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

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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, $\langle \vec{R}^2_N \rangle = A_N^{2\nu_0}(1 + a(0)N^{-1} + b(0)N^{-\Delta_1} + \cdots)$, and the persistence length $\lambda_N = \langle \vec{R}_N \cdot \vec{u}_1 \rangle$, 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 $\lambda_N$ for the square lattice, such as $\ln(N)$ and $N^\delta$ or even $\lambda = cte$ [2], on which we shed some light after establishing the Inner Persistence Length: $I_j = \langle \vec{R}_j \cdot \vec{u}_j \rangle [3]$. Starting from $I_j$, the relation $\langle \vec{R}_N^2 \rangle = \langle \vec{R}_{N-1}^2 \rangle + 2\lambda_N - 1$ could be written. Observing that $\lambda_N$ is not the discrete derivative of $\langle \vec{R}_N^2 \rangle$, 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 $\lambda_N$. 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 $\lambda_N$ 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 $\lambda_\infty$ from $\approx 2.60$ to $\approx 2.78$. We expect more accurate estimate of $\lambda_\infty$ 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 $\lambda_N$. Also, we generalize the scaling approach to obtain $\lambda_N$ using only one $N$-step ensemble.