8.2: Self-Avoiding Walks

To account for excluded volumes, one can enumerate polymer configurations in which no two beads occupy the same site. Such configurations are called **self-avoiding walks** (SAWs). Theoretically it is predicted that the number of configurations for a random walk on a cubic lattice should scale with the number of beads as $\Omega_p(n) \propto z^n n^{\gamma-1}$, where γ is a constant which is equal to 1 for a random walk. By explicitly evaluating self-avoiding walks (SAWs) on a cubic lattice it can be shown that

$$\Omega_p(n) = 0.2\alpha^n n^{\gamma-1}$$

where $\alpha = 4.68$ and $\gamma = 1.16$, and the chain entropy is

$$S_p(n) = k_B[n \ln \alpha + (\gamma - 1)\ln n - 1.6].$$

Comparing this expression with our first result $\Omega_P = Mz(z-1)^{n-2}$ we note that in the limit of a random walk on a cubic lattice, α=z=6, when we exclude only the back step for placing the next bead atop the preceeding one $\alpha = (z-1) = 5$, and the numerically determined value is $\alpha = 4.68$.

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2. C. Vanderzande, Lattice Models of Polymers (Cambridge University Press, Cambridge, UK, 1998).