Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Collapse transition for self-avoiding random walks with hydrophobic interaction on a 2 dimensional lattice MATHIEU GAUDREAULT, JORGE VINALS, Department of Physics, McGill University, Canada — We study the collapse transition of a protein model with an explicit coarse-grained model of solvent hydrophobicity using Monte Carlo simulation. The protein is modelled as self- avoiding random walk with nearest neighbour interaction on a two dimensional lattice by using the pivot algorithm. Without the solvent, universal quantities of the chain around the transition temperature are well known. Hydrophobicity is modelled through a lattice of solvent molecules in which each molecule can have q states, depending of an orientation variable. Only one state is energetically favoured, when two neighbouring solvent molecules are both in the same state of orientation. The monomers are placed in interstitial position of the solvent lattice, and are only allowed to occupy sites surrounded by solvent cells of the same orientation. The potential of mean force between two interstitial solute molecules is calculated, showing that the strength of attraction increases by increasing the free energy of H-bond formation while its range decreases. We also show that the temperature of the collapse transition is shifted in the presence of solvent, while the universal quantities of the protein transition are conserved.

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Date submitted: 15 Nov 2006 Electronic form version 1.4