Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Structure in the Condensate Occupation of Trapped Hard Sphere Bosons JONATHAN L. DUBOIS, K. BIRGITTA WHALEY, Department of Chemistry and Pitzer Center for Theoretical Chemistry, University of California, Berkeley, CA 94720-1460 — We have performed detailed variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) calculations of the ground state and condensate properties for small numbers ($1 < N < 100$) of hard sphere bosons in a harmonic trap. Condensate properties are obtained by evaluating the eigenvectors (Natural Orbitals) and eigenvalues (Occupation numbers) of the one body density matrix. For macroscopic systems with weak interactions, $na^3 \ll 1$, the OBDM description of the condensate in terms of a single large eigenvalue with large occupation and the "condensate wave-function" of Gross-Pitaevskii (GP) theory are equivalent. Unlike GP theory, however, condensate properties obtained within the OBDM formulation are a property of the full ground state wave-function of the many-body Hamiltonian and are equally valid for any number of particles and interaction strength. We find that in the mesoscopic regime, $N < 30$ & $na^3 > 10^{-3}$, the N dependence of the fraction of particles in the condensate orbital $n_0(N)$ is not a simple monotonically decreasing function of N. Quite remarkably, we find that there are instead "magic" particle numbers for which the condensate experiences anomalous depletion. This structure in the condensate fraction will be described fully and possible implications for experiment will be discussed.

Jonathan L. DuBois

Date submitted: 05 Jan 2005 Electronic form version 1.4