

Abstract Submitted  
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**Correlation functions of flexible macromolecules<sup>1</sup>** DONALD JACOBS, DENNIS LIVESAY, OLEG VOROV, UNC at Charlotte — We present an ab initio calculation of conformational entropy, radii of gyration, X-ray and neutron scattering form-factors, correlation functions, and other observables describing proteins, polypeptides, nucleic acids, related macromolecules and artificial polymers [1]. The analytic form of the method minimizes computational costs and reveals relations between observables. We apply these methods to study thermodynamics of protein unfolding. The presented results agree with the results from experiment and simulation [2].

[1] O.K.Vorov, A.Y.Istomin, D.R.Livesay, D.J.Jacobs, *subm. to Phys.Rev.Lett.*, 2007. [2] O.K.Vorov, D.R.Livesay, D.J.Jacobs, *to be subm. to Proc. Natl. Acad. Sci.*, 2007, in preparation.

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