

M05T.2 - Defects in a Cubic Crystal

Problem

A cubic crystal contains N atoms. The atoms can exist at lattice sites or an atom may find itself displaced from its normal site into the center of one of the 8 adjacent unit cells as suggested by the figure. (Note that the figure shows only a small part of the crystal, N is very large.) When an atom is displaced, its energy is increased by $\epsilon > 0$ over its energy at the normal lattice site. Suppose the crystal is in equilibrium at temperature T . assume $k_B T \ll \epsilon$ so the chance that two displaced atoms try to occupy the same cell is negligible. Calculate the partition function, the entropy, the energy (relative to the energy the crystal would have if all atoms were at their normal sites), and the number of atoms in displaced sites.

