Book Review: Statistical Mechanics and Stability of Macromolecules

Statistical Mechanics and Stability of Macromolecules. Earl Prohofsky, Cambridge University Press, Cambridge, 1995.

This is a compendium of recent work by Prohofsky and his collaborators on different aspects of bond disruption, base pair separation, melting, and drug dissociation of DNA. It contains a thorough exposition of the effective harmonic bond theory coupled to a Bogolyubov–Feynman variational Ansatz that forms the core of Prohofsky's approach to the statistical mechanical analysis of the subject. The book is not, however, meant to be an introduction of the method, so all the technical details are conveniently relegated to the appendices. They are nevertheless sufficiently detailed so that the interested reader will find them a good starting point to actually learn something about the method itself.

In general the book is well written, but I had immense problems with the discussion of bounded interaction potentials in Chapter 2. It is argued that the boundedness of the molecular bond potentials leads to the conclusion that the dissociated state is the equilibrium state. I cannot generally concur with this conclusion. There are in fact two parts to this problem, one connected with the practical simulation of systems with particular intermolecular potentials and the other one being a fundamental issue in statistical mechanics. First, in any simulation done in an infinite space the entropy is eventually going to win except if one is dealing with singular potentials (e.g., point charge particles). One therefore has to make the system finite, usually by introducing some brute force boundary as in standard cell models. The author's reasoning applies to such situations. As for the fundamental statistical mechanical problem, there is, in fact, none because of the way the statistical limit is taken, i.e., the volume of the system as well as the number of the particles approach infinity in such a way that the density is kept fixed. This means that the effective volume available to each particle is finite and the maximal entropy therefore remains a bounded quantity.

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Most of the book is devoted to the analysis of specific problems connected with DNA conformations and interactions. The main idea in these sections is to use effective harmonic potentials where the harmonic force constants are determined variationally from real (i.e., nonharmonic) potentials. The whole procedure is very close to the original Feynman-Kleinert variational principle, which is applicable to both quantum mechanical and polymer problems. The main thrust of Prohofsky's work is that of describing a variety of phenomena such as bond disruption, conformational changes in DNA, and interactions between the DNA helix and various other molecules in the language of phonons. In this framework different phonon characteristics such as mean square displacement or bond length probabilities are used as descriptors of the conformational transitions of the helix or interactions with other probe molecules.

This program ultimately leads to a quite sophisticated analytical undertaking. One is surprised to see how such complicated phenomena as the cutting and splicing of the DNA helix can be formulated in the language of harmonic vibrations. I believe it is at present not completely clear what the impact of this work is going to be on current models in molecular biology or biopolymer physics in general. One can safely assume that, as with any other theory presently on the scene, the comparison of theoretical results with experimental data will decide on the ultimate utility of this type of analysis.

> Rudi Podgornik Laboratory of Structural Biology Division of Computer Research and Technology National Institutes of Health Bethesda, Maryland 20892