Diffusion on Self-Avoiding Walks with Bridges

In a recent Letter[1] Helman, Coniglio, and Tsallis investigated the phenomenon of a random walk (RW) on self-avoiding-walk (SAW) configurations and suggested that additional hoppings across the so-called "bridges" (bonds connecting the sites, visited by the SAW, which are not nearest neighbors along the SAW but which are nearest neighbors on the embedding lattice) could remove the inconsistencies between theoretical[1] and experimental[2] estimates of the fractal dimension d_w associated with a RW. Our Monte Carlo[3] (MC) as well as small-cell renormalization[4] results for the same problem indicated that the hoppings across the bridges do, indeed, have a nontrivial effect on the diffusion. But, contrary to Ref. 1, d_w increases rather than decreases to 2 because of these additional hoppings. In our earlier investigation,[3] the hopping probabilities along "streets" (nearest-neighbor bonds along the SAW) and bridges were assumed to be identical. However, in reality, these two hopping probabilities may be quite different[1,5] because of the difference in the nature of the corresponding bonds in linear polymers. The aim of this note is to study the effect of the variation of the ratio of these two hopping probabilities on the end-to-end distance exponent of the RW's on SAW configurations by means of MC simulation on a square lattice.

SAW configurations of lengths $N=70$ and 50 were generated by MC simulation.[3] The ratio (W) of the weights of a street and of a bridge were then specified. The probability of hopping at every site was then normalized to unity, with the number of bridges connected to the site taken into account. The mean square end-to-end distance $\langle R_t^2 \rangle$ of t-step RW's for $0 \leq W \leq 100$ were measured as before.[3] The data for $W > 1$ are similar to those for $W < 1$.

For $W=0$, the random walker gets trapped between the end points of the first bridge(s) it encounters and then it remains localized in a small finite part of the (infinite) SAW. The random walker diffuses (anomalously) for all $0 < W < \infty$ and $\langle R_t^2 \rangle$, for a given N (the SAW configuration being much longer[3] than the RW), varies as $\langle R_{t_2} \rangle \propto t^{2\nu}$, where $\nu = 0.72$ (Fig. 1). We see in Fig. 1 no change of the dimensionality d_w ($=\nu^{-1}$) of the RW for any finite nonzero W. This contradicts a recent conjecture[5] and agrees with the findings of Stinchcombe.[6] For $W=\infty$, the walker moves only along the streets and hence the corresponding exponent ν crosses over to 0.75. The saturation of $\langle R_t^2 \rangle$ observed for $W \neq 0$ at large t ($t \sim N^2$) is a consequence of the finite length of the SAW. On the other hand, the saturation of $\langle R_t^2 \rangle$ for $W=0$ occurs at much smaller t which is determined by the topology of the SAW.

The disagreement between the experiments[2] on hemeproteins and the results of the nearest-neighbor hopping model[1,3] on a SAW is, therefore, unlikely to arise from different hopping probabilities along the streets and the bridges. However, a change of the random-walk dimensionality due to long-range hoppings[7] or due to protein-solvent interaction[8] cannot be ruled out.

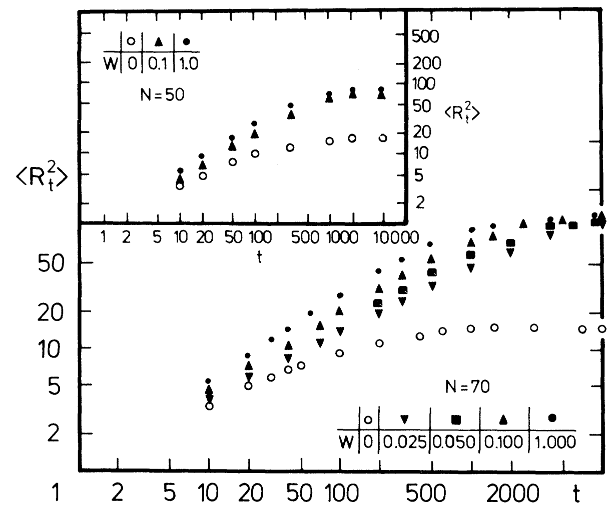

FIG. 1. Plots of $\langle R_t^2 \rangle$ of RW's for various W on SAW configurations of length $N=70$. The inset shows the same for $N=50$.

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