Contribution ID: **57** Type: **ORAL**

On the Feasibility of Solving the Time Independent Schrödinger Equation using Neural Network and Block Form with Rayleigh Quotient Loss Function

Wednesday, April 1, 2026 3:30 PM (20 minutes)

In the HBCU Chips 2025 conference, M.R. Hadizadeh, B. Sarker, and M.A. Khan presented an approach for solving 1D quantum systems using machine learning. Here, we present a discussion and feasibility consideration of numerical methods for computing multiple eigenpairs of Hamiltonian matrix $A \in \mathbb{R}^{n\times n}$ using a block formulation of the Rayleigh quotient in either Python or Julia in a closely related problem. This approach reformulates the classical eigenvalue problem $A\mathbf{v} = \lambda\mathbf{v}$ into a block structured optimization framework. This block formulation may enable simultaneous computation of multiple eigenpairs and provide enhanced numerical stability through the use of structured matrix operations. The method will attempt to leverage the geometric properties of the Rayleigh quotient in block space, where the gradient and Hessian structure are exploited for efficient optimization. The proposed technique discussed may combine elements of the Rayleigh quotient iteration with possible block Krylov subspace methods, towards achieving convergence rates compared to traditional power iteration approaches for small blocks. The algorithm's computational complexity is considered and may scale favorably with problem dimensions, particularly for computing the k smallest eigenpairs. Numerical experiments will be discussed.

Academic or Professional Status

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Session Classification: Technical Session 2

Track Classification: Education & Workforce Development