Protein Thermodynamics from Maxwell Constraint Counting
DONALD JACOBS, Department of Physics and Optical Science, UNC-Charlotte,
DENNIS LIVESAY, Department of Bioinformatics and Genomics, UNC-Charlotte,
OLEG VOROV, Department of Physics and Optical Science, UNC-Charlotte —
Topological properties of network rigidity explain essential aspects of structural
phase transitions and thermodynamic stability in proteins [1]. We present an exact
transfer matrix method within a Distance Constraint Model (DCM) that maps inter-
actions into distance constraints having energy and entropy contributions. Confor-
mational entropy is reduced by interactions that rigidify structure, associated with
independent constraints. Here, we solve the DCM using a mean-field treatment
that assumes distance constraints are well distributed throughout the structure,
meaning a distance constraint is independent until the structure is globally rigid.
Experimental heat capacity curves are described markedly well with a few adjustable
parameters. The universal character of this theory is analogous to the van der Waals
model for a liquid-gas transition. This work is supported by NIH R01 GM073082.