Abstract Submitted
for the APR17 Meeting of
The American Physical Society

Computing Critical Properties with Yang-Yang Anomalies

GERASSIMOS ORKOULAS, Widener University, CLAUDIO CERDEIRINA, Universidad de Vigo, Spain, MICHAEL FISHER, University of Maryland — Computation of the thermodynamics of fluids in the critical region is a challenging task owing to divergence of the correlation length and lack of particle-hole symmetries found in Ising or lattice-gas models. In addition, analysis of experiments and simulations reveals a Yang-Yang (YY) anomaly which entails sharing of the specific heat singularity between the pressure and the chemical potential. The size of the YY anomaly is measured by the YY ratio $R_\mu = \tilde{C}_\mu / C_V$ of the amplitudes of $\tilde{C}_\mu = -T\, d^2\mu/dT^2$ and of the total specific heat C_V. A "complete scaling" theory, in which the pressure mixes into the scaling fields, accounts for the YY anomaly. In Phys. Rev. Lett. 116, 040601 (2016), compressible cell gas (CCG) models which exhibit YY and singular diameter anomalies, have been advanced for near-critical fluids. In such models, the individual cell volumes are allowed to fluctuate. The thermodynamics of CCGs can be computed through mapping onto the Ising model via the seldom-used great grand canonical ensemble. The computations indicate that local free volume fluctuations are the origins of the YY effects. Furthermore, local energy-volume coupling (to model water) is another crucial factor underlying the phenomena.

Gerassimos Orkoulas
Widener University

Date submitted: 28 Sep 2016