Quantum Computing for Dispersion Bands of Phononic Crystals

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Abstract

Investigating the vibro-elastic dispersion relations of architected materials presents a significant challenge due to the complex interplay between the material's microstructure, inherent physical properties, and wave propagation characteristics. We present dispersion band predictions for architected materials using the Dual-Adapt framework, which integrates adaptive ansatz and adaptive penalty with the Variational Quantum Deflation (VQD) method. Our algorithm (Dual-Adapt-VQD) significantly improves the accuracy of predictions for multiple high-lying excited states, marking a pivotal step in equipping the metamaterials research community for the forthcoming quantum computing era.

Main Objectives

- Improving VQD performance for circuit efficiency and convergence rate.
- Circumventing the ADAPT-VQE pipeline w.r.t. growing-depth operators and steepest descent of cost function gradient.
- Adjusting the penalty factors without prior knowledge of state gaps in the studied system.

Reference

[1] Y. Liu, J. Liu, J. R. Raney, and P. Wang. Quantum computing for solid mechanics and structural engineering–a demonstration with variational quantum eigensolver. *Extreme Mechanics Letters*, 67:102117, 2024.

Acknowledgements

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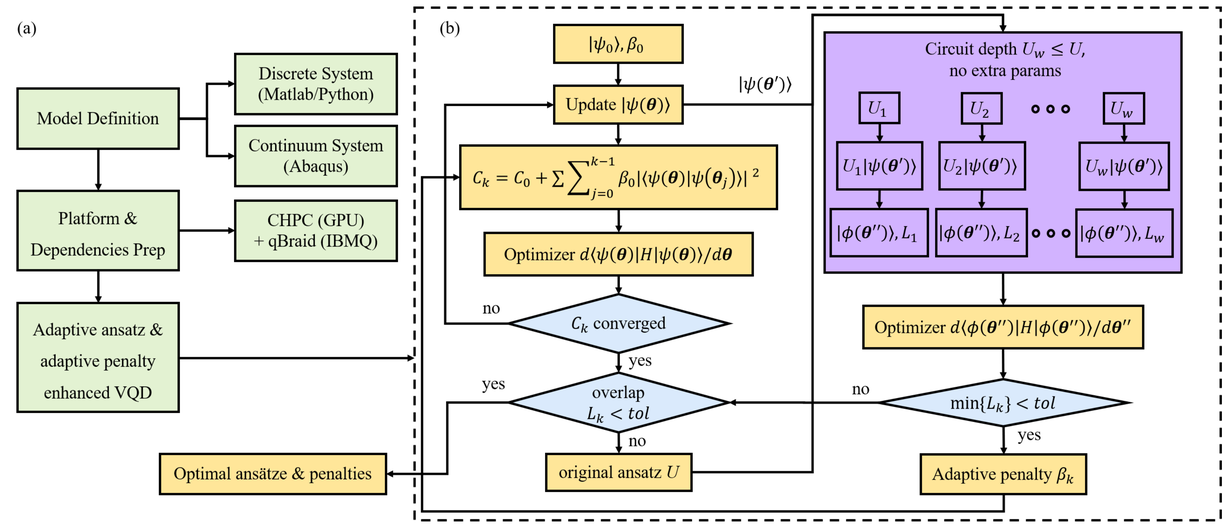
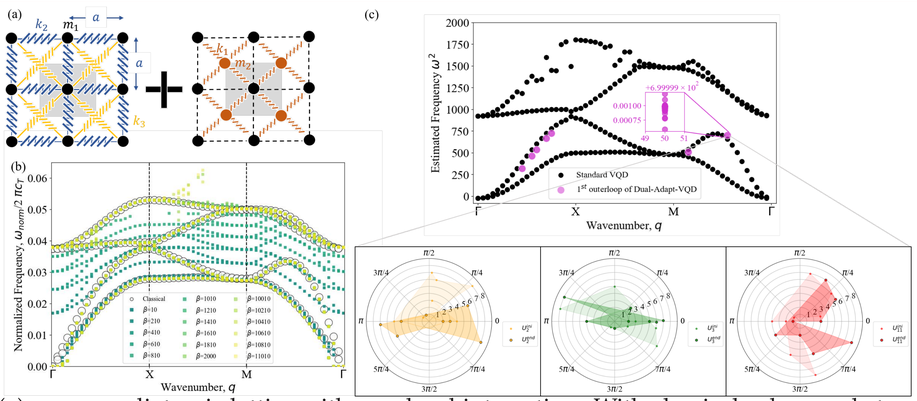
Method



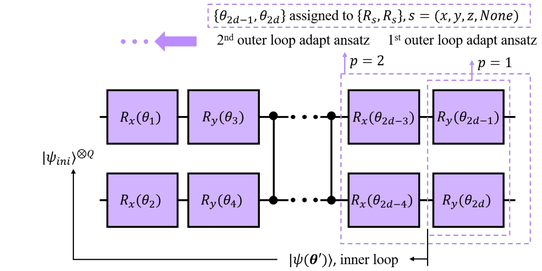
With the reliable adaptive ansatz U_w, orthogonality between excited state $|\psi(\boldsymbol{\theta}_k)\rangle$ and the previously determined states $|\psi(\boldsymbol{\theta}_0)\rangle, ..., |\psi(\boldsymbol{\theta}_{k-1})\rangle$ for k-th excited level are ensured, achieving a user-specified tolerance of $tol = 1e\text{-}6$. By applying the filter process for the minimum overlap $\min(\bar{L}_k)$, we obtain the expectation values C_k and C_{k-1}, as well as the penalty factor $\beta_k = (C_k - \sum C_{k-1})/\min(\bar{L}_k)$.

Example & Initial Prediction



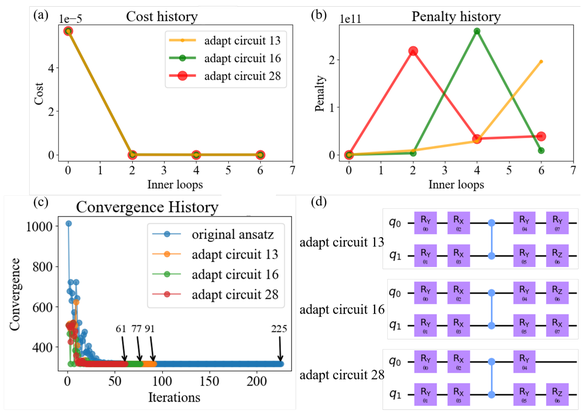
The model is (a) a square diatomic lattice with non-local interaction. With classical solver and standard VQD, we obtain the dispersion bands (b) with user-defined penalty factors. Further, we implement the Dual-Adapt-VQD algorithm. The highlighted (purple) scatters denote orthogonal eigenstates from parameter space (shallow: before optimization, dark: after optimization) of reliable adaptive ansätze U_2, U_3, and U_{11} when wavenumber $p = 51$.

Dual-Adapt-VQD Improvement



At each wavenumber p, our goal is to obtain all precise excited states. For the k-th state, if orthogonality with lower states is not achieved, we adaptively reconstruct quantum ansätze by exploring all possible gate sequences and parameter assignments in the last k layers. Parameter optimization is facilitated through multiple inner loops for each ansatz, while the outer loops search for higher excited states.

As an example, we present the Dual-Adapt-VQD improvement for 1^{st} excited state regarding overlaps, penalty factors, and convergence rate at $p = 9$.



Conclusions

- Adaptive circuits improve the dispersion band predictions with high-fidelity orthogonal states.
- Optimal ansatz adapts precise penalty for deflation with efficient circuit depth and higher convergence rate.
- Available for high-lying states prediction in arbitrary architected materials.