Study of the behavior of the persistence length in self-avoiding random walks using the pivot algorithm

C.R.F. Granzotti[1], A.S. Martinez[1], M.A.A. da Silva[2]

[1]Departamento de Física , Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto, Universidade de São Paulo, Brazil

[2]Departamento de Física e Química, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Brazil

The self-avoiding random walk (SAW) can be seen as a path on a lattice that visits a site just once [1]. The characterization of the set of trajectories with N steps is based on the scaling behavior of conformational quantities. In our study, the quantities of interest include the mean square end-to-end distance, $\langle \vec{R}_N^2 \rangle_N = AN^{2\nu_0}(1 + a^{(0)}N^{-1} + b^{(0)}N^{-\Delta_1} + \cdots)$, and the persistence length $\lambda_N = \langle \vec{R}_N \cdot \vec{u}_1 \rangle_N$, defined as the projection of the end-to-end vector along the first step. The N^{-i} and $N^{-\Delta_i}$ terms are the analytical and non-analytical corrections (i being integer and $\Delta_i > 0$). There exist controversial estimates of λ_N for the square lattice, such as $\ln(N)$ and N^{δ} or even $\lambda = cte$ [2], on which we shed some light after establishing the Inner Persistence Length: $\mathcal{I}_j = \langle \vec{R}_j \cdot \vec{u}_j \rangle_N$ [3]. Starting from $\mathcal{I}_j$, the relation $\langle \vec{R}_N^2 \rangle_N = \langle \vec{R}_{N-1}^2 \rangle_N + 2\lambda_N - 1$ could be written. Observing that λ_N is not the discrete derivative of $\langle \vec{R}_N^2 \rangle_N$, one formulates the scaling ansatz: $\lambda_N = \lambda_\infty + \alpha_1 N^{\varpi_1} + \alpha_2 N^{\varpi_2} + \cdots$, where the values $\varpi_1 = 2\nu_0 - 2$ and $\varpi_2 = 2\nu_0 - \Delta_1 - 1$ provided a good fitting of λ_N. By using walks with $N < 100$ steps one finds the asymptotic value $\lambda_\infty = 2.52$, and $\lambda_\infty = 1.42$, for square and cubic lattice respectively [3]. Here, we investigate the convergence of λ_N with accurate data obtained with the pivot algorithm [4]. We performed the simulations for SAWs up to $N = 1000$ and $N = 800$ steps in the square and cubic lattice, respectively. Preliminary results confirm the $\lambda_\infty \approx 1.42$ value for the cubic lattice. However, the estimates for the square lattice, using the fitting or extrapolation graphs, provide λ_∞ from ≈ 2.60 to ≈ 2.78. We expect more accurate estimate of λ_∞ with the data obtained with up to $N = 8000$ steps, currently being generated. Simulations are being carried out with hexagonal and diamond lattices in order to check the universal behavior of λ_N. Also, we generalize the scaling approach to obtain λ_N using only one N-step ensemble.

[l] E.J. Janse van Rensburg, J. Phys. A-math. Gen **42**, 323001 (2009).

[2] E. Eisenberg and A. Baram, J. Phys. A-math. Gen **36(8)**, L121 (2003).

[3] C.R.F. Granzotti, et. al., Phys. Rev. E **93**, 052116 (2016).

[4] N. Madras and A. Sokal, J. Stat. Phys. **50(1-2)**, 109 (1988).