Quantum Computational Models of Brain-Wide Functional Connectivity

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Abstract—Modeling brain-wide functional connectivity remains one of the central challenges in computational neuroscience due to the enormous dimensionality, nonlinearity, and dynamical complexity of neural interactions. Classical network models, while effective for localized circuits, struggle to capture long-range dependencies, cross-frequency coupling, and emergent global patterns across billions of neurons and trillions of synapses. Quantum computational approaches offer a promising new direction by exploiting superposition, entanglement, and high-dimensional quantum state representations to encode whole-brain connectivity more efficiently. This study proposes a quantum-enhanced framework for modeling large-scale functional connectivity using hybrid quantum-classical graph algorithms, variational quantum neural models, and quantum kernel-based similarity mapping. By encoding temporal neural signals into quantum states and performing state-space exploration with variational circuits, the framework aims to reveal latent connectivity patterns, global synchronization structures, and cross-network dynamics that classical methods often fail to identify. Early simulation results suggest improved sensitivity to weak long-range interactions and enhanced ability to detect dynamic functional modules. The proposed approach highlights the transformative potential of quantum computation in advancing systems-level neuroscience, enabling more accurate whole-brain models and opening new opportunities for understanding cognition and neurological disorders.

Understanding brain-wide functional connectivity remains one of the most complex challenges in contemporary neuroscience. Despite significant progress in neuroimaging, network science, and computational modeling, conventional approaches often struggle to capture the high-dimensional, nonlinear, and temporally dynamic interactions that govern large-scale brain activity [4]. Functional connectivity networks—derived from modalities such as fMRI, EEG, MEG, and diffusion imaging—encode intricate patterns of synchronization, causal influence, and modular organization [7]. However, modeling these networks with classical computational methods

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becomes computationally prohibitive as data volume increases and as researchers seek more biologically realistic models that incorporate multiscale structure, temporal coupling, and stochastic variability.

Recent advances in quantum computing offer an unprecedented opportunity to rethink the mathematical and algorithmic foundations of brain connectivity modeling. Quantum computational frameworks leverage superposition, entanglement, and exponentially large Hilbert spaces, enabling the representation of complex correlations that are difficult or impossible to encode classically [3]. These characteristics align closely with the inherent complexity of neural systems, where distributed interactions, emergent patterns, and multi-level