

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Spherical Proteins and Viral Capsids Studied by Theory of Elasticity** ZHENG YANG, Department of Physics & Astronomy, University of Pittsburgh, IVET BAHAR, Department of Computational Biology, University of Pittsburgh, MICHAEL WIDOM, Department of Physics, Carnegie Mellon University — Coarse-grained elastic network models have been successful in elucidating the fluctuation dynamics of proteins around their native conformations. It is well established that the low-frequency collective motions derived by simplified normal mode analysis depend on the overall 3-dimensional shape of the biomolecule. Given that the large scale collective motions are usually involved in biological function, our objective in this work is to gain more insights into large scale collective motions of spherical proteins and virus capsids by considering a continuous model with perfect spherical symmetry. To this end, we compare the global dynamics of proteins and the analytical solutions from an elastic wave equation with spherical boundary conditions. In addition, an icosahedral discrete model is generated and analyzed for validating our continuous model. Applications to lumazine synthase, satellite tobacco mosaic virus and other viruses shows that the spherical elastic model can efficiently provide insights on collective motions that are otherwise obtained by detailed elastic network models.

Zheng Yang  
Department of Physics & Astronomy, University of Pittsburgh

Date submitted: 22 Nov 2007

Electronic form version 1.4