Structures on lattices: Some useful relations

Yu.I. Dublenych

Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Street, 79011 Lviv, Ukraine
E–mail: dubl@icmp.lviv.ua

In many methods for the determination of the ground states of lattice-gas models (or equivalent spin models) the global ground-state structures are constructed with local configurations of some subset of the lattice (cluster). We show that there exist some linear relations between fractional contents of these configurations in any structure that they generate.

Consider cluster $\boldsymbol{K}$, which covers the lattice with overlaps and a set of its configurations $\{\boldsymbol{K}_l\}$ $(l = 1, 2, ..., L)$. Consider subcluster $\boldsymbol{Q}$ of this cluster. Let the subcluster occupy M *nonequivalent* positions in the cluster $(m = 1, 2, ..., M)$. Let each cluster $\boldsymbol{Q}$ on the lattice be contained in c_m clusters $\boldsymbol{K}$ as subcluster $\boldsymbol{Q}$ in position number m. Consider a structure $\boldsymbol{S}$ on the lattice generated by the set of cluster configurations $\{\boldsymbol{K}_l\}$. This means that each cluster $\boldsymbol{K}$ on the lattice has one of the configurations of the set. We denote the fractional content of configuration $\boldsymbol{K}_l$ in structure $\boldsymbol{S}$ by k_l $(\sum_l k_l = 1)$.

Consider a subcluster configuration $\boldsymbol{Q}_t$ from the set of all possible subcluster configurations $\{\boldsymbol{Q}_t\}$ and calculate its content in structure $\boldsymbol{S}$. This can be done in different ways, depending on the position of the subcluster in the cluster. Let it be position m. Then the number of configurations $\boldsymbol{Q}_t$ per one cluster $\boldsymbol{K}$ is equal to $\sum_l \frac{k_l n_{ml}}{c_m}$, where n_{ml} is the number of configurations $\boldsymbol{Q}_t$ occupying position m in configuration $\boldsymbol{K}_l$ of the cluster. The number of configurations $\boldsymbol{Q}_t$ should not depend on m. Therefore the following relation holds: $\sum_l \frac{k_l n_{m_1 l}}{c_{m_1}} = \sum_l \frac{k_l n_{m_2 l}}{c_{m_2}}$, where m_1 and m_2 are arbitrary *nonequivalent* positions of subcluster $\boldsymbol{Q}$ in cluster $\boldsymbol{K}$. This equality gives a relation between fractional contents k_l. Considering different pairs of positions of the subcluster in the cluster or another subclusters, we obtain other relations. Such relations can be useful for the determination of the ground states of lattice-gas models.

[1] Yu.I. Dublenych, Phys. Rev. E, 2011, **83**, 022101.