Residual entropy and waterlike anomalies in the repulsive one dimensional lattice gas

F. Barbosa, V. da Silva, F.A. Oliveira, and M.A.A. Barbosa
IFB

Water is special fluid for its biological relevance and technological applications but most intriguing is that it presents thermodynamic and dynamic properties with anomalous (or unusual) behavior. The origin of its anomalous properties is actively discussed in the literature, with different thermodynamic scenarios competing to describe its behavior on regular and metastable regimes. Among alternative views on water thermodynamics, it should be relevant to mention the second critical point hypothesis and the singularity free scenario, which will be relevant in the context of the current work.
In this work, we proceed on this direction by investigating the repulsive 1D lattice gas, which is even simpler than our previous models and presents waterlike anomalies in density, thermodynamic response functions, and self-diffusion constant. The model was studied through transfer matrix technique, the Takahashi method (within a two-states approximation, as will be discussed later), and Monte Carlo simulations. With the results obtained from these techniques, a connection between temperature of maximum density and GSTP was found as in a previous work with more complex models. In addition, it was also found that GSPT does present a residual entropy, due to phase mixing, and it is shown that this property is fundamental in determining waterlike anomalies for the model considered here. Finally, a comparison between regions with density and diffusion anomaly indicated that this model presents so called hierarchy of anomalies.
In the ground state, the model presents a phase transition between a softened fluid and a dense fluid, which is characterized by a mixture between two states. The main consequence of this mixed state is a residual entropy in a single point in the pressure vs. temperature phase diagram. Using thermodynamic relations, it was argued that the presence of a residual entropy in a single point is consistent with a temperature of maximum density line (= 0) emanating from the ground state phase transition. Considering this it is possible to state that ground state phase transition, residual entropy, and density anomalies are the thermodynamic properties of our model which are intrinsically related and cannot be dissociated from each other.

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