# Residual entropy in the repulsive one-dimensional lattice model of liquid water

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The thermodynamic and kinetics of the one dimensional lattice gas with repulsive interaction is investigated using transfer matrix technique and Monte Carlo simulations. This simple model is shown to exhibit waterlike anomalies in density, thermal expansion coefficient and self diffusion. A unified description for the thermodynamic anomalies in this model is achieved based on the ground state residual entropy which appears in the model due to mixing entropy in a ground state phase transition. Lattice models of fluid have been extensively used to investigate the above mentioned anomalous properties of water due to possibility of obtaining simple and analytically (or numerically) solvable results, while exploring a wide range of physical parameters. In this direction, both thermodynamics and kinetics [1] where investigated in lattice models with waterlike behavior. Nevertheless, approximations employed in two and three dimensions(3D), and even some analytical solutions in one dimension (1D), tend to generate complex sets of equations whose analysis is often performed numerically. Thus, it should desired to design models for which one could obtain simple analytical expressions connecting thermodynamic anomalous behavior to phase transitions and critical behavior. To achieved this goal we previously investigate 1D lattice models with pair interaction between the first neighboring molecules, with interactions spanning two [2] and three lattice sites [3]. While in Ref. [2] both van der Waals and hydrogen bond like interactions were used, resulting in a line of temperature of maximum density (TMD) associated to a ground state phase transition (GSPT), in Ref. [3] it was proposed a core-softened fluid with pair interactions up to three sites, resulting in two TMD lines associated to two GSPT. Besides obtaining exact results,
in the latter work we used an analytical approximation in the neighborhood of the critical point to obtain a simple expression for Gibbs free energy, and used it mathematically study the relation between anomalous density behavior and GSPT.

In this work we proceed on this direction by investigating the repulsive 1D lattice gas (RLG1D), which is even simpler than our previous models and presents waterlike anomalies in density, thermal response functions and self diffusion constant. The model was studied through transfer matrix technique, the Takahashi method and Monte Carlo simulations (for obtaining the self diffusion constant) and its simplicity allowed us to find a connection between temperature of maximum density and GSTP, as before [3]. 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 the present model has the so called hierarchy of anomalies.

References

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