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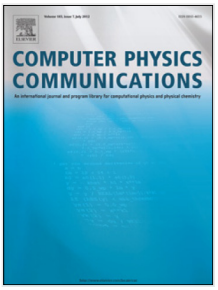

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Efficient algorithm for computing exact partition functions of lattice polymer models

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Abstract

Polymers are important macromolecules in many physical, chemical, biological and industrial problems. Studies on simple lattice polymer models are very helpful for understanding behaviors of polymers. We develop an efficient algorithm for computing exact partition functions of lattice polymer models, and we use this algorithm and personal computers to obtain exact partition functions of the interacting self-avoiding walks with N monomers on the simple cubic lattice up to $N = 28$ and on the square lattice up to $N = 40$. Our algorithm can be extended to study other lattice polymer models, such as the HP model for protein folding and the charged HP model for protein aggregation. It also provides references for checking accuracy of numerical partition functions obtained by simulations.

Keywords: Lattice polymer; Exact enumeration; Interacting self-avoiding walk; Complex polymer system

1. Introduction

The purpose of statistical mechanics is to understand the macroscopic behavior of a system from interactions of its microscopic components. Sta-

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