inclusion of hopping elements t_{ij} with odd range $D = \|\boldsymbol{r}_i - \boldsymbol{r}_j\| \geq 3$ will reintroduce infinite-ranged low-energy tails and thus destroy the sharp band edge, one of the prominent features of t-t' DOS in $d = \infty$. This issue will be treated in a broader context in Sec. 2.3. For the DMFT computation of transport properties for the t-t' lattice, see subsection 4.5.3.

For a discussion of the hyperdiamond lattice, see App. B.

2.1.3 Magnetic Frustration and Asymmetry of the DOS

One important question in the context of the DMFT is whether magnetic frustration, in particular the suppression of antiferromagnetism, is closely related to other properties like the DOS and the optical conductivity or whether it can be regarded as being essentially independent, at least in high dimensions. While it is immediately clear that unfrustrated particle-hole symmetric systems have a symmetric DOS, the converse statement is not generally true for $Z = \infty$. In fact, when extended hopping only along the cartesic axes is introduced for the hypercubic lattice, the DOS remains Gaussian while for suitably chosen hopping matrix elements antiferromagnetic order is suppressed (Müller-Hartmann, 1989*a*). In the following, we will outline an argument why this behavior (and not only the model) should be regarded as pathological. First, we observe that for fixed hopping matrix elements t_D to D^{th}-nearest neighbors along the cartesic axes the DOS in d dimensions can be obtained from folding the one-dimensional DOS $d-1$ times with itself. Since the DOS is symmetric in $d = 1$ if and only if the system is unfrustrated (i.e., $t_{2n} = 0$ for integer n) the same applies for all finite dimensions d. In Sec. 1.2 we have seen that perfect anticorrelation in the two-particle density of states $D_{\boldsymbol{q}}(\epsilon_1, \epsilon_2)$ at the antiferromagnet wave vector $\boldsymbol{Q}$, i.e., $\eta(\boldsymbol{Q}) = -1$ is associated with a strong antiferromagnetic instability due to particle-hole symmetry. More generally, an instability at vector $\boldsymbol{q}$ occurs for $\eta_{\boldsymbol{q}} \equiv \eta(\boldsymbol{q}) \approx -1$. It seems thus reasonable to associate magnetic frustration with the deviation of the minimum of η from -1. For the lattice under consideration it is clear that all extrema are on the diagonal $\{\boldsymbol{q}; \boldsymbol{q} = \lambda\boldsymbol{Q}; 0 \leq \lambda \leq 1\}$. For this line, we have[11] (Müller-Hartmann, 1989*a*)

$$\eta(\lambda\boldsymbol{Q}) = \frac{1}{t^2}\sum_{D=1}^{\infty} t_D^2 \cos(D\lambda\pi)\,, \tag{2.20}$$

where $t^2 = \sum_{D=1}^{\infty} t_D^2$. First, we note that $\eta(\lambda\boldsymbol{Q}) \geq -1$ and that $\eta(\boldsymbol{Q}) = -1$ only in the unfrustrated case where $t_{2n} = 0$ for all n. For a fully quantitative analysis, we restrict hopping to NN and to NNN (along the cartesic axes). Then, the minimum of $\eta(\lambda\boldsymbol{Q})$ is for unit variance (${t_1^*}^2 + {t_2^*}^2 = 1$)

$$\eta_{\min} = \begin{cases} -1 + 2{t_2^*}^2 & \text{for } {t_2^*}^2 \leq 0.2 \\ -\frac{9{t_2^*}^4 - 2{t_2^*}^2 + 1}{8{t_2^*}^2} & \text{for } 0.2 < {t_2^*}^2 \leq 1 \end{cases}\,. \tag{2.21}$$

[11] Note that (in this special case) we can use either scaled or unscaled hopping matrix elements since the scaling factor is independent of the hopping range.