Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Static and Dynamic Anomalies in a Repulsive Spherical Ramp Liquid: Theory and Simulation PRADEEP KUMAR, Center for Polymer Studies and Department of Physics Boston University, Boston, MA 02215, SERGEY V. BULDYREV, Yeshiva University, Department of Physics, 500 W 185th Street, FRANCESCO SCIORTINO, EMANUELA ZACCARELLI, Dipartimento di Fisica and INFM CRS-SOFT: Complex Dynamics in Structured Systems, Università di Roma La Sapienza, Rome, Italy, H.E. STANLEY, Center for Polymer Studies and Department of Physics Boston University, Boston, MA 02215 USA — We compare theoretical and simulation results for static and dynamic properties for a model of particles interacting via a spherically symmetric repulsive ramp potential. The model displays anomalies similar to those found in liquid water, namely, expansion upon cooling and an increase of diffusivity upon compression. In particular, we calculate the phase diagram from the simulation and successfully compare it with the phase diagram obtained using the Rogers-Young (RY) closure for the Ornstein-Zernike equation. Both the theoretical and the numerical calculations confirm the presence of a line of isobaric density maxima, and lines of compressibility minima and maxima. Indirect evidence of a liquid-liquid critical point is found. Along constant temperature paths, as the density increases, the dynamics alternates several times between slowing down and speeding up. Finally we confirm that mode coupling theory successfully predicts the behavior of dynamics and the presence of multiple glass phases.

Pradeep Kumar
Center for Polymer Studies and
Department of Physics Boston University, Boston, MA 02215

Date submitted: 08 Dec 2004 Electronic form version 1.4