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The study of identical state-nematic phase transition in a confined monolayer of hard cylindrical rods using Onsager and Parsons-Lee theories

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Abstract

We studied the identical-nematic (I-N) phase transition of hard cylinders confined between two hard walls when $H < L$ using Onsager and Parsons-Lee theories and the Zwanzig approximation. The obtained results show the difference in predicting the I-N phase transition of the systems studied by these two theories. The results of Onsager theory are consistent with the previous paper, but the results of Parsons-Lee predict a completely different behavior. Compared to the previous results, our results occur at higher densities, which is due to the use of the Zwanzig approximation. Since Onsager model is accurate for highly elongated particles, we expect the two theories to provide a more accurate and similar answer for elongated particles, which was met in the investigations. Therefore, it seems that Onsager theory provides more appropriate result in the studied cases. It should be noted that what can give a more accurate judgment about these results is the simulation of a similar system of limited cylinders in a quasi-two-dimensional space. According to the literature review, the Parsons-Lee theory has given very good results for three dimensional systems, where two or more layers can form in the pores, however, it does not work properly for a monolayer of confined hard cylinders. Therefore, for such systems, it is necessary to modify the Parsons-Lee pre-factor to provide reliable results. This pre-factor has been calculated for three-dimensional systems in which the geometrical shape of particles is mapped to spheres of the same volume, not for two-dimensional systems. Because the image of a cylinder in two dimensions is a rectangle, and hard rectangles must map to hard disks, it is necessary to formulate a pre-factor and the Carnahan-Starling equation for disks in two-dimensional and quasi-two-dimensional systems.

Keywords: phase transition, liquid crystal, nematic, identical state, monolayer

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