Generating Generalised Ground-State Ansatzes from Few-Body Examples

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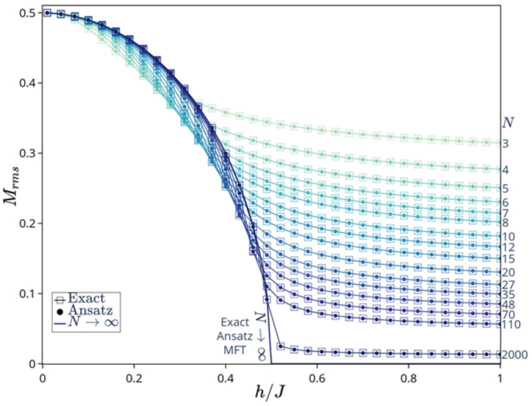
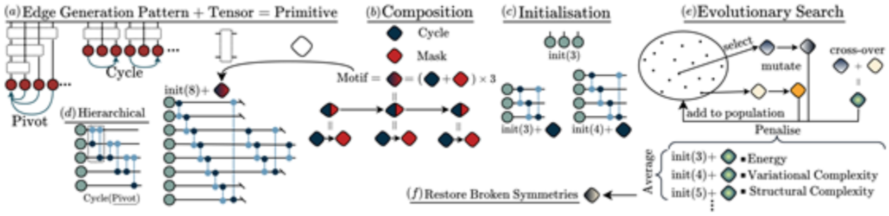
We present a systematic approach to ansatz design for quantum many-body problems. The approach is based on a custom symbolic language that compactly encodes modular, size-scalable, and hierarchically composable wavefunction structures. With this language, evolutionary search can be carried out on few-body instances, yet the resulting wavefunctions extrapolate to arbitrary system sizes without modification. This enables efficient fitness evaluation and the capture of robust wavefunction structures. Applied to ground-state problems, the method autonomously rediscovers a mean-field description and extends it to incorporate correlations, producing simple, interpretable wavefunctions that remain analytically tractable. For both the Lipkin-Meshkov-Glick model and the transverse-field Ising model, the search converges on the same compact, two-parameter ansatz [1], showcasing its ability to identify network structures with some degree of universality. Owing to its structure, we obtain closed-form expressions for the expectation values of local observables as well as for correlation functions. We find that this ansatz effectively encodes correlations, captures finite-size effects, accurately predicts ground-state energies, and offers a good description of critical phenomena. The core of our approach lies in the interplay between the symbolic language and the fitness criteria. The former enables fitness evaluation on small system sizes, which is computationally efficient and allows the capture of system-size scaling. The latter favours ansatzes with low variational and structural complexity while preserving accuracy. This results in expressive ansatzes which tend to break the underlying model's symmetries, but due to their simple structure, these symmetries can be restored analytically, thus providing a systematic way to improve the ansatz. Beyond ground-state problems, our approach can be applied to any physical system that is amenable to a variational treatment in terms of tensor network states. For example, finding time evolution approximations would entail a train-by-example strategy. In the context of quantum algorithm design, we use such a strategy and show that our framework is able to automatically generate the N-qubit realisations of popular quantum algorithms (Deutsch–Jozsa, QFT, Grover) by considering only examples up to five qubits [2]. Applied to quantum phase recognition, we show that it discovers an ansatz that outperforms a commonly used architecture [3] while reducing the number of required variational parameters by two orders of magnitude.





References

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