Density of states for one-particle system

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1. Energy level in 3D system

We consider the Schrödinger equation of a spin-less particle, which is confined to a cube of edge L.

$$H\psi_{\boldsymbol{k}} = \frac{\boldsymbol{p}^2}{2m}\psi_{\boldsymbol{k}} = -\frac{\hbar^2}{2m}\nabla^2\psi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}}\psi_{\boldsymbol{k}}. \tag{1}$$

It is convenient to introduce wavefunctions that satisfy periodic boundary conditions.

Boundary condition (Born-von Karman boundary conditions).

$$\psi_{\mathbf{k}}(x+L, y, z) = \psi_{\mathbf{k}}(x, y, z),$$

$$\psi_{\mathbf{k}}(x, y+L, z) = \psi_{\mathbf{k}}(x, y, z),$$

$$\psi_{\mathbf{k}}(x, y, z+L) = \psi_{\mathbf{k}}(x, y, z).$$

The wavefunctions are of the form of a traveling plane wave.

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{2}$$

with

$k_x = (2\pi/L)\, n_x$, ($n_x = 0, \pm 1, \pm 2, \pm 3, \ldots$),

$k_y = (2\pi/L)\, n_y$, ($n_y = 0, \pm 1, \pm 2, \pm 3, \ldots$),

$k_z = (2\pi/L)\, n_z$, ($n_z = 0, \pm 1, \pm 2, \pm 3, \ldots$).

The components of the wavevector $\boldsymbol{k}$ are the quantum numbers. The energy eigenvalue is given by

$$\varepsilon(\boldsymbol{k}) = \frac{\hbar^2}{2m}({k_x}^2 + {k_y}^2 + {k_z}^2) = \frac{\hbar^2}{2m}\boldsymbol{k}^2. \tag{3}$$

Here

$$\boldsymbol{p}\psi_k(\boldsymbol{r}) = \frac{\hbar}{i}\nabla_k\psi_k(\boldsymbol{r}) = \hbar\boldsymbol{k}\psi_k(\boldsymbol{r}). \tag{4}$$

So that the plane wave function $\psi_k(\boldsymbol{r})$ is an eigenfunction of $\boldsymbol{p}$ with the eigenvalue $\hbar\mathbf{k}$. The ground state of a system of N electrons, the occupied orbitals are represented as a point inside a sphere in $\boldsymbol{k}$-space.

2. Density of states

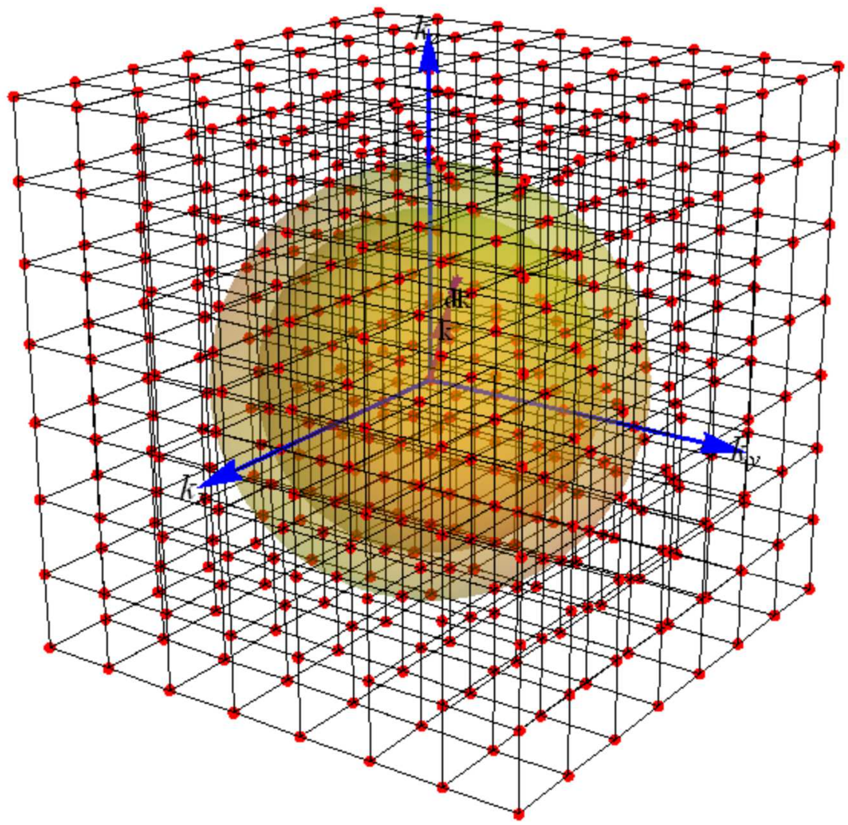

Fig. Density of states in the 3D $\boldsymbol{k}$-space. There is one state per $(2\pi/L)^3$. Each state is denoted by red points.

There is one state per volume of $\boldsymbol{k}$-space $(2\pi/L)^3$. We consider the number of one-particle levels in the energy range from ε to ε+dε; $D(\varepsilon)$dε

$$D(\varepsilon)d\varepsilon = \frac{L^3}{(2\pi)^3}4\pi k^2 dk = \frac{V}{(2\pi)^3}4\pi k^2 dk\,, \tag{5}$$

where $V = L^3$, and $D(\varepsilon)$ is called a density of states. Since $k = (2m/\hbar^2)^{1/2}\sqrt{\varepsilon}$, we have

$$dk = (2m/\hbar^2)^{1/2} d\varepsilon/(2\sqrt{\varepsilon})\,.$$

Then we get the density of states

$$D(\varepsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} = \frac{2\pi(2m)^{3/2}}{h^3}V\varepsilon^{1/2}. \tag{6}$$

The number of states for the energy (0 - ε)

$$N(\varepsilon) = \int_0^{\varepsilon} D(\varepsilon)d\varepsilon = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{\varepsilon_F}\sqrt{\varepsilon}d\varepsilon = \frac{V}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon^{3/2}. \tag{7}$$