Comment on ''Exact solution of a one-dimensional continuum percolation model''

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In a recent article [Phys. Rev. E **55**, 3878 (1997)], Drory obtains the exact pair-connectedness function of a one-dimensional hard-rod fluid by using a mapping between continuum percolation and a Potts fluid. The purpose of this Comment is to note that the main formula in that paper was already reported some years ago by Vericat, Gianotti, and Rodríguez [J. Phys. A **20**, 6155 (1987)]. They calculated it by a direct diagrammatic analysis of the expression for the pair-correlation function in the canonical ensemble. According to Drory, it appears that in order to discuss continuum percolation in general models there is at the moment no method more powerful than the Potts fluid mapping. However, our calculation seems to show that to achieve the pair-connectedness function for the one-dimensional model under consideration (as well for extensions that include short-range tails) the mapping method should overcome difficulties of a nature similar to those found by standard statistical-mechanics techniques for one-dimensional liquids. [S1063-651X(97)08411-0]

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Very recently, Drory considered the exact solution of a one-dimensional continuum percolation model [1]. The system is an ensemble of $N+1$ hard rods of length σ on a closed ring of circumference L. To study clustering and percolation he takes as a criterion that two such particles are directly connected if they are closer than a connectivity distance $d>\sigma$. Two particles of the system belong to the same cluster if they are either directly connected or indirectly connected through a path of directly connected intermediary particles.

For this model he calculates, in the thermodynamic limit ($N,L\to\infty$ and $N/L=\rho\leqslant 1/\sigma$), the pair-connectedness function by using an interesting, previously described mapping between the percolation problem and a Potts fluid [2]. He also evaluates the mean cluster size in two different ways: (i) by directly using the analogy with the Potts fluid susceptibility and (ii) by integrating the analytical expression he found for the pair-connectedness function.

Therefore, a central object in Drory's paper [1] is the pair-connectedness function $\rho^{\dagger}(x_1,x_2)=\rho^2 g^{\dagger}(x_1,x_2)$, which is the density probability of finding two particles in differential elements dx_1 and dx_2 around the positions x_1 and x_2, respectively. Because of the periodic conditions, implicit in the ring geometry, the system is translationally invariant so that $g^{\dagger}(x_1,x_2)=g^{\dagger}(r)$, with $r=|x_2-x_1|$. The closed analytical expression he obtains for $g^{\dagger}(r)$ [Eqs. (3.25) and (4.2) of [1]] is

$$g^{\dagger}(r)=\frac{1}{\rho}\sum_{k=1}^{\infty}\sum_{j=0}^{k}(-1)^j\binom{k}{j}\left(\frac{\rho}{1-\rho\sigma}\right)^k \times\frac{[r-k\sigma-j(d-\sigma)]^{k-1}}{(k-1)!}\,\Theta(r-k\sigma-j(d-\sigma)) \times\exp\left[-\frac{\rho(r-k\sigma)}{1-\rho\sigma}\right], \tag{1}$$

where $\Theta(z)$ is the Heaviside step function. (Note the minus sign before j in the argument of Θ instead of the plus sign that appears in [1].)

Here we wish to note that ten years ago two of us reported in Ref. [3] the same formula [Eq. (1)] for the pair-connectedness function of a hard-rod fluid. The model and the connectivity criterion considered in [3] were basically the same ones as those used in [1]. The only difference is that the hard rods in [3] were constrained to move on a line segment $[0,L]$, not on a ring as in [1]. The consequence is that points 0 and L act as the container walls for the hard rods and the translational invariance near the walls is, in principle, lost.

To evaluate the pair-connectedness function in [3] we started from its canonical definition. For N hard rods we have

$$\rho(x_1,x_2)=\frac{N!}{(N-2)!}\frac{1}{Z(L,N)}\int\cdots\int dx_3\cdots dx_N \times\prod_{i<j}^{N}\exp[-v(x_i,x_j)/k_BT], \tag{2}$$

with $Z(L,N)$ the configurational integral and $v(x_i,x_j)$ the pair potential for hard rods. Following the standard approaches [4,5], the Boltzmann factors $e(x_i,x_j)=\exp[-v(x_i,x_j)/k_BT]$ are split up into connectivity $(e^{\dagger}(x_i,x_j)=\exp[-v^{\dagger}(x_i,x_j)/k_BT])$ and blocking $(e^{*}(x_i,x_j)=\exp[-v^{*}(x_i,x_j)/k_BT])$ parts $e=e^{\dagger}+e^{*}$, so that also the pair-connectedness function separates into a similar form

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$\rho(x_1,x_2)=\rho^{\dagger}(x_1,x_2)+\rho^{*}(x_1,x_2)$. The effective pair potential $v^{\dagger}$ (v^{*}) between bound (unbound) particles equals v for interparticle distances shorter (longer) than d and is infinity otherwise.

In order to calculate $\rho^{\dagger}(x_1,x_2)$ we replace $e\rightarrow e^{\dagger}+e^{*}$ in Eq. (2) and expand the right-hand side as a sum of all terms that are possible arrangements of the factors $e^{\dagger}$ and e^{*} evaluated between the $N(N-1)/2$ pairs of particles. Then $\rho^{\dagger}(x_1,x_2)$ is built by selecting among all these summands those that have at least one path of $e^{\dagger}$ bonds between particles at positions x_1 and x_2. For hard rods, a simple diagrammatic analysis shows that particles 1 and 2, with $x_1<x_2$, belong to the same cluster if, independently of what happens in the external intervals $[0,x_1]$ and $[x_2,L]$, all the particles inside the interval $[x_1,x_2]$ form a chain of $e^{\dagger}$-bonded nearest neighbors. This is equivalent to the factorization occurring in [1]. We must remark here that the condition $\sigma<d<2\sigma$ that we imposed in [3] is completely unnecessary and the result is valid for any $d>\sigma$.

Thus, in [3] we obtained an expression for the pair-connectedness function valid for $d>\sigma$, N and L being, in principle, arbitrary. However, due to the mentioned lack of translational invariance in our system, we can take the thermodynamic limit only for densities $\rho<1/2\sigma$ [3]. These densities are compatible with the existence of a region of translational invariance in the system. Thus the formula we found in [3] is valid just for $\rho<1/2\sigma$ when we consider a container with impenetrable walls, but it is also valid for any density $0<\rho\leqslant 1/\sigma$ whenever the translational symmetry is ensured. Accordingly, calculations in [1] and [3] give the same connectedness formula for the ring geometry.

A comparison between calculations in [1] and [3] seems to show that the difficulties of the two methods to obtain the pair-connectedness function for the one-dimensional hard-rod model are of a similar nature. What makes the model exactly solvable in both approaches is that the pair-connectedness function can be written as convolution integrals [see, for example, Eq. (3.3) of [1]]. This is possible for arbitrary d because of the particular form of the hard-rod potential that is trivially of the nearest-neighbor type and a treatment similar to those of Takahashi [6] or Salsburg, Zwanzig, and Kirkwood [7] is enough. Things become complicated if one wishes to consider an additional tail in the potential. In this case the existence of an exact solution for some particular tail forms would still be possible (by both ways), but at the cost of restricting the connectivity distance to a limited region (i.e., $\sigma<d<2\sigma$).

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