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COMMENT

Detecting knots in self-avoiding walks

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Abstract. In this comment, we discuss problems in the method recently proposed by Windwer for computing knot probability in self-avoiding walks on the simple cubic lattice.

In a recent letter to the editor, Windwer (1989) reported calculations of the knot probability in self-avoiding walks (SAWs) on the simple cubic lattice in 3-space. His numerical work was based on theoretical work (Sumners and Whittington 1988) where it was proved that all but exponentially few sufficiently long self-avoiding walks on the simple cubic lattice contain a knotted arc, and all but exponentially few sufficiently long self-avoiding polygons on the simple cubic lattice are knotted. Windwer was interested in finding the probability of knot formation as a function of length in SAWs, and comparing that with extant results (Vologodskii *et al* 1974, Michels and Wiegel 1982) on the probability of knot formation in self-avoiding polygons (SAPs).

In this comment, we point out two problems with Windwer's approach. The concept of knotting in self-avoiding walks (Sumners and Whittington 1988, pp 1690-2) is rather technical. This is due to the fact that, in the pure topological sense, no arc consisting of finitely many straight edges can be knotted in R^3. Just as one can untangle an extension cord by pulling the ends through any entanglement, one can likewise untangle any SAW in R^3. In the special case of a SAW on the simple cubic lattice, however, it is possible to exploit volume exclusion to obtain a topologically well defined notion of knotting in a confined region of 3-space for a SAW. One way to do this is via *tight knots*, where the tightness shields the knotted portion from the rest of the SAW. Briefly, every SAW generates a unique confined region of 3-space which surrounds it, namely the union of the Wigner-Seitz cubes dual to the occupied vertices of the walk. It sometimes happens that this union of Wigner-Seitz cells is homeomorphic to a 3-ball. In this case, one can prolong the walk through the 2-sphere boundary of this 3-ball, obtaining an arc (1-ball) whose endpoints lie in the boundary 2-sphere, and we say that the arc is *properly embedded* in the 3-ball. This resulting *ball pair* can be knotted. This means that when the endpoints of the arc are constrained to remain in the boundary 2-sphere and the interior of the arc is constrained to remain in the interior of the 3-ball, it is impossible to undo the entanglements which occur inside the 3-ball; in this situation we say that the SAW forms a *knotted arc*. See, for example, figure 1 of Sumners and Whittington (1988), and the discussion thereof. If a SAW contains a subwalk which forms a knotted arc, and if that SAW is closed up by any path which misses the surrounding 3-ball associated with the knotted subwalk, one can be certain that the circle so constructed is knotted in R^3. Hence, if any subwalk of a SAP forms a knotted arc, that SAP must be knotted.

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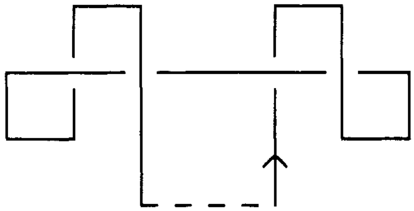

Figure 1. An unknot which is detected as a knot by the crossing invariant.

The problem is that the knotting characteristics of an arc depend entirely on which portion of 3-space one chooses as the surrounding region. For example, any given SAW is unknotted in R^3, and is unknotted in many 3-balls which properly contain it; likewise, that same SAW is knotted in many other 3-balls which properly contain it. In other words, knotting depends on *both* the 3-ball and the SAW. One does not encounter this 'surrounding 3-space' problem when discussing knotting of circles, where the surrounding space is R^3.

In the computation of Windwer, SAWs are generated, and the surrounding 3-space is taken to be R^3, where no knotted arcs can exist. Moreover, the 'crossing invariant' employed to detect knots is not an invariant, even when applied to circles in 3-space. A knot invariant may fail to detect some knotted circles (as does the 'crossing invariant'), but it must never identify an unknotted circle as a knotted circle—no false positives are allowed. The 'crossing invariant' detects that some unknotted circles are knotted; see for example the circle whose projection appears in figure 1.

Nevertheless, the question of computing knot probability for SAWs remains an interesting one. The algorithm for detecting that a SAW contains a knotted arc may be difficult to construct, however. First, one must decide whether or not the union of some Wigner–Seitz cells is homeomorphic to a 3-ball and, if so, one must then decide whether or not the resulting ball pair is knotted. This final problem of knottedness of the ball pair is perhaps the most difficult of the two, because one usually employs knot projections in order to compute knot invariants. For a ball pair contained in R^3, however, one cannot simply project the arc using a projection of R^3 onto a hyperplane—such a projection does not take into account the structure of the surrounding 3-ball. One must first choose a homeomorphism of the surrounding 3-ball to the standard 3-ball (all vectors in R^3 of length $\leqslant 1$). This homeomorphism takes the SAW to an arc in the standard 3-ball in R^3, and the standard 3-ball can then be projected onto an equatorial 2-disc via projection induced by a projection of R^3. In other words, one must first straighten out the surrounding 3-ball before one can obtain a projection for a ball pair, and that projection will depend on the homeomorphism chosen from the surrounding 3-ball to the standard 3-ball.

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