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Hybrid Quantum-Classical Strategy for Spectra Computation

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We introduce a hybrid classical–quantum algorithm designed to efficiently compute molecular spectra. Our approach combines classical methods with sample-based quantum diagonalization, using snapshots of the quantum system's evolution at selected times we construct a tailored subspace. By integrating these classical techniques with a post-evolution sampling strategy, we effectively capture the dominant dynamical features of molecular excitations. This strategy enables the accurate estimation of spectral quantities with limited resource demands and enhanced robustness against quantum noise, paving the way for scalable simulations of complex molecular systems.

Presenter: SANTINI, Alessandro (CPHT, Ecole Polytechnique)