

# ML-Based Error Mitigation Approach for Overcoming NISQ Hardware Constraints in Fermionic Nanoelectronic Simulations

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**Abstract**—Simulating time-evolution dynamics of nanoelectronic systems on Noisy Intermediate-Scale Quantum (NISQ) hardware suffers from severe decoherence and gate errors, was replicated using device-calibrated noise models. To improve approximation to noiseless dynamics, a Machine Learning-based Quantum Error Mitigation (QEM) strategy is proposed. Tested on an asymmetric 3-site quantum wire using device-calibrated noisy simulators, presented approach captures non-linear dynamics on an unseen noise profile with millisecond-scale training overhead, demonstrating the potential viability of ML-assisted quantum Electronic Design Automation (EDA).

**Keywords**—Quantum Computing, NISQ, Machine Learning, Quantum Error Mitigation, Post-processing

## I. INTRODUCTION

Simulating simplified nanoelectronic systems on quantum hardware is hindered by rapid decoherence and coherent gate errors. We model a single electron propagating through an asymmetric 3-site tight-binding system ( $J_1 = 1.0, J_2 = 0.5$ ). For quantum compilation, fermionic operators are mapped to qubits via the Jordan-Wigner transformation [1], yielding:

$$H = \frac{J_1}{2}(X_0X_1 + Y_0Y_1) + \frac{J_2}{2}(X_1X_2 + Y_1Y_2). \quad (1)$$

Implementing time evolution on gate-based quantum circuits requires approximating the exact operator via a Lie-Trotter-Suzuki decomposition. In the research, a Trotter step  $\Delta t = 0.4$  was employed as a practical baseline balancing algorithmic accuracy against hardware noise [2].

## II. ML-BASED MITIGATION AND RESULTS

To mitigate residual hardware errors, a classical post-processing QEM filter [3] is proposed. Radial Basis Function (RBF) Kernel Ridge Regression (KRR) was applied to learn an empirical correction mapping between noisy and ideal observables.

The approach utilized Qiskit’s noisy simulators parameterized by real device calibration data, training the model on 500 stochastically generated Hamiltonians using the FakeManilaV2 noise profile, and testing on an unseen configuration from FakeBelemV2.

Fig. 1 shows unmitigated noisy simulation drifting toward a highly mixed state. The QEM post-processing accurately reproduces the damped amplitude.

Tab. 1 shows a significant reduction in Mean Squared Error (MSE) and a consistent improvement in Classical Fidelity across all sites.

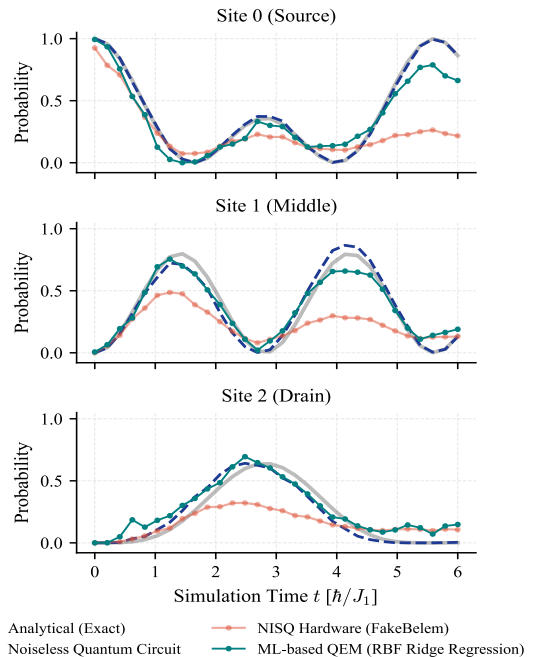


Fig. 1. Cross-backend testing results using the FakeBelem noise model. The ML-based QEM closely approximates the analytical signal from the degraded output.

TABLE I  
STATISTICAL METRICS FOR BASELINE AND QEM PERFORMANCE

Node	MSE (Noisy)	MSE (QEM)	MAE (Noisy)	MAE (QEM)	Fidelity (Noisy)	Fidelity (QEM)
Site 0	0.0916	0.0119	0.1958	0.0841	0.8875	0.9701
Site 1	0.0561	0.0053	0.1802	0.0588	0.9351	0.9869
Site 2	0.0271	0.0080	0.1203	0.0770	0.9546	0.9678

## III. CONCLUSION

Combining a practical Trotter baseline with a lightweight RBF-KRR QEM protocol successfully approximates physical electron dynamics from simulated, degraded NISQ outputs. This hybrid method bypasses physical error correction overhead, offering a potentially scalable pathway for future quantum EDA.

## REFERENCES

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