Fourier space for a system in a periodic box

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There are many situations where we will want to consider a system (say, a crystal) with finite volume V. Real systems have surfaces and edges, and including these in calculations is usually unpleasant. Fortunately it is also often unnecessary. If the volume V is large (and it usually is in condensed matter physics), and we are interested in "bulk" properties to which *all* the atoms contribute, then the contribution of atoms near surfaces is negligible. This is true simply because the surface-to-volume ratio goes to zero when V gets large – there are comparatively very few atoms near the surface.

Given this discussions, we often take advantage of a mathematical trick that gets rid of surfaces entirely: we imagine our system fills a box with periodic boundary conditions. For simplicity, in these notes we will assume this box is a cube with sides of length L ($V = L^3$); later on we will see that this works just about the same for more general periodic boxes. We will often need to work in Fourier space, so it is important to recall how to do that for a system with periodic boundary conditions.

Consider a function $f(\boldsymbol{r})$ defined in infinite, three-dimensional space. (It is not hard to generalize the discussion here to dimensions other than 3.) This function has a Fourier transform $\tilde{f}(\boldsymbol{k})$, defined by

$$f(\boldsymbol{r}) = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tilde{f}(\boldsymbol{k}) \tag{1}$$

$$\tilde{f}(\boldsymbol{k}) = \int d^3\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{r}), \tag{2}$$

where both the $\boldsymbol{r}$- and $\boldsymbol{k}$-integrals are taken over infinite three-dimensional space. The fact that these two equations are consistent with one another follows from the Dirac delta-function identity

$$(2\pi)^3 \delta(\boldsymbol{k} - \boldsymbol{k}') = \int d^3\boldsymbol{r}\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}. \tag{3}$$

Now instead suppose $f(\boldsymbol{r})$ is some physical property of our periodic system. This means that

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + L\boldsymbol{x}) = f(\boldsymbol{r} + L\boldsymbol{y}) = f(\boldsymbol{r} + L\boldsymbol{z}). \tag{4}$$

If we take a look back at Eq. (1), we see that, for the right-hand side to be consistent with periodicity [Eq. (4)], we need to have

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}+L\boldsymbol{x})} \implies e^{iLk_x} = 1, \tag{5}$$

and similarly for k_y and k_z. The most general $\boldsymbol{k}$ that satisfies this constraint is

$$\boldsymbol{k} = \frac{2\pi}{L}(n_x\boldsymbol{x} + n_y\boldsymbol{y} + n_z\boldsymbol{z}), \tag{6}$$

where n_x, n_y, n_z are integers. We see that periodicity in real space makes Fourier space discrete. Also, as V (and hence L) gets large, Fourier space gets more and more continuous, because the allowed values of $\boldsymbol{k}$ get closer together.

To deal with this discreteness, we can define the Fourier transform of our periodic function as follows:

$$f(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tilde{f}(\boldsymbol{k}) \tag{7}$$

where the sum is over all allowed $\boldsymbol{k}$-values. We can also invert this to find

$$\tilde{f}(\boldsymbol{k}) = \int_{\boldsymbol{r}\in\text{cube}} d^3\boldsymbol{r}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{r}), \tag{8}$$

where the integral is over a single cube, that is the region $0 \le r_x, r_y, r_z \le L$. This can be derived from Eq. (7) by using the identity

$$\frac{1}{V}\int_{\boldsymbol{r}\in\text{cube}} d^3\boldsymbol{r}\, e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k},\boldsymbol{k}'}, \tag{9}$$

where $\delta_{\boldsymbol{k},\boldsymbol{k}'}$ is the Kronecker delta defined by

$$\delta_{\boldsymbol{k},\boldsymbol{k}'} = \begin{cases} 1, & \boldsymbol{k} = \boldsymbol{k}' \\ 0, & \boldsymbol{k} \neq \boldsymbol{k}' \end{cases} . \tag{10}$$

In the limit $V \to \infty$, the allowed points in $\boldsymbol{k}$-space get closer and closer together, and we can approximate this by allowing $\boldsymbol{k}$ to be continuous. In this limit, using the fact that the density of points in $\boldsymbol{k}$-space is $V/(2\pi)^3$, we have the very important identity

$$\sum_{\boldsymbol{k}} \to V \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}. \tag{11}$$

It is also useful to understand what happens to $\delta_{\boldsymbol{k},\boldsymbol{k}'}$ in this limit, because a Kronecker delta does not make much sense for a continuous variable. To do this, note that

$$\sum_{\boldsymbol{k}} \delta_{\boldsymbol{k},\boldsymbol{k}'} = 1. \tag{12}$$

Since the sum goes to an integral according to Eq. (11), we must have

$$\delta_{\boldsymbol{k},\boldsymbol{k}'} \to \frac{(2\pi)^3}{V} \delta(\boldsymbol{k} - \boldsymbol{k}'), \tag{13}$$

where the Kronecker delta has become a Dirac delta. This is the correct choice because it vanishes for $\boldsymbol{k} \neq \boldsymbol{k}'$, and because we have

$$1 = \sum_{\boldsymbol{k}} \delta_{\boldsymbol{k},\boldsymbol{k}'} \to V \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} \frac{(2\pi)^3}{V} \delta(\boldsymbol{k} - \boldsymbol{k}') = 1. \tag{14}$$