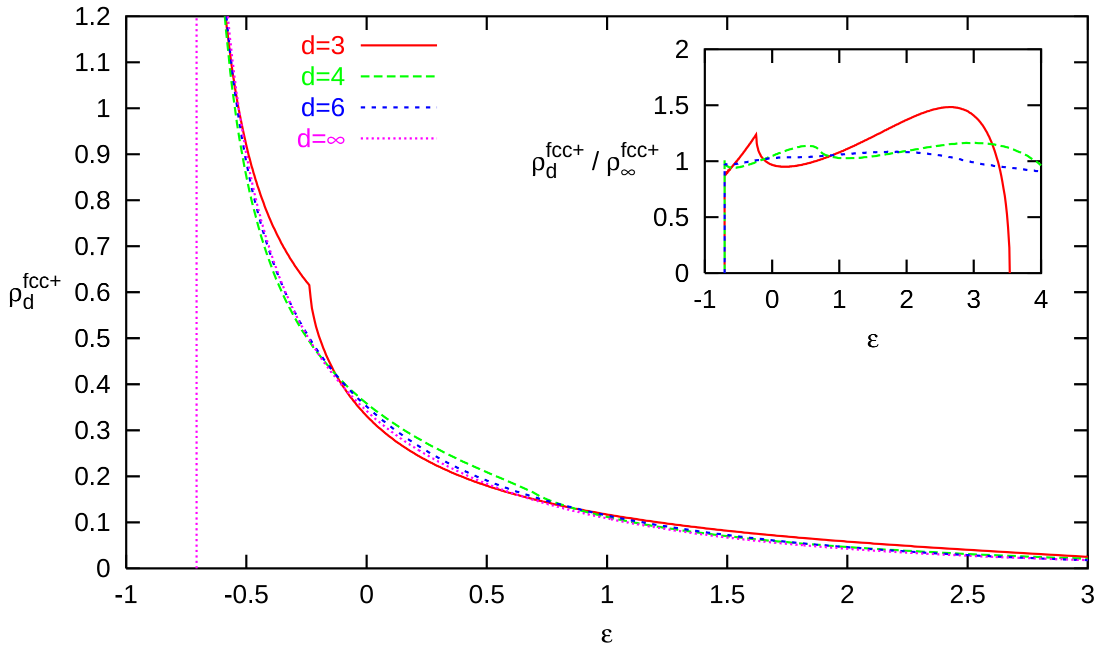

Figure 2.8: DOS of the fcc lattice with extended hopping along the axes.

Both the prefactor and the first two terms in the square bracket of (2.17) are $\mathcal{O}(1)$ while the third term is $\mathcal{O}(1/\sqrt{d})$ in high dimensions. Consequently, we can write

$$\epsilon_{\boldsymbol{k}}^{\text{fcc}} = \frac{(t')^*}{\sqrt{2}} \left[(\epsilon_{\boldsymbol{k}}^{\text{hc}}/t^*)^2 - 1 \right] + \mathcal{O}(1/\sqrt{d}) \tag{2.18}$$

which for $d \to \infty$ implies[9] a square-root singularity in the DOS broadened by a Gaussian of width $1/\sqrt{d}$. Strictly in $d = \infty$, the DOS of the fcc lattice is given by

$$\rho^{\text{fcc}} = 2 \frac{\mathrm{e}^{-(1+\sqrt{2}\epsilon)/2}}{\sqrt{1+\sqrt{2}\epsilon}\sqrt{2\pi}} \,. \tag{2.19}$$

Since the third term in (2.17) corresponds to extended hopping along the axes it can be cancelled by adding a corresponding term in the Hamiltonian in which case there is a square-root singularity in any dimension as shown in Fig. 2.8. Densities of states obtained via such a transformation $\epsilon_{\boldsymbol{k}} = f(\epsilon_{\boldsymbol{k}}^{\text{hc}})$ cannot show a stronger dimensional dependence than the hc DOS itself.[10] Indeed, the curves for $d > 3$ in Fig. 2.8 are hardly distinguishable. Even $d = 3$ only stands out only by the Van-Hove singularity at $\epsilon = -\sqrt{2}/6$, but has the same square-root singularity at the lower band edge.

While the dramatic changes of the DOS introduced by NNN hopping clearly show that extended hopping matrix elements are important we wish to point out that the

[9] As is apparent from (2.1), a DOS (which may be seen as probability distribution) transforms under change of variables like a delta-function, see (2.56).

[10] This fact will be utilized in Sec. 2.3.