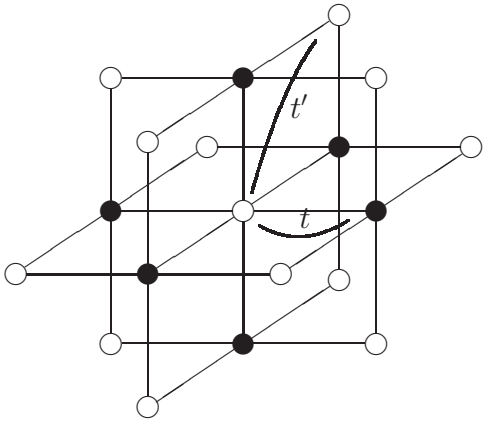

Figure 2.1: Cubic lattice with NN (t) and NNN hopping (t'); (from Schlipf (1998)).

where L is the number of lattice sites $\boldsymbol{R}_i$ and $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote NN pairs and NNN pairs, respectively. The variance of the resulting DOS can be easily computed for arbitrary dimension from the sum of squares of all hopping terms (cf. subsection 2.2.2):

$$\langle\epsilon^2\rangle_{\rho(\epsilon)} = \langle\epsilon_{\boldsymbol{k}}^2\rangle_{\boldsymbol{k}} = 2dt^2 + d(d-1)(t')^2. \tag{2.7}$$

Here, we have introduced the expectation values[7]

$$\langle f(\epsilon)\rangle_{\rho(\epsilon)} = \int_{-\infty}^{\infty} \mathrm{d}\epsilon f(\epsilon)\rho(\epsilon) \tag{2.8}$$

$$\langle f(\boldsymbol{k})\rangle_{\boldsymbol{k}} = \frac{1}{N}\sum_{\boldsymbol{k}} f(\boldsymbol{k})\,. \tag{2.9}$$

When t and t' are scaled with the inverse number of NN and NNN, respectively, and we introduce the ratio a^* of these scaled amplitudes,

$$t = \frac{t^*}{\sqrt{2d}}, \quad t' = \frac{t'^*}{\sqrt{d(d-1)}}, \quad a^* = \frac{t'^*}{t^*} \tag{2.10}$$

we obtain for the variance

$$\langle\epsilon_{\boldsymbol{k}}^2\rangle_{\boldsymbol{k}} = (t^*)^2 + (t'^*)^2 = t^{*2}\left(1 + a^{*2}\right)\,. \tag{2.11}$$

For given ratio $a^* < \infty$ the variance can thus be fixed to 1 by setting $t^* = 1/\sqrt{1+a^{*2}}$.

[7]Note that the definitions are obviously consistent, i.e., $\langle f(\epsilon_{\boldsymbol{k}})\rangle_{\boldsymbol{k}} = \langle f(\epsilon)\rangle_{\rho(\epsilon)}$ for constant functional dependence f; consequently, the appropriate definition of the average usually follows from the argument and may be omitted.