Contribution ID: **51** Type: **Oral Presentation**

Effects of virtual gauge degrees of freedom in the variational optimization of projected entangled pair states

Projected entangled-pair states (PEPS) constitute a powerful variational ansatz for two-dimensional quantum systems, but accurately computing and minimizing the energy expectation value remains challenging. A recent work [Tang et al., Phys. Rev. B 111, 035107 (2025)] showed that virtual gauge degrees of freedom can significantly affect the accuracy of tensor network contractions, raising questions about their impact on PEPS optimization. In this work, we consider a U(1)-symmetric PEPS with point group symmetry, reducing the gauge degrees of freedom to a single class, which enables an efficient manifold optimization scheme that fixes the gauge throughout the optimization. Applying this method to the prototypical Bose-Hubbard model, we find that the gradients during unconstrained PEPS optimization typically contain components along gauge directions, causing the tensor network contraction to become increasingly inaccurate and producing artificially low variational energies. In contrast, in gauge-fixed PEPS optimization, this effect can be largely suppressed, resulting in a more robust and reliable optimization. Our study paves the way for future efforts to systematically increase the robustness and reliability of PEPS optimization in general settings.

Author: TANG, Wei (Ghent University)

Co-authors: HAEGEMAN, Jutho; VANDERSTRAETEN, Laurens (Université Libre de Bruxelles)

Presenter: TANG, Wei (Ghent University)

Session Classification: B - Contributed Talk