Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Efficient free energy calculations of quantum systems through computer simulations ALEX ANTONELLI, Universidade Estadual de Campinas, RAFAEL RAMIREZ, CARLOS HERRERO, Instituto de Ciencia de Materiales de Madrid, EDUARDO HERNANDEZ, Institut de Ciencia de Materials de Barcelona
— In general, the classical limit is assumed in computer simulation calculations of free energy. This approximation, however, is not justifiable for a class of systems in which quantum contributions for the free energy cannot be neglected. The inclusion of quantum effects is important for the determination of reliable phase diagrams of these systems. In this work, we present a new methodology to compute the free energy of many-body quantum systems [1]. This methodology results from the combination of the path integral formulation of statistical mechanics and efficient non-equilibrium methods to estimate free energy, namely, the adiabatic switching and reversible scaling methods. A quantum Einstein crystal is used as a model to show the accuracy and reliability the methodology. This new method is applied to the calculation of solid-liquid coexistence properties of neon. Our findings indicate that quantum contributions to properties such as, melting point, latent heat of fusion, entropy of fusion, and slope of melting line can be up to 10% of the calculated values using the classical approximation. [1] R. M. Ramirez, C. P. Herrero, A. Antonelli, and E. R. Hernández, Journal of Chemical Physics **129**, 064110 (2008)

Alex Antonelli
Universidade Estadual de Campinas

Date submitted: 20 Nov 2008 Electronic form version 1.4