Finite clusters in high intensity Zwanzig model

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Introduction

Zwanzig (1963) studied a system of non-overlapping hard rods in the continuum.
The orientation of the rods are restricted to a finite set.
He observed that as the density of rods increased a phase transition occurred from an isotropic phase to a nematic phase, i.e.
from a phase where the rods are placed chaotically to a phase where the rods are oriented in a fixed direction.

Lately there has been a considerable interest among physicists in this model.

Hard rods being renamed as hard needles.

This interest is kindled by the connection between the entropic properties and the the phases of the system.

see, e.g., Dhar, Rajesh and Stilck [2011], Gurin and Varga [2011]

Our study is for the 2-state and the 3-state Zwanzig model with overlapping hard needles.
The needles form a Boolean fibre process
(see e.g., Hall [1990], Stoyan Kendall and Mecke [1995]).
In the case when the centres of the needles are placed according to a homogenous Poisson point process of density λ, the overlapping needles form a percolating cluster and the system displays phase transition (see Roy [1991]) as the density increases from a regime which does not admit an unbounded connected component of needles to one where such a component exists.

We study the structure of finite connected components in a high density supercritical regime.
We establish the nematic behaviour as observed by Zwanzig by showing that any finite cluster consists of
all but one needle bunched together in a given direction,
the other needle providing the connectivity by lying across these oriented needles.
Needles of which direction and which length are preferred in such a finite cluster depend on the parameters of the process.

2-state Zwanzig model

The needles are placed according to a Poisson point process of density λ.
Needles being of two distinct orientations,
needles of the same orientation being of the same length
but needles of different orientations allowed to be of different lengths.

Consider a finite cluster comprising of m needles in a high density λ percolating regime.

For m large, the cluster typically consists of $m - 1$ needles of one orientation with only one needle in the other orientation connecting them to form a cluster.

The choice of the orientation of the cluster depends on which orientation of the needles is more probable, and not on either the angle of orientation or the length of the sticks.

This is a consequence of the affine invariance of the model.

Also the $(m-1)$ needles in one direction are bunched together with their centres very tightly packed (with a density much larger than the ambient density of sticks in the chosen direction),

whereas the lone needle in the other direction is the only needle in its directeion placed with its centre uniformly distributed in the parallelogram such that it intersects the other $(m-1)$ sticks (thus having a density much less than the ambient density of sticks in its direction).

These densities follow the compression and rarefaction phenomenon in the case of the Poisson Boolean model with spheres of fixed radius (Alexander 1996) and random radius (Sarkar 1998).

An interesting observation of our model is that if $p_{\lambda,m}(k,l)$ denotes the probability that in a cluster of size m there are k needles of one orientation and l needles of the other orientation, then,
in the situation where $(k/m) \to s \in [0,1]$ as $m \to \infty$ and where each of the directions is equally likely, we have

$$\lim_{\substack{m\to\infty \\ (k/m)\to s}} \frac{1}{m} \lim_{\lambda\to\infty} \log p_{\lambda,m}(k,\ell) = s\log s + (1-s)\log(1-s),$$

thereby suggesting a link between entropy and the structure of large finite clusters.

In this case (when $p = 1/2$ and $k/m \to s$) what happens is that

the packing densities of the centres of both the bunches of needles is much larger than their ambient density,

however the centres are uniformly placed in the appropriate parallelogram.

And it is this uniform placement which gives the entropic term.

3-state Zwanzig model

Here three distinct orientations of the needles are allowed.
The affine invariance of the model breaks down;
and for high density λ,
the finite clusters consist of sticks in only two directions,
the surviving directions being dependent on both the angles and the lengths of the needles in different orientations as well as the probabilities of orientations of the needles.
The equivalent of $p_{\lambda,m}(k,l)$ is not as explicit as the entropy-like expression in the case of needles with the 2-state Zwanzig model.

Notation

Let $\mathcal{R} = \mathbb{R}^2 \times [0, \pi) \times (0, \infty)$, and

$$\mathcal{M} = \mathcal{M}(\mathcal{R}) := \{\xi = \{\xi_i, i \in \mathbb{N}\} : \xi_i = (x_i, \theta_i, r_i) \in \mathcal{R}\}.$$

For $(x, \theta, r) \in \mathcal{R}$,
$S(x, \theta, r) = \{x + ue_\theta, u \in [-r, r]\}$
is the needle with centre x, angle θ and length $2r$, where
$e_\theta = (\cos\theta, \sin\theta)$.
We define the collection of needles for $\xi \in \mathcal{M}$ as
$S(\xi) = \{S(x, \theta, r) : (x, \theta, r) \in \xi\}$.

Two needles S and S' are connected $S \overset{\xi}{\leftrightarrow} S'$
if there exist needles $S_1, S_2, \dots S_k \in S(\xi)$ such that
$S \cap S_1 \neq \emptyset$, $S' \cap S_k \neq \emptyset$ and $S_i \cap S_{i+1} \neq \emptyset$ for every
$i = 1, 2, \dots, k-1$.
If $S(\xi)$ contains a needle $S_{\mathbf{0}}$ centred at the origin $\mathbf{0}$, we denote by
$C_{\mathbf{0}}(\xi)$ the cluster of needles containing $S_{\mathbf{0}}$, i.e.

$$C_{\mathbf{0}}(\xi) = \{y \in S : S \in S(\xi), S \overset{\xi}{\leftrightarrow} S_{\mathbf{0}}\}.$$

We put
$C_{\mathbf{0}}(\xi) = \emptyset$,
if $S(\xi)$ does not contain any needle with centre $\mathbf{0}$.
However for our results we take a typical point of the Poisson process to be the origin so as to exclude the possibility of $C_{\mathbf{0}} = \emptyset$.

Let ρ be the Radon measure on $\mathcal{R}$ defined by

$$\rho(dxd\theta dr) = dx \sum_{j=1}^{d} p_j \delta_{\alpha_j}(d\theta)\delta_{R_j}(dr),$$

where
$\alpha_1 = 0 < \alpha_2 < \alpha_3 < \cdots < \alpha_d < \pi$,
$p_j \geq 0, \sum_{j=1}^{d} p_j = 1,\ R_j > 0,\ j = 1, 2, \ldots, d$
and
δ_* denotes the usual Dirac delta measure.
We denote by μ_ρ the Poisson point process on $\mathcal{M}(\mathcal{R})$ with intensity measure ρ.

Let

$$\Gamma_0 := \{\xi \in \mathcal{M} : (\mathbf{0}, \alpha_j, R_j) \in \xi \text{ for some } j = 1, 2, \ldots, d\},$$

and for $\mathbf{k} = (k_1, k_2, \ldots, k_d) \in (\mathbb{N} \cup \{0\})^d$,
let $\Lambda(\mathbf{k})$ be the set of clusters containing exactly $|\mathbf{k}| = \sum_j^d k_j$ needles
with k_j needles at an orientation α_j, $j = 1, 2, \ldots, d$.

Theorem 1

Suppose that the needles are of two types:-
Needles oriented horizontally of length R_0 each
and
needles at an angle $\alpha \in (0, \pi)$ of length R_α each.
The probability that a randomly chosen needle is horizontal (respectively vertical) is p (respectively $1 - p$).
$\Lambda(k, \ell)$ is the set of clusters containing k horizontal needles and ℓ needles at an angle α.
Let $m = k + l$.

Theorem

As $\lambda \to \infty$, we have

(i) $\mu_{\lambda\rho}(C_0 \in \Lambda(k,\ell) \mid \Gamma_0)$

$$\sim \left(\frac{1}{\lambda R_0 R_\alpha \sin\alpha}\right)^{m-3} e^{-\lambda R_0 R_\alpha \sin\alpha}(pq)^{-2(m-1)} m p^{3k} k! q^{3l} \ell!,$$

(ii)

$p_{\lambda,m}(k,\ell) := \mu_{\lambda\rho}(\# C_0 = (k,\ell) \mid \# C_0 = (k',\ell'),\ k' + \ell' = m)$

$$\sim \frac{p^{3k} k! q^{3\ell} \ell!}{\sum_{k+\ell=m} p^{3k} k! q^{3\ell} \ell!}.$$

As $\lambda \to \infty$, from (ii) we see that the conditional probability $p_{\lambda,m}(k, \ell)$ of the needles comprising the *finite* cluster C_0, is independent of both the angles and the lengths of the needles. This, as noted earlier is not surprising because the model is invariant under affine transformations.

Let $p_m(k,\ell) := \lim_{\lambda\to\infty} p_{\lambda,m}(k,\ell)$. We also observe from (ii) that, as $m \to \infty$,

$$\begin{aligned} p_m(m-1,1) &\to 1 && \text{for } p > q, \\ p_m(1,m-1) &\to 1 && \text{for } p < q, \\ p_m(1,m-1) = p_m(m-1,1) &\to \frac{1}{2} && \text{for } p = q. \end{aligned}$$

Moreover, let k and m both approach infinity in such a way that $(k/m) \to s$, for some $s \in [0,1]$, then we have

$$\lim_{\substack{m\to\infty \\ (k/m)\to s}} \frac{1}{m} \log p_m(k,\ell) = H(s),$$

where

$$H(s) = s\log s + (1-s)\log(1-s) + \begin{cases} 3(1-s)\log(q/p), & \text{if } p > q, \\ 3s\log(p/q), & \text{if } p < q, \\ 0, & \text{if } p = q, \end{cases}$$

From the above we have
as $m \to \infty$, for $0 \le a \le b \le 1$,
the proportion (k/m) of horizontal needles in the cluster lies between a and b has probability
$\sim \exp\{\sup_{s \in (a,b)} H(s)\}$.

Needles of three types

Now we assume that
there are needles with only three orientations – $0, \alpha$ and β, with lengths of R_0, R_α and R_β along these orientations.
The absence of any affine invariance leads to the dependence of the results on both the lengths and orientations of the needles through the following quantities

$$H_\alpha = \frac{R_\alpha}{\sin\beta},$$

$$H_\beta = \frac{R_\beta}{\sin\alpha},$$

$$H_0 = \frac{R_0}{\sin(\beta - \alpha)}.$$

By a suitable scaling we take

$$H_0 = 1 \text{ and let } H_\alpha = a, \;\; H_\beta = b.$$

Our theorem shows that, as $\lambda \to \infty$, the asymptotic composition of the finite cluster contains needles of only two distinct orientation, while the third does not figure at all.
Here we use the shorthand "$A(x, y)$ occurs" to mean that as $\lambda \to \infty$ the asymptotic shape of C_0 consists of needles only in the directions x and y.

Theorem

Given that C_0 consists of m needles,

1. for $a, b \geq 2$;
   (i) if $(ab - a + 1/4)p_\beta + a < (ab - b + 1/4)p_\alpha + b$, then $A(0, \alpha)$ occurs,
   (ii) if $(ab - a + 1/4)p_\beta + a > (ab - b + 1/4)p_\alpha + b$, then $A(0, \beta)$ occurs, and
   (iii) if $(ab - a + 1/4)p_\beta + a = (ab - b + 1/4)p_\alpha + b$, then both $A(0, \alpha)$ and $A(0, \beta)$ have positive probabilities of occurrence;

2. for $1/2 < \min\{a, b\} < 2$ and $a \neq b$, $a, b \neq 1$ and for $x, y, z \in \{0, \alpha, \beta\}$ let

$$f(x, y, z) := p_x H_x \max\{H_y, H_z\} + p_x \min\{H_y, H_z\}^2/4 + (1-p_x) H_y H_z,$$

(i) $A(\alpha, \beta)$ occurs when $f(0, \alpha, \beta) < \min\{f(\beta, 0, \alpha), f(\alpha, \beta, 0)\}$

(ii) $A(0, \alpha)$ and $A(0, \beta)$ have positive probabilities of occurrence, when $f(\beta, 0, \alpha) = f(\alpha, \beta, 0) < f(0, \alpha, \beta)$, and

(iii) $A(\alpha, \beta)$, $A(0, \alpha)$ and $A(0, \beta)$ all have positive probabilities of occurrence when $f(\beta, 0, \alpha) = f(\alpha, \beta, 0) = f(0, \alpha, \beta)$;

3. for $0 < a = b < 1$, and,

(i) for $p_0 \leq \min\{p_\alpha, p_\beta\}$, $A(\alpha, \beta)$ occurs,

(ii) for $p_0 > \min\{p_\alpha, p_\beta\}$,

if $a < \mathbf{l}_1(p_0, p_\alpha, p_\beta) := 1 - \frac{p_0 - \min\{p_\alpha, p_\beta\}}{4 - 3p_0 - \min\{p_\alpha, p_\beta\}}$, then $A(\alpha, \beta)$ and fixation occurs, while,

if $a \geq \mathbf{l}_1(p_0, p_\alpha, p_\beta)$, $A(0, \alpha)$ occurs for $p_\alpha > p_\beta$ and both $A(0, \alpha)$ and $A(0, \beta)$ have positive probability of occurrence for $p_\alpha = p_\beta$;

4. for $1 < a = b < 2$, and,

(i) for $p_0 < \min\{p_\alpha, p_\beta\}$,
if $a < \mathbf{I}_2(p_0, p_\alpha, p_\beta) :=$
$\frac{2\max\{p_\alpha, p_\beta\} + \sqrt{4\max\{p_\alpha, p_\beta\}^2 + 4p_\alpha p_\beta + p_0 \min\{p_\alpha, p_\beta\}}}{4\max\{p_\alpha, p_\beta\} + p_0}$, then $A(\alpha, \beta)$ and fixation occurs, while,
if $a \geq \mathbf{I}_2(p_0, p_\alpha, p_\beta)$, $A(0, \alpha)$ occurs for $p_\alpha > p_\beta$ and both $A(0, \alpha)$ and $A(0, \beta)$ have positive probability of occurrence for $p_\alpha = p_\beta$,

(ii) for $\min\{p_\alpha, p_\beta\} \leq p_0$, $A(0, \alpha)$ occurs for $p_\alpha > p_\beta$ and both $A(0, \alpha)$ and $A(0, \beta)$ have positive probability of occurrence for $p_\alpha = p_\beta$;

5. for $a = b = 1$, fixation always occurs and
   (i) $A(x, y)$ occurs when $p_z < \min\{p_x, p_y\}$,
   (ii) with equal probability $A(x, y)$ and $A(x, z)$ occur when $p_y = p_z < p_x$, and
   (iii) with equal probability $A(x, y)$, $A(y, z)$ and $A(z, x)$ occur when $p_x = p_y = p_z$;