Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Phase diagram of the one dimensional Hubbard-Holstein Model at 1/2 and 1/4 filling[1] RAHUL HARDIKAR, TORSTEN CLAY, Mississippi State University — We present a detailed study of the phase diagram of the Hubbard Holstein model at 1/2 filling and 1/4 filling, including finite-frequency quantum phonons within the numerically exact Stochastic Series Expansion quantum Monte Carlo method. In one dimension at 1/2 filling, the electron-phonon (e-ph) coupling gives a Peierls charge density wave, while Hubbard onsite U promotes antiferromagnetic correlations and a Mott insulating state. Our previous study revealed a third Intermediate phase when the electron-electron and e-ph interaction are closely balanced. We show here from direct calculations of charge and spin susceptibilities that (i) as the e-ph coupling strength is increased first a spin gap transition and then the Peierls transition occurs, (ii) transitions between Mott/Intermediate and Intermediate/Peierls states are of the Kosterlitz-Thouless type, (iii) for large U, the two transitions merge into a single fist order transition. Our data is consistent with a renormalization of the Luttinger Liquid exponent K_ρ, which gives a slightly larger intermediate region as determined from susceptibilities than in previous calculations of K_ρ. At 1/4 filling we find a very similar phase diagram.

[1]Supported by the American Chemical Society (Petroleum Research Fund) and DOE

Rahul Hardikar
Mississippi State University

Date submitted: 17 Nov 2006 Electronic form version 1.4