Bipartite Lattices and Perfect Nesting

Independent of hopping range and dimension, a hc lattice may be split into two sublattices A and B,

$$A = \{\boldsymbol{r}; (-1)^{\|\boldsymbol{r}\|} = 1\}, \quad B = \{\boldsymbol{r}; (-1)^{\|\boldsymbol{r}\|} = -1\}, \tag{2.12}$$

which is visualized in Fig. 2.1 by using empty circles for A sites and filled circles for B sites, respectively. Since the origin has no special meaning, both sublattices A and B are equivalent. Note that each sublattice constitutes a face centered cubic lattice in 3 dimensions so that we can use either of the two sets in (2.12) in order to define a generalized face centered cubic (fcc) lattice in arbitrary dimensions $d > 2$. The tendency towards breaking this $A - B$ symmetry by staggered charge or spin order is largest when hopping matrix elements are nonvanishing only between (as opposed to within) the sublattices. The simplest example for such a *bipartite lattice* is the hc with NN hopping only; the most general case (on a full hypercubic host lattice) can be expressed by the requirement $t_{ij} = 0$ for $(-1)^{\|\boldsymbol{r}_i - \boldsymbol{r}_j\|} = 1$. It is easily seen that (for real t_{ij}) all such bipartite Bravais lattices have symmetric DOSs by performing the particle-hole transformation $\hat{c}_{i\sigma} \to \hat{c}^{\dagger}_{i\sigma}$ for $\boldsymbol{r}_i \in A$ and $\hat{c}_{j\sigma} \to -\hat{c}^{\dagger}_{j\sigma}$ for $\boldsymbol{r}_j \in B$. A prominent example for a non-bipartite lattice is the generalized fcc lattice mentioned above which corresponds to the limit $t \to 0$ (while $t' \neq 0$) of (2.5).

For the hypercubic lattice the particle hole symmetry can be expressed in $\boldsymbol{k}$-space ($\boldsymbol{Q} = (\pi, \pi, \dots)$)

$$\epsilon_{\boldsymbol{k}+\boldsymbol{Q}} = -\epsilon_{\boldsymbol{k}}\,, \tag{2.13}$$

which implies *perfect nesting* at half filling ($n = 1$): the Fermi surface (all $\boldsymbol{k}$ points with $\epsilon_{\boldsymbol{k}} = 0$) is mapped on itself for $\boldsymbol{k} \to \boldsymbol{k} + \boldsymbol{Q}$ which amounts to an effective doubling of the unit cell (or halving of the Brillouin zone) and again implies a potential instability against $A - B$ symmetry breaking. A trivial consequence of (2.13) is a symmetric DOS, i.e., $\rho(-\epsilon) = \rho(\epsilon)$.

2.1.2 Numerical Results

The DOS of the hc lattice with NN hopping is shown in Fig. 2.2. For $d \geq 3$, $\rho^{\text{hc}}(\epsilon) < \infty$ at all energies. Apart from Van-Hove singularities with infinite slope for $d = 3$ and a jump in the slope for $d = 4$ the overall shape is quite regular with no visible qualitative changes for $d > 6$. For $d \to \infty$, more spectral weight is transferred from $|\epsilon| \approx 3/2$ to $\epsilon \approx 0$ while the exponentially small tails extend to $\pm\infty$. An application of $d = \infty$ results to $d = 3$ apparently misses the Van-Hove singularities (as it must for any lattice type) and (for $n = 1$) slightly overestimates the DOS at the Fermi level but does not introduce artificial features – except for the infinite energy tails.

Switching on additional NNN hopping destroys the symmetry of the DOS as illustrated in Fig. 2.3 for $a^* = (t')^*/t^* = -0.25$ which introduces an important aspect of realistic tight-binding calculations. Except for $d = 2$ and the Van-Hove singularities visible for $d = 3$ (at $\epsilon = \pm\sqrt{2/3}$) and $d = 4$ (at $\epsilon = 0$), Fig. 2.3 implies a rapid qualitative convergence with few differences between $d = 4$ and $d = 5$. This