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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 interactions into distance constraints having energy and entropy contributions. Conformational 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.

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