# Reply to 'Detecting knots in self-avoiding walks'



1990 J. Phys. A: Math. Gen. 23 1473

(http://iopscience.iop.org/0305-4470/23/8/023)

J. Phys. A: Math. Gen. 23 (1990) 1473-1474. Printed in the UK

## COMMENT

# Reply to 'Detecting knots in self-avoiding walks'

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Received 30 November 1989

In a recent letter to the editor (Windwer 1989) I was interested in finding the probability of knot formation in self-avoiding walks and comparing that with previous work (Michels and Wiegel 1982) on the probability of knot formation in self-avoiding polygons (SAP). Michels and Wiegel found a power law relationship between the probability of knot formation and the size of the SAP. SAWs and SAPs have shown similar power law relationships (Kremer and Binder 1988).

Sumners and Whittington (1990) correctly note that the SAWs which I generated on a five-choice cubic lattice is not a mathematical knot since one can pull the ends through the entanglement to form an untangled linear chain. It is however a loop (Wiegel 1986) which is related to knots.

In their theoretical work, Sumners and Whittington (1988) showed how SAWs can be mathematically knotted. One way was via tight knots which, because of the tightness of the knot, cannot be rethreaded to give an unknot. They demonstrate this (p 1692) by a SAW on a five choice cubic lattice of 18 steps. This 18-step walk contains 10 nearest neighbours. This translates into 10 opportunities for the walk to terminate in just an 18-step generation process. The generation of SAWs with large numbers of nearest neighbours is very difficult mainly because of the large probability of self-intersection (Wall *et al* 1962). By an ingenious construction they showed how the self-avoiding condition itself may generate a space which would give rise to a topologically equivalent knot (see their figures 1(*b*) and 1(*d*)). Whether this can actually be constructed keeping the self-avoiding condition valid is still open.

Given what I perceive as the difficulties in proceeding with the mathematical paradigm of a knot for SAWs I investigated SAWs loops whose endpoints could be connected by an arc without violating the excluded volume condition. As I noted earlier they could be rethreaded to yield the unknot.

Sumners and Whittington also point out that the 'crossing invariant' which I used to detect knots is not an invariant. I also note this in my paper and show in some detail how twists can yield the same crossing information as a knot. I give one detailed example of how to distinguish between a twisted chain and a knot. As the number of crossing points increase, the difficulties in distinguishing between twists and knots increases at a much greater rate. Their figure 1 is two twists on either side of the chain which can be distinguished from a $4_1$ knot. It should also be stated that my work never intended to distinguish between two topologically different knots, but only count their crossings.

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