

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Solvable model of mechanical unfolding of biopolymers<sup>1</sup>** DONALD JACOBS, DENNIS LIVESAY, OLEG VOROV, UNC at Charlotte — We present exact analytical results for a hairpin to coil transition induced through mechanical pulling of dsDNA or peptides (beta-hairpin) within a distance constraint model [1], taking into account geometry of conformations. Starting from ab initio considerations, the configuration partition function is calculated exactly. Among other thermodynamic response functions, an expression for the end-to-end extension as a function of the applied force at a given temperature is derived. Our theoretical results agree well with data from single-molecule stretching experiments [2]. The employed method is general, and promises to remain a tractable computational approach when applied to larger, more complicated macromolecules. This work is supported by NIH R01 GM073082.

[1] O.K. Vorov, D.R. Livesay and D.J. Jacobs, ENTROPY, v.10 (3) 285-308 (2008).  
[2] O.K. Vorov, D.R. Livesay and D.J. Jacobs, to be subm. to Phys. Rev. Lett., in preparation.

<sup>1</sup>This work is supported by NIH R01 GM073082.

Oleg Vorov  
UNC at Charlotte

Date submitted: 14 Dec 2009

Electronic form version 1.4