Resource-efficient Quantum Algorithm for Protein Folding

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Summary

The study presents a quantum algorithm for addressing the protein folding problem on a regular tetrahedral lattice, which involves predicting the three-dimensional structure of a protein based on its amino acid sequence. Traditional protein folding solutions using classical computers, even with the Hydrophobic-Polar model, have been resource-intensive due to the NP-hard complexity of the problem. This research proposes a quantum variational method to represent and simulate the folding of protein chains on a lattice. A model Hamiltonian, scaling at $O(N^4)$, was developed, which reflects many of the protein's physicochemical properties, bridging the gap between granular and mere lattice models. The paper demonstrates the algorithm's effectiveness by simulating the folding of two proteins: a 10-amino acid protein called angiotensin and a 7-amino acid peptide.

Limitations

1. **Limitation in Side Chain Length**: The algorithm currently supports side chains of lengths up to 1 amino acid. This limitation restricts its applicability to proteins with relatively simple side-chain structures.

2. **Simplified Interactions for Side Chains**: While the algorithm utilizes the Miyazawa-Jernigan interaction and a random interaction for the main chain, it employs a simplified random interaction (random value between -5 and -1) for side chains. This approach might only partially capture the complexities of side-chain interactions in some proteins.