frac{m}{2\hbar^2 E}} \tag{5}$$

A factor of $2S+1$ multiplies the density of state, where S is the spin of the particle.

Values of the DoS varies depending on dimension. The following examples should make things crystal clear:

1.1 1 Dimension

Box of Size L:

1.1.1 Mode Counting

$$N(k) = \frac{kL}{\pi} = \frac{\textit{length of line in k space}}{\textit{length of interval between points}} \tag{6}$$

$$G = \frac{N}{L} = \frac{k}{\pi} = \sqrt{\frac{2mE}{\hbar^2}}\frac{1}{\pi} \tag{7}$$

$$g = \frac{dG}{dE} = \frac{d}{dE}\left(\sqrt{\frac{2mE}{\hbar^2}}\frac{1}{\pi}\right) = \sqrt{\frac{m}{2\hbar^2 E}}\frac{1}{\pi} \tag{8}$$

1.1.2 Phase Space

$$G = \frac{1}{h}\int dp = 2\frac{1}{h}p = 2\frac{1}{h}\hbar k = \frac{1}{2\pi}\sqrt{\frac{2mE}{\hbar^2}} = \frac{1}{\pi}\sqrt{\frac{mE}{2\hbar^2}} \tag{9}$$

$$g = \frac{dG}{dE} = \frac{d}{dE}\left(\sqrt{\frac{2mE}{\hbar^2}}\frac{1}{\pi}\right) = \sqrt{\frac{m}{2\hbar^2 E}}\frac{1}{\pi} \tag{10}$$

1.1.3 General Comments

Note that in the above, the dispersion relation $k = \sqrt{\frac{2mE}{\hbar^2}}$ has been used in glorious abundance in order to

change from $G(k)$ to $G(E)$. Finally, note that both mode counting and phase space approaches yield the same value for both the number of states G

and the

density of state g. The phase space approach does not require worrying about multiplying a factor to reduce the calculation to that

of just one quadrant, while in the mode counting approach, one must be wary of this, lest one is off by a non-trivial factor.

1.2 2 Dimension

Box of Width L_x and Length L_y:

1.2.1 Mode Counting

$$N(k) = \frac{\pi k^2}{4}\frac{L_x L_y}{\pi^2} = \frac{\textit{area of quarter circle in k space}}{\textit{area per point}} \tag{11}$$

$$G = \frac{k^2}{4\pi} = \frac{1}{4\pi}\frac{2mE}{\hbar^2} \tag{12}$$

$$g = \frac{dG}{dE} = \frac{d}{dE}\left(\frac{1}{4\pi}\frac{2mE}{\hbar^2}\right) = \frac{1}{4\pi}\frac{2m}{\hbar^2} \tag{13}$$

1.2.2 Phase Space

$$G = \frac{1}{h^2}\int d^2p = \frac{1}{h^2}\int pdp\int_0^{2\pi} d\theta = \frac{1}{h^2}\pi p^2 = \frac{\pi\hbar^2}{h^2}k^2 = \frac{1}{4\pi}\frac{2mE}{\hbar^2} \tag{14}$$

$$g = \frac{dG}{dE} = \frac{d}{dE}\left(\frac{1}{4\pi}\frac{2mE}{\hbar^2}\right) = \frac{1}{4\pi}\frac{2m}{\hbar^2} \tag{15}$$

Indeed, both G and g are the same for both methods.[1] From now on, g will be calculated just once.

1.3 3 Dimension

1.3.1 Mode Counting

$$N(k) = \frac{1}{8}\frac{4\pi k^3}{3}\frac{L_x L_y L_z}{\pi^3} = \frac{\textit{volume of quadrant of sphere}}{\textit{volume per point}} \tag{16}$$

$$G = \frac{N}{L_x L_y L_z} = \frac{k^2}{6}\frac{1}{\pi^2} = \frac{1}{6}\left(\frac{2mE}{\hbar^2}\right)^{3/2}\frac{1}{\pi^2} \tag{17}$$

[1] Rather obvious, if you realize that the only difference between G and g is the derivative with respect to E.

1.3.2 Phase Space

$$G = \frac{1}{h^3}\int d^3p = \frac{4\pi}{h^3}\int p^2 dp = \frac{4\pi}{h^3}\int (\hbar k)^2 \hbar dk = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int E^{1/2} dE \tag{18}$$

$$g = \frac{dG}{dE} = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \tag{19}$$

1.4 n Dimension

1.4.1 Mode Counting

1.4.2 Phase Space

2 Relativistic particle in a box:

The dispersion relation for the relativistic particle is elegant:

$$E = pc = \hbar k c, \tag{20}$$

where $p = \hbar k$, as usual.

2.1 1 Dimension

$$G(k) = \frac{1}{h}\int dp = 2\frac{p}{h} = \frac{E}{\pi h c} \tag{21}$$

$$g = \frac{dG}{dE} = \frac{1}{\pi \hbar c} \tag{22}$$

2.2 2 Dimension

$$G(k) = \frac{1}{h^2}\int d^2p = \frac{1}{h^2}\int p dp d\theta = \frac{\pi p^2}{h^2} = \left(\frac{E}{2\hbar c\pi}\right)^2 \pi \tag{23}$$

$$g = \frac{dG}{dE} = \frac{E}{2\hbar^2 c^2 \pi} \tag{24}$$

2.3 3 Dimension

$$G(k) = \frac{1}{h^3}\int d^3p = \frac{4\pi}{h^3}\int p^2 dp = \frac{1}{6\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2} \tag{25}$$

$$g = \frac{dG}{dE} = \frac{1}{h^3}\int d^3p = \frac{4\pi}{h^3}\int p^2 dp = \frac{1}{2\pi^2}\frac{E^2}{(\hbar c)^3} \tag{26}$$