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Title:	Investigation of Equilibrium and Non-equilibrium behavior of Symmetrical Binary Liquid Mixtures
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Abstract:	We study the Phase separation in simple binary liquid mixture in the first part of thesis. The binary liquid mixture, near its consolute point, exhibits critical fluctuations in their local composition. They fall into the universality class of the three dimensional Ising model with short-range interactions. Although finite system size, in general challenges the study of phase transition, we employ finite size scaling analysis to solve this problem and arrive at the critical properties. Typically, such analysis requires the simulation of a vast number of system sizes. Here we present an alternative approach whereby a single extensive system is simulated and finite-size scaling is done using a sub-system analysis. The correlation length and the concentration susceptibility are determined from the time-averaged static structure factor for the order parameter fluctuations and are shown to diverge as $\xi \propto T - T_c ^{-\nu}$ and $\chi \propto T - T_c ^{-\gamma}$ respectively. We also find the critical amplitudes of susceptibility and correlation length. Finally, to get the estimate of critical temperature we use the intersection criterion for Binder cumulant of the different subsystems. The second part of the thesis deals with active Brownian motion of symmetrical binary liquid mixture which is a modification to my first work. The two types of particles are distinguished from one another by the opposite propulsion velocity and different interaction strength. We expected a non-equilibrium phase separation into different particle types due to their different motilities, but however this was not observed. So several checks were done to test the dynamics of system which gave the expected results. We can safely conclude that attractive interaction in force-shifted LJ potential is affecting the non-equilibrium phase transition. More work has to be done to confirm this. The third part of thesis deals with self-diffusiophoresis in the near-critical binary mixture. Gold capped Janus particles immersed in a near-critical fluid mixture can be propelled using illumination to a temperature below T_c . We attribute this motion of the particle to the slip-velocity of the fluid around the particle, caused by the local-demixing of fluid due to the asymmetric heating. The aim is to quantify the dependency of orientational and translational dynamics on the wetting parameters and heating of the particle. Although this work is not complete, I have arrived at some initial simulation results.
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