Multicanonical Monte Carlo ensemble growth algorithm

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We present an ensemble Monte Carlo growth method to sample the equilibrium thermodynamic properties of random chains. The method combines two elegant techniques: the ensemble (breath-first) growth and the Wang-Landau sampling, for computing the density of states of a polymer chain in the energy space. The density of states is the central quantity for computing all the microcanonical and canonical thermodynamic quantities, including the free energy, entropy, and thermal averages. The algorithm was validated against exact enumeration and numerical results for several well-studied cases, and employed to confined polymers. One of the notable benefits of the new algorithm is that it can be easily parallelized across multiple nodes, relaxing the memory constraints imposed by other breath-first algorithms.
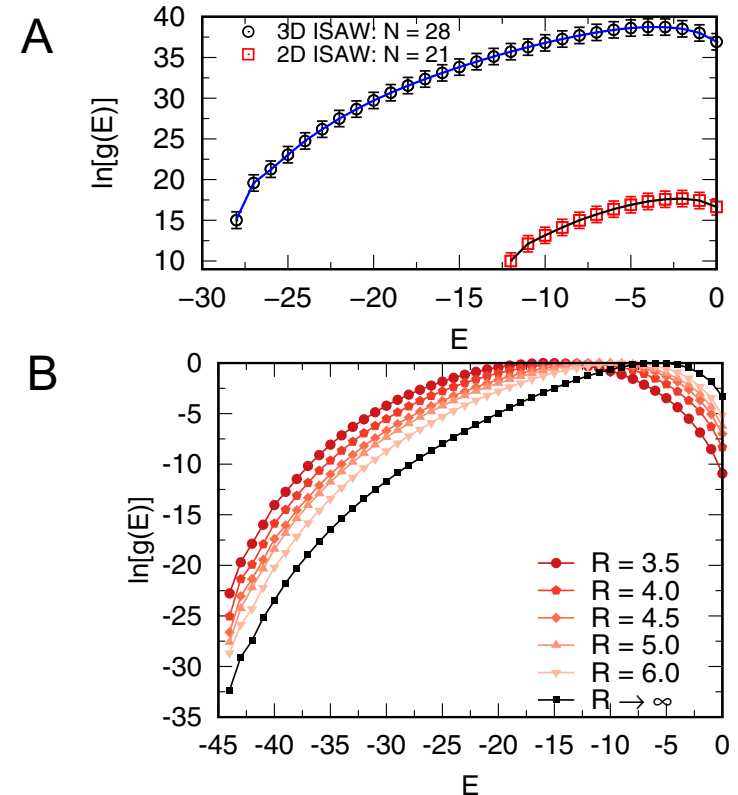
A) Density of states, g(E), for a N = 28-mer interacting self-avoiding walk (ISAW) chain on a 3D cubic lattice, and N = 21-mer ISAW on a 2D square lattice. Solid black lines are exact values from enumeration.

B) Density of states of a 40-mer ISAW confined in a spherical cavity of radius R (in the unit of lattice spacing).

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