Adaptive Majorana-Neural Propagation for Non-Hermitian Quantum Many-Body Dynamics

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Abstract

We propose the **Adaptive Majorana-Neural Propagation (AMNP)** framework, unifying autoregressive neural quantum states with Majorana string truncation for simulating **non-Hermitian** strongly correlated fermionic systems. The framework addresses three fundamental gaps in current methods: (1) the optimizer incompatibility between Stochastic Reconfiguration and RNN wave functions, (2) Majorana truncation rules breaking for non-Fock variational states, and (3) restriction of fermionic neural Gibbs states to Hermitian closed systems. We introduce three novel algorithmic contributions: **Geometry-Aware Stochastic Reconfiguration (GASR)**, **Non-Hermitian Trotter-Consistent Truncation (NHTCT)**, and **Thermofield-Extended Neural Gibbs States (TENGS)**. These innovations enable accurate simulation of dissipative Fermi-Hubbard dynamics, non-Hermitian kagome lattices, and open-system quantum transport beyond existing classical methods.

1 Introduction and Motivation

Neural quantum states (NQS) have emerged as powerful variational representations for quantum many-body systems [1,2]. Recent advances demonstrate that recurrent neural network (RNN) wave functions achieve state-of-the-art accuracy for frustrated spin systems [3], while Majorana string propagation enables efficient 2D fermionic dynamics simulation [4]. Simultaneously, fermionic neural Gibbs states capture finite-temperature correlations in doped Fermi-Hubbard models [5]. However, critical limitations prevent these methods from addressing **non-Hermitian** quantum systems—central to dissipative dynamics, quantum transport, and open quantum systems.

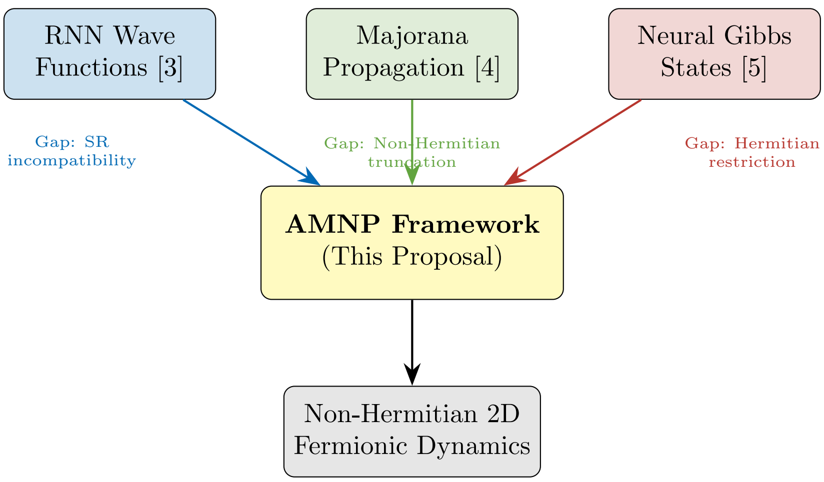

Figure 1: Research landscape: AMNP unifies three recent advances while addressing their identified limitations.

2 Problem Statement and Identified Gaps

2.1 Gap 1: Optimizer Incompatibility in Autoregressive NQS

Recent work on kagome lattice Rydberg arrays [3] demonstrates that "*Stochastic Reconfiguration is not as effective as Adam optimizer when applied to RNN wave functions*." The quantum geometric tensor $S_{kk'} = \langle \Delta O_k^* \Delta O_{k'} \rangle$ becomes ill-conditioned for autoregressive architectures due to sequential sampling correlations, causing convergence instabilities.

2.2 Gap 2: Majorana Truncation for Non-Hermitian Systems

The Majorana string propagation framework [4] introduces Trotter-consistent truncation: discard strings with unpaired Majoranas $w_s(v) > S$. However, this assumes **Fock-state initial conditions**—the overlap condition $\langle n_1 \cdots n_N | \mu(v) | n_1 \cdots n_N \rangle \neq 0$ requires $v_{2k-1} = v_{2k}$. For variational initial states or non-Hermitian Hamiltonians with complex eigenvalues, these truncation rules fail to preserve Trotter accuracy.

2.3 Gap 3: Hermitian Restriction in Neural Thermal States

The fermionic neural Gibbs states [5] achieve accurate thermal energies via thermofield-double purification with work-operator evolution. However, the framework assumes Hermitian Hamiltonians: $W = \hat{H} \otimes \tilde{I} - \frac{\beta_0}{\beta} \hat{I} \otimes \tilde{H}_0$. Extensions to "*real-time dynamics and non-Hermitian steady states require new theoretical frameworks*" [5].

3 Proposed Innovations

3.1 Geometry-Aware Stochastic Reconfiguration (GASR)

We propose an adaptive optimizer interpolating between curvature-aware (SR) and first-order (Adam) updates based on gradient signal-to-noise ratio:

$$G_{\text{GASR}} = (1-\alpha)S + \alpha J^T J + \lambda I \tag{1}$$

where S is the quantum geometric tensor, J is the Jacobian of log-amplitudes, and $\alpha = \sigma(\log \rho - \tau)$ adapts based on effective signal-to-noise $\rho = \|g\|^2 / \text{Var}[g]$.

Algorithm 1 Geometry-Aware Stochastic Reconfiguration (GASR)

Require: Ansatz $|\psi_\theta\rangle$, learning rate η, threshold τ

1: Sample configurations $\{x_i\}_{i=1}^{N_s}$ from $|\psi_\theta|^2$
2: Compute local energies $E_{\text{loc}}(x_i) = \langle x_i | \hat{H} | \psi_\theta \rangle / \psi_\theta(x_i)$
3: Compute gradient $g_k = \langle O_k^* (E_{\text{loc}} - \langle E \rangle) \rangle$
4: Estimate SNR: $\rho \leftarrow \|g\|^2 / \text{Var}[g]$
5: Adaptive interpolation: $\alpha \leftarrow \sigma(\log \rho - \tau)$
6: Construct $G_{\text{GASR}} = (1-\alpha)S + \alpha J^T J + \lambda I$
7: Update: $\theta \leftarrow \theta - \eta \cdot G_{\text{GASR}}^{-1} g$
8: **return** Updated parameters θ

3.2 Non-Hermitian Trotter-Consistent Truncation (NHTCT)

For non-Hermitian Hamiltonians $H = H_{\text{Herm}} + i\Gamma$, complex eigenvalues cause exponential growth/decay. We introduce **decay-bounded truncation**:

$$\text{Truncate if: } w_s(v) > S \text{ OR } |\text{Im}[\lambda_v]| > \Gamma_{\max} \tag{2}$$

where $\Gamma_{\max} = -\frac{1}{\delta\tau} \ln(\epsilon_{\text{Trotter}})$ ensures truncation errors remain within Trotter accuracy.

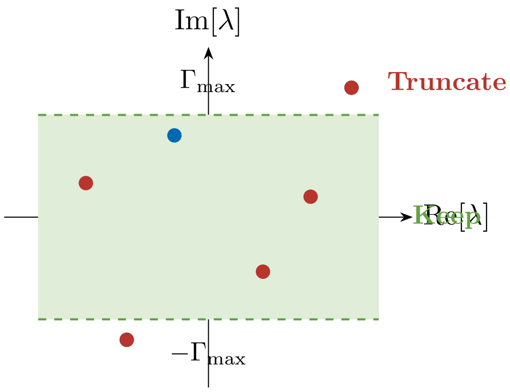

Figure 2: NHTCT eigenvalue truncation in complex plane. Strings with eigenvalues outside $[-\Gamma_{\max}, \Gamma_{\max}]$ are pruned.

3.3 Thermofield-Extended Neural Gibbs States (TENGS)

We extend the work operator to non-Hermitian systems:

$$W_{\mathrm{NH}} = \hat{H} \otimes \tilde{I} - \frac{\beta_0}{\beta} \hat{I} \otimes \tilde{H}_0 + i\Gamma \otimes \tilde{I} \tag{3}$$

The dissipator Γ captures particle loss, gain, or dephasing. Imaginary-time evolution via Taylor-root expansion projected ITE (tre-pITE) [5] generalizes to complex-time contours.

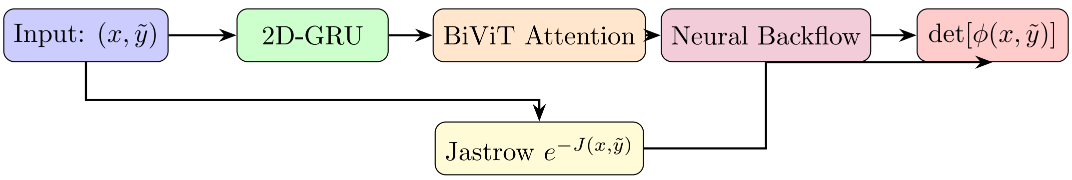

Figure 3: TENGS neural architecture: BiViT attention captures inter-species correlations between physical and auxiliary fermions.

Algorithm 2 TENGS Evolution for Non-Hermitian Systems

Require: Mean-field state $|\Psi_0(\beta_0)\rangle$, target β, dissipator Γ

Initialize pair orbitals $\phi \leftarrow \phi_0$ from mean-field
Construct work operator $W_{\mathrm{NH}} = \hat{H} \otimes \tilde{I} - \frac{\beta_0}{\beta} \hat{I} \otimes \tilde{H}_0 + i\Gamma \otimes \tilde{I}$
for $\tau = 0$ to $\beta/2$ by $\delta\tau$ **do**
    Sample $(x, \tilde{y}) \sim |\Psi_\theta|^2$
    Compute fidelity gradient via tre-pITE [5]
    Update θ using GASR optimizer
end for
return Thermal state $|\Psi(\beta)\rangle$

4 Target Systems and Validation

Validation Protocol: Following variational benchmarks [1], we report v-scores comparing energy accuracy against exact diagonalization (small systems) and quantum Monte Carlo (where applicable). Correlation functions $C_{ss}(\mathbf{d})$ and structure factors $S(\mathbf{q})$ verify physical consistency.

Table 1: Target systems and comparison with existing methods

System	**AMNP**	**MPS/fPEPS**	**QMC**
Dissipative Fermi-Hubbard	✓	Limited	Sign problem
Non-Hermitian kagome	✓	×	×
Open-system transport	✓	1D only	×
Finite-T non-Hermitian	✓	×	×

5 Expected Contributions

1. **Theoretical:** First framework unifying NQS with non-Hermitian dynamics; complexity bounds for NHTCT; convergence analysis of GASR optimizer.
2. **Algorithmic:** Three novel algorithms (GASR, NHTCT, TENGS) with open-source NetKet implementation.
3. **Practical:** Benchmarks for dissipative 2D fermionic systems beyond tensor network capabilities; protocols for quantum simulator validation.

6 Conclusion

The AMNP framework addresses fundamental limitations in current neural quantum state methods by introducing geometry-aware optimization, non-Hermitian truncation schemes, and thermofield extensions to dissipative systems. This research will advance our capability to simulate strongly correlated fermionic dynamics in regimes inaccessible to existing classical methods, with direct applications to quantum materials, superconductivity, and quantum device physics.

References

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