

Density of States

Franz Utermohlen

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1 Preface

In these notes, the expressions V_d denotes the volume of a d -dimensional sphere of radius R and Ω_{d-1} denotes the solid angle a d -dimensional sphere (or equivalently, the surface area of a d -dimensional sphere of unit radius).¹ These expressions are given by

$$V_d = \frac{\pi^{d/2}}{\Gamma(1 + \frac{d}{2})} R^d, \quad \Omega_{d-1} = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})}. \quad (1)$$

For example, for $d = 1, 2$, and 3 , these are

$$\begin{aligned} d = 1 : \quad V_1 &= 2R, & \Omega_0 &= 2, \\ d = 2 : \quad V_2 &= \pi R^2, & \Omega_1 &= 2\pi, \\ d = 3 : \quad V_3 &= \frac{4}{3}\pi R^3, & \Omega_2 &= 4\pi. \end{aligned}$$

¹The $d - 1$ subscript refers to the fact that the surface area of a d -dimensional sphere is $(d - 1)$ -dimensional. It's also useful to use $d - 1$ as the subscript, since the surface area of a d -dimensional sphere of radius R is given by $S_{d-1} = \Omega_{d-1} R^{d-1}$.

2 Summation definition

Intensive quantities A can generally be expressed in the form

$$A = \frac{1}{V_d} \sum_i a(\epsilon_i), \quad (2)$$

where V_d is the d -dimensional volume of the system, the sum is over all possible single-particle states i , and ϵ_i is the energy of the single-particle state i . In the continuum limit (thermodynamic limit), we can similarly define intensive quantities through

$$A = \int_{-\infty}^{\infty} a(\epsilon)g(\epsilon) d\epsilon, \quad (3)$$

where $g(\epsilon)$ is called the *density of states* (DOS). Setting Eqs. 2 and 3 equal to each other, we obtain

$$\frac{1}{V_d} \sum_i a(\epsilon_i) = \int_{-\infty}^{\infty} a(\epsilon)g(\epsilon) d\epsilon, \quad (4)$$

which implies that the DOS is given by

$$\boxed{g(\epsilon) = \frac{1}{V_d} \sum_i \delta(\epsilon - \epsilon_i)}, \quad (5)$$

as we can verify by inserting this into the right-hand side of Eq. 4:

$$\begin{aligned} \int_{-\infty}^{\infty} a(\epsilon)g(\epsilon) d\epsilon &= \int_{-\infty}^{\infty} a(\epsilon) \left[\frac{1}{V_d} \sum_i \delta(\epsilon - \epsilon_i) \right] d\epsilon \\ &= \frac{1}{V_d} \sum_i \int_{-\infty}^{\infty} a(\epsilon)\delta(\epsilon - \epsilon_i) d\epsilon \\ &= \frac{1}{V_d} \sum_i a(\epsilon_i). \quad \checkmark \end{aligned}$$

2.1 Examples of Eqs. 2 and 3 for a fermionic system

As concrete examples of Eqs. 2 and 3, let's consider a fermionic system, whose distribution is the Fermi–Dirac distribution

$$n_F(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1}. \quad (6)$$

We can describe the system's number density $n \equiv N/V_d$ and energy density $u \equiv U/V_d$ (where $U = E_{\text{tot}}$) as

$$n = \frac{1}{V_d} \sum_i n_F(\epsilon_i) = \int_{-\infty}^{\infty} n_F(\epsilon) g(\epsilon) d\epsilon, \quad (7)$$

$$u = \frac{1}{V_d} \sum_i \epsilon_i n_F(\epsilon_i) = \int_{-\infty}^{\infty} \epsilon n_F(\epsilon) g(\epsilon) d\epsilon. \quad (8)$$

2.2 Example: Ideal Fermi gas

Consider an ideal, nonrelativistic Fermi gas comprised of electrons of mass m with an energy–momentum relation

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m}. \quad (9)$$

The DOS is given by Eq. 5, which reads

$$g(\epsilon) = \frac{1}{V_d} \sum_i \delta(\epsilon - \epsilon_i). \quad (10)$$

We can rewrite the sum over single-particle states as a sum over single-particle momenta

$$\sum_i \rightarrow 2 \sum_{\mathbf{k}_i}, \quad (11)$$

where the factor of 2 is due to the fact that there are two different single-particle states corresponding to a given momentum \mathbf{k}_i (spin up and spin down). In the continuum limit, we use the prescription

$$\boxed{\sum_{\mathbf{k}_i} \rightarrow V_d \int \frac{d^d k_i}{(2\pi)^d}} \quad (12)$$

to rewrite Eq. 10 as

$$g(\epsilon) = 2 \int \delta(\epsilon - \epsilon_i) \frac{d^d k_i}{(2\pi)^d} = \frac{2}{(2\pi)^d} \int \delta(\epsilon - \epsilon') d^d k'. \quad (13)$$

We can use rotational invariance to rewrite the integration element as $d^d k' = \Omega_{d-1} k'^{d-1} dk'$, so we obtain

$$g(\epsilon) = \frac{2\Omega_{d-1}}{(2\pi)^d} \int_0^\infty \delta(\epsilon - \epsilon') k'^{d-1} dk' = \frac{2\Omega_{d-1}}{(2\pi)^d} \int_0^\infty \delta(\epsilon - \epsilon') k'^{d-1} dk'.$$

Changing the integral to an energy integral through

$$k' = \frac{\sqrt{2m\epsilon'}}{\hbar}, \quad dk' = \frac{1}{\hbar} \sqrt{\frac{m}{2\epsilon'}} d\epsilon', \quad (14)$$

we obtain

$$\begin{aligned}
g(\epsilon) &= \frac{2\Omega_{d-1}}{(2\pi)^d} \int_0^\infty \delta(\epsilon - \epsilon') \left(\frac{\sqrt{2m\epsilon'}}{\hbar} \right)^{d-1} \frac{1}{\hbar} \sqrt{\frac{m}{2\epsilon'}} d\epsilon' \\
&= \frac{m^{d/2} \Omega_{d-1}}{2^{d/2} \pi^d \hbar^d} \epsilon^{(d-2)/2} \theta(\epsilon) \\
&= \frac{m^{d/2}}{2^{d/2-1} \pi^{d/2} \hbar^d \Gamma(\frac{d}{2})} \epsilon^{(d-2)/2} \theta(\epsilon) \\
&= \frac{m^{d/2} d}{2^{d/2} \pi^{d/2} \hbar^d \Gamma(1 + \frac{d}{2})} \epsilon^{(d-2)/2} \theta(\epsilon).
\end{aligned}$$

We thus find that the DOS for an ideal d -dimensional Fermi gas is given by

$$g(\epsilon) = \frac{m^{d/2} d}{(2\pi)^{d/2} \hbar^d \Gamma(1 + \frac{d}{2})} \epsilon^{(d-2)/2} \theta(\epsilon). \quad (15)$$

3 Derivative definition

For a d -dimensional thermodynamic system of volume V_d , the DOS $g(\epsilon)$ is defined by

$$\boxed{g(\epsilon) \equiv \frac{dn}{d\epsilon}}. \quad (16)$$

Then, $g(\epsilon) d\epsilon$ is the number of states per unit volume in the energy interval $(\epsilon, \epsilon + d\epsilon)$.

3.1 Example: Ideal Fermi gas

Consider an ideal, nonrelativistic Fermi gas comprised of electrons of mass m with an energy–momentum relation

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m} \quad (17)$$

in a d -dimensional box of volume $V_d = L^d$. Since all of the energies are nonnegative, we will multiply $g(\epsilon)$ by the step function $\theta(\epsilon)$ to make sure that we only integrate from $\epsilon = 0$ to ∞ if we use the DOS inside an integral:

$$g(\epsilon) = \frac{dn}{d\epsilon} \theta(\epsilon). \quad (18)$$

We can rewrite this using the chain rule as

$$g(\epsilon) = \frac{dn}{dk} \frac{dk}{d\epsilon} \theta(\epsilon). \quad (19)$$

The derivative on the right can simply be obtained from Eq. 17:

$$\frac{dk}{d\epsilon} = \frac{d}{d\epsilon} \frac{\sqrt{2m\epsilon}}{\hbar} = \frac{\sqrt{2m}}{2\hbar\sqrt{\epsilon}} = \frac{1}{\hbar} \sqrt{\frac{m}{2}} \epsilon^{-1/2}. \quad (20)$$

For the other derivative, we need to find an expression for n . In this d -dimensional box of volume L^d , n is given by

$$n = \frac{N}{L^d}. \quad (21)$$

We need to find N now, which we will find by looking at the problem in d -dimensional \mathbf{k} -space.

For a given value of \mathbf{k} , we can consider a corresponding sphere of radius $k \equiv |\mathbf{k}|$ in d -dimensional \mathbf{k} -space whose volume is

$$V_d(k) = \frac{\pi^{d/2}}{\Gamma(1 + \frac{d}{2})} k^d. \quad (22)$$

We now imagine dividing this sphere into cubic cells of length k_{cell} and volume k_{cell}^d . In the large k limit ($k \gg k_{\text{cell}}$), the number of cells that fit inside the sphere is therefore

$$N_{\text{cells}} = \frac{V_d(k)}{k_{\text{cell}}^d}. \quad (23)$$

Now, we know that we can only have two particles (with opposite spins) of momentum \mathbf{k} per \mathbf{k} -space volume $(2\pi/L)^d$, which means that for this problem we can use

$$k_{\text{cell}} = \frac{2\pi}{L} \quad (24)$$

to find the number of particles that fit in a d -dimensional \mathbf{k} -space sphere of radius k :

$$N = 2N_{\text{cells}} = \frac{2V_d(k)}{k_{\text{cell}}^d} = \frac{2\pi^{d/2}k^d}{\Gamma(1 + \frac{d}{2})} \left(\frac{L}{2\pi}\right)^d = \frac{L^d k^d}{2^{d-1}\pi^{d/2}\Gamma(1 + \frac{d}{2})}. \quad (25)$$

Inserting this into Eq. 21, we find

$$n = \frac{k^d}{2^{d-1}\pi^{d/2}\Gamma(1 + \frac{d}{2})}. \quad (26)$$

We can now compute the k derivative of n :

$$\frac{dn}{dk} = \frac{k^{d-1}d}{2^{d-1}\pi^{d/2}\Gamma(1 + \frac{d}{2})}. \quad (27)$$

In terms of ϵ , this is

$$\frac{dn}{dk} = \frac{d}{2^{d-1}\pi^{d/2}\Gamma(1 + \frac{d}{2})} \left(\frac{2m\epsilon}{\hbar^2}\right)^{(d-1)/2} = \frac{m^{(d-1)/2}d}{2^{(d-1)/2}\pi^{d/2}\hbar^{d-1}\Gamma(1 + \frac{d}{2})} \epsilon^{(d-1)/2}. \quad (28)$$

Using this derivative and the one we computed in Eq. 20, we have

$$\begin{aligned} g(\epsilon) &= \frac{m^{(d-1)/2}d}{2^{(d-1)/2}\pi^{d/2}\hbar^{d-1}\Gamma(1+\frac{d}{2})}\epsilon^{(d-1)/2}\frac{1}{\hbar}\sqrt{\frac{m}{2}}\epsilon^{-1/2}\theta(\epsilon) \\ &= \frac{m^{d/2}d}{2^{d/2}\pi^{d/2}\hbar^d\Gamma(1+\frac{d}{2})}\epsilon^{(d-2)/2}\theta(\epsilon). \end{aligned}$$

We thus find that the DOS for an ideal d -dimensional Fermi gas is given by

$$\boxed{g(\epsilon) = \frac{m^{d/2}d}{2^{d/2}\pi^{d/2}\hbar^d\Gamma(1+\frac{d}{2})}\epsilon^{(d-2)/2}\theta(\epsilon)}, \quad (29)$$

which agrees with Eq. 15.

4 Useful expressions

The DOS is useful for computing thermodynamic quantities, such as the following:

$$n \equiv \frac{N}{V_d} = \frac{1}{V_d} \sum_i n_{F/B}(\epsilon_i) = \int_{-\infty}^{\infty} n_{F/B}(\epsilon)g(\epsilon) d\epsilon, \quad (30)$$

$$u \equiv \frac{U}{V_d} = \frac{1}{V_d} \sum_i \epsilon_i n_{F/B}(\epsilon_i) = \int_{-\infty}^{\infty} \epsilon n_{F/B}(\epsilon)g(\epsilon) d\epsilon, \quad (31)$$

where $U = E_{\text{tot}}$ is the system's total energy and $n_{F/B}(\epsilon)$ denotes the system's distribution, i.e. the Fermi–Dirac distribution $n_F(\epsilon)$ or the Bose–Einstein distribution $n_B(\epsilon)$.

For a fermionic system at $T = 0$, the Fermi–Dirac distribution is just $n_F(\epsilon) = \theta(-\epsilon)\theta(\epsilon - \mu)$. The chemical potential at $T = 0$ is called the Fermi energy:

$$E_F \equiv \mu(T = 0) = \frac{\hbar^2 k_F^2}{2m}, \quad (32)$$

so the integral expressions for n and u become

$$n = \int_0^{E_F} g(\epsilon) d\epsilon, \quad (33)$$

$$u = \int_0^{E_F} \epsilon g(\epsilon) d\epsilon. \quad (34)$$