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Physica A 224 (1996) 279–286

PHYSICA A

Protein folding and spin glass

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Abstract

We explicitly show the connection between the protein folding problem and spin glass transition. This is then used to identify appropriate quantities that are required to describe the transition. A possible way of observing the spin glass transition is proposed.

1. Introduction

Proteins are linear polymers, resulting from the joining of tens to thousands of monomer units (amino acids), in a repeating chain, called polypeptide chain or "backbone chain". This sequence of monomers is also known as the "primary structure". A typical protein would have a few hundreds of amino acids, from a choice of 20 amino acids. This would result in an astronomical number of conformations. Under appropriate circumstances, the chain folds into a close-packed globule like structure. This is the working (functional) protein, known as tertiary structure or the native structure. If a protein has to explore all the possible configurations to reach its biologically active form, then the time required would be $\sim 10^{10}$ years compared to the real situation, which is of the order of few milliseconds to few seconds [1]. This is the Levinthal paradox, whose resolution seems to hinge on the similarities between this biologically important problem and the concept of a rugged free energy landscape of a spin glass in condensed matter physics [2,3]. Attempts have also been made to study the dynamics directly, but so far these are necessarily restricted to small chains. Our purpose in this paper is to establish the connection with the spin glass quantitatively, and thereby identify the appropriate quantities that one should look at in experiments.

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SSDI 0378-4371(95)00325-8