

SPIN CHEMISTRY SIMULATION VIA HYBRID-QUANTUM MACHINE LEARNING

Trevor J. Brokowski¹, Farhan T. Chowdhury², Luke D. Smith², Pedro Alvarez³, Samarth Sandeep⁴, Clarice D. Aiello¹

¹Department of Electrical and Computer Engineering, UCLA ²Department of Physics, University of Exeter ³Universidade Estadual de Campinas ⁴If and Only If Technologies

The radical pair mechanism can be simulated using NISQ methods

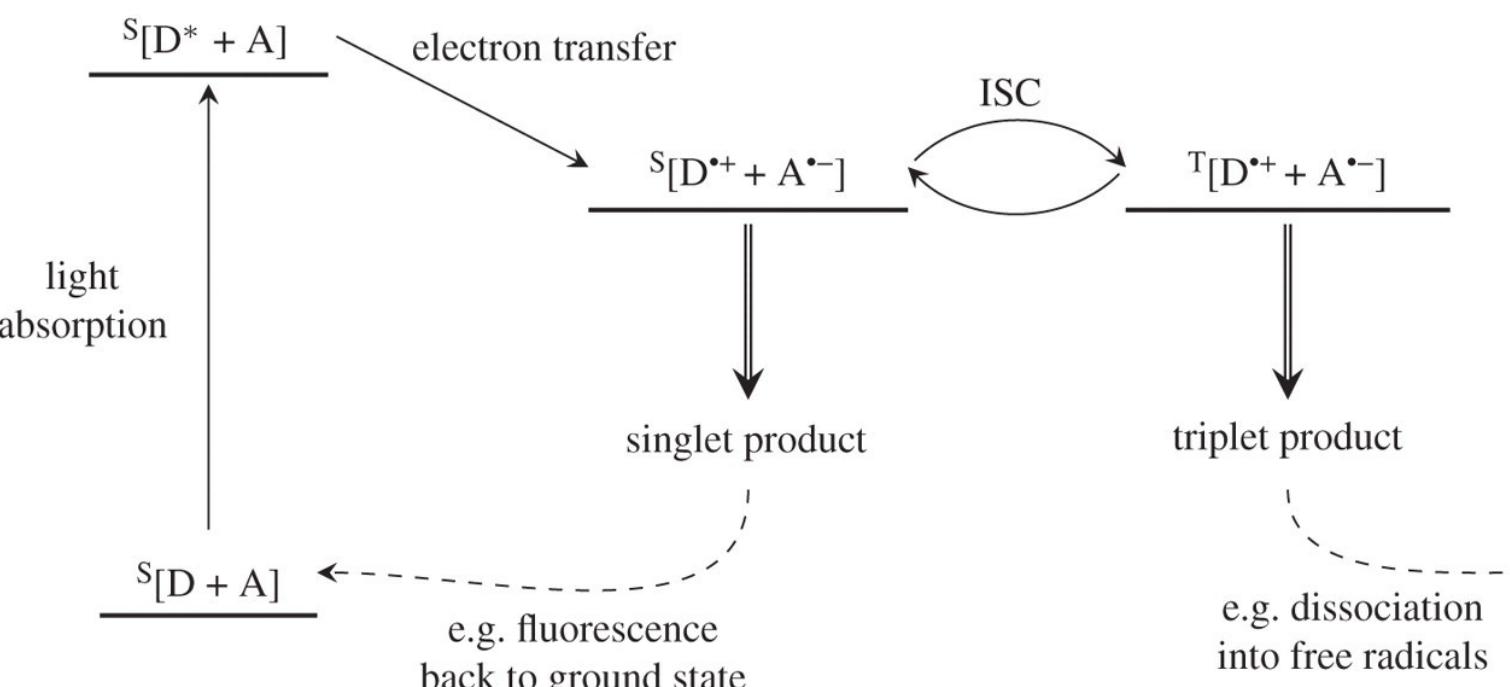


Fig. 1: Example Radical Pair System. Used with permission of The Royal Society (U.K.) from "Decoherence in the chemical compass: the role of decoherence for avian magnetoreception", Tiersch Markus and Briegel Hans J., Phil. Trans. R. Soc. A, **370**: 4517-4540, 2012; permission conveyed through Copyright Clearance Center, Inc.

The radical pair mechanism:

- Weak magnetic fields modulate the kinetics of radical recombination reactions.
- Underlies a variety of processes in spin chemistry and quantum biology.

However, in modeling the relevant processes, as the system scales in size by incorporating a greater number of electronic and nuclear spins, the system quickly reaches bottlenecks in current classical simulation capabilities. This makes spin chemistry systems ideal to probe and explore on noisy intermediate-scale quantum devices. To that end, we propose a hybrid quantum machine learning protocol to simulate an example toy radical pair spin system as a minimum working example.

Optimisation of the variational quantum Ansatz

Using the final singlet population yields as our training data, we employ a hybrid quantum machine learning protocol to simulate the time evolution of our radical pair system on a noisy quantum device. We construct a variational quantum ansatz with parameters representing the Zeeman and hyperfine interactions of the Hamiltonian and measure the expectation value of the singlet yields on the device. Parameters are classically optimized using both the Scipy gradient optimizer and a modified gradient-free Simultaneous Perturbation Stochastic Approximation (SPSA) protocol until the expectation value of the circuit is similar to singlet yields computed via the Lindblad Master Equation Solver, shown right. Through our procedure, we demonstrate that the Scipy 'classic' gradient optimizer is not sufficient in optimizing noisy quantum functions and that the noisy SPSA protocol is more accurate, immune to local minima, and faster than its classic counterpart.

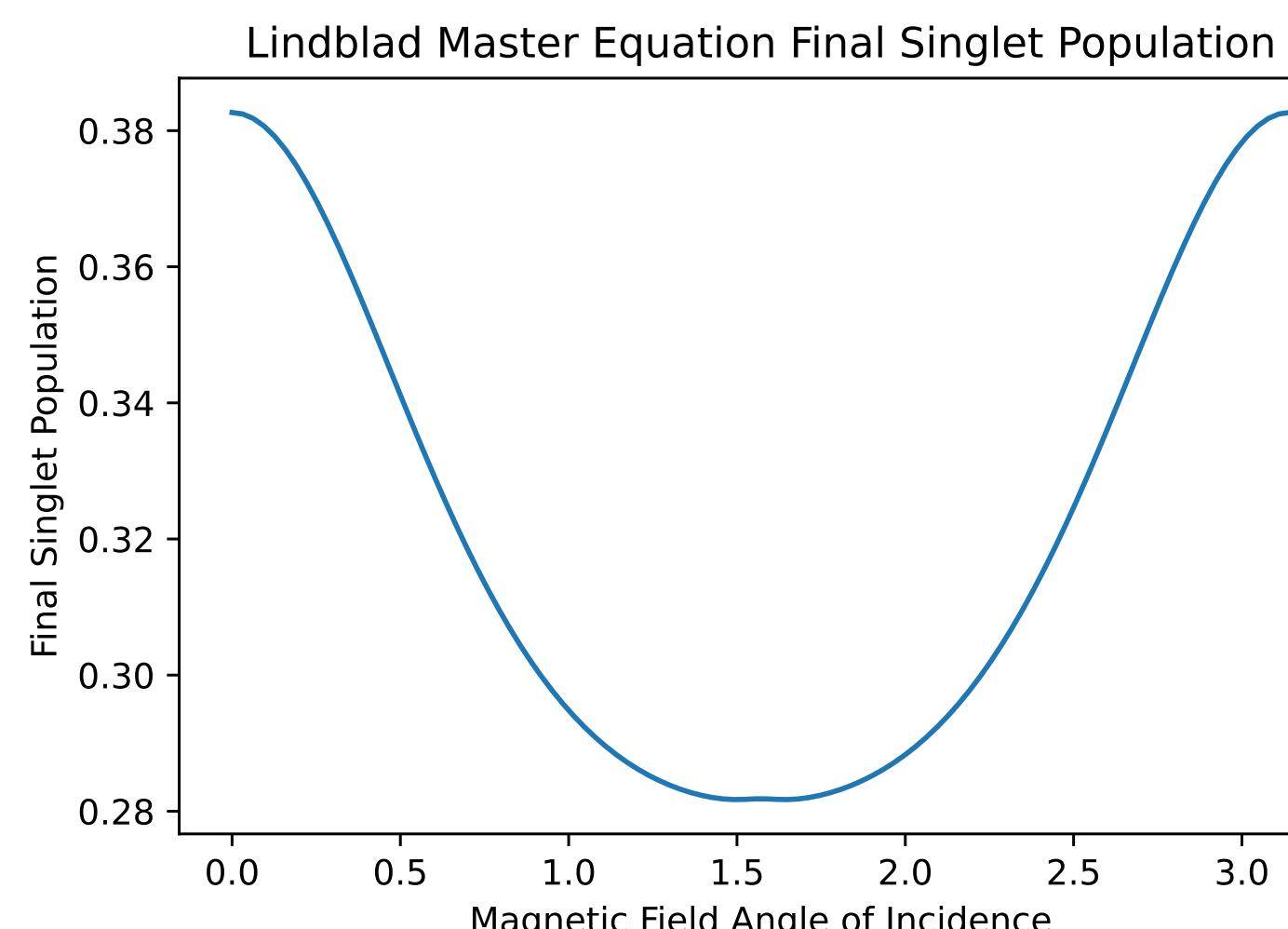


Fig. 2: Singlet yields obtained from Lindblad simulation – used to minimize the variational circuit.

Mapping the spin system Hamiltonian to a circuit simulable Hamiltonian

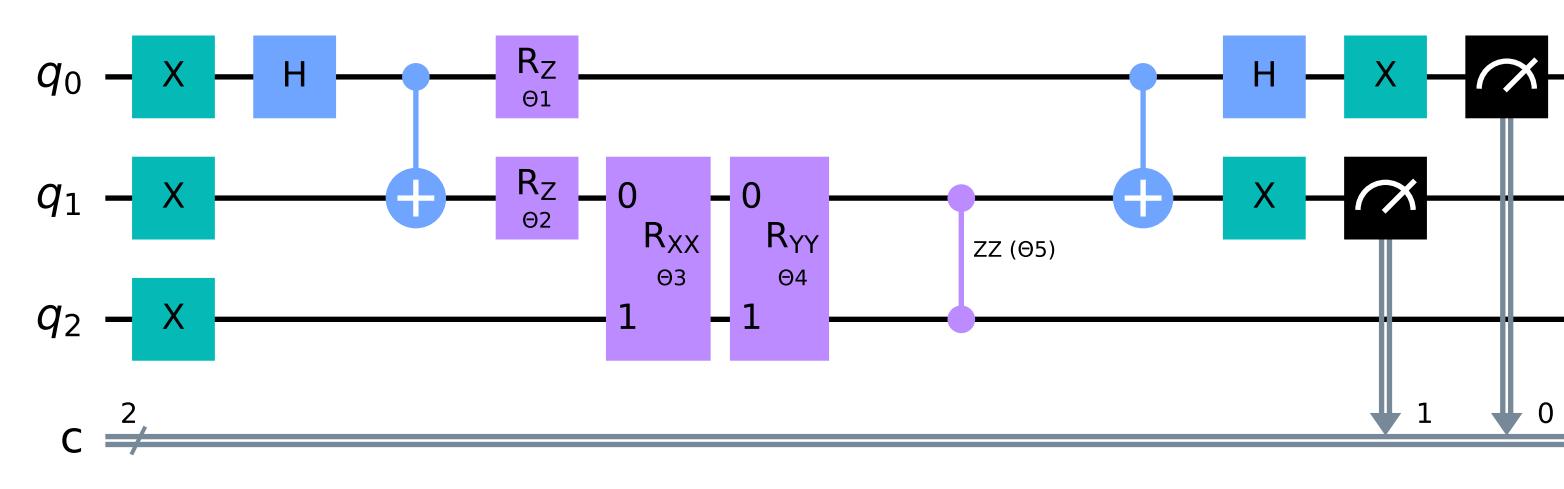


Fig. 3: Quantum Circuit with Nuclear Spin Down.

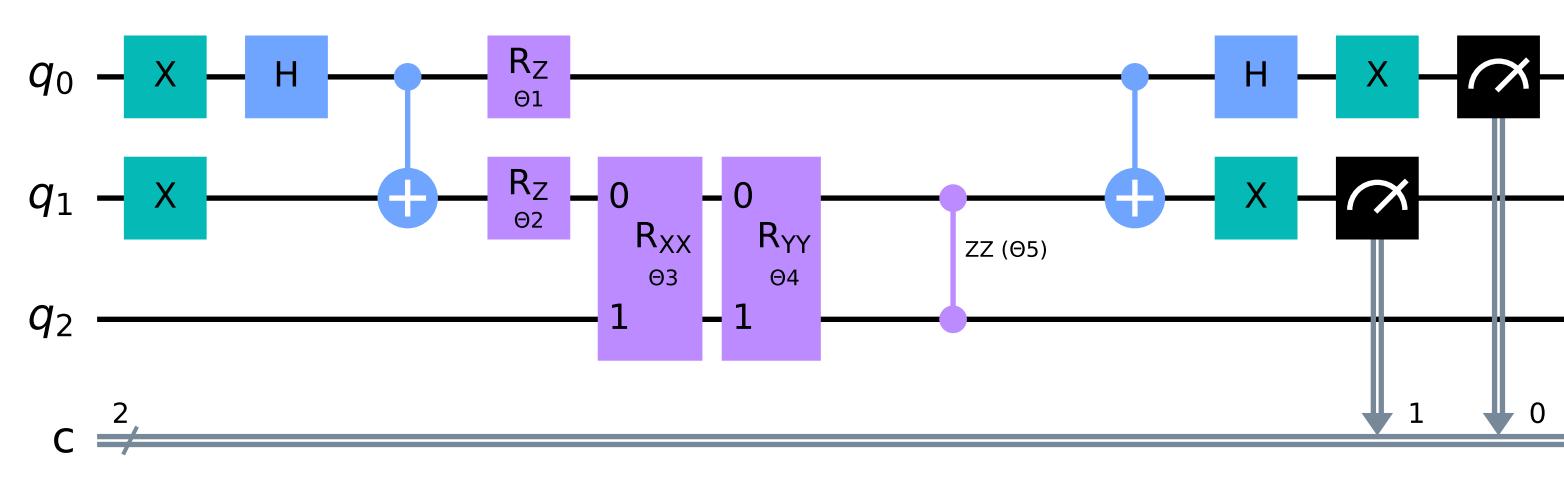


Fig. 4: Quantum Circuit with Nuclear Spin Up.

To map our spin system to a Hamiltonian that can be simulated in a quantum computer, we utilize a variational quantum circuit where we employ a series of rotations and use a hybrid quantum-classical method to obtain the final circuit representing the evolution of the system. We construct a 3-qubit circuit where q0 maps to \hat{e}_1 , q1 maps to \hat{e}_2 and q3 maps to I. We initialize the system in a singlet state, by applying gate operations to q1 and q2, then we employ a series of rotation gates that represent the Zeeman and hyperfine interactions. As the Zeeman interactions only affect the electron spins along the z-axis, we only apply a z-axis rotation gate. Then, as the nuclear hyperfine interaction can modulate the state of the electron spin along the x,y, and z axes, we apply an XX, YY, and an ZZ rotation gate that represents the interaction between the nuclear and electron spins. Then, we perform a measurement by applying the singlet initialiser gates in reverse and count the percentage of shots that result in '00', as that represents the final singlet population yield. Because the nuclear spin can either be up or down, we add the results from both circuits where one circuit has the nuclear spin up and the other with the nuclear spin down.

Model system

Our example system consists of two spatially separated spin-correlated electrons (\hat{e}_1 and \hat{e}_2) interacting with an external magnetic field via the zeeman interaction and one electron spin coupled to an external nuclear spin (\hat{I}) via hyperfine interaction with a tensor represented by A . The complete Hamiltonian for the system is

$$\hat{H} = \gamma_e B \cdot (\hat{e}_1 + \hat{e}_2) + \hat{e}_2 \cdot A \cdot \hat{I}_1$$

Using QuTiP's Lindblad Master Equation Solver, we construct 8 basis states for the system (one for each total spin configuration), evolve our initial singlet density matrix, and then measure the partial trace of the density matrix for each collapse operator. We project each of the two possible singlet state configurations onto an added shelving state to store the new singlet population, resulting in the final singlet population at the end of the simulation.

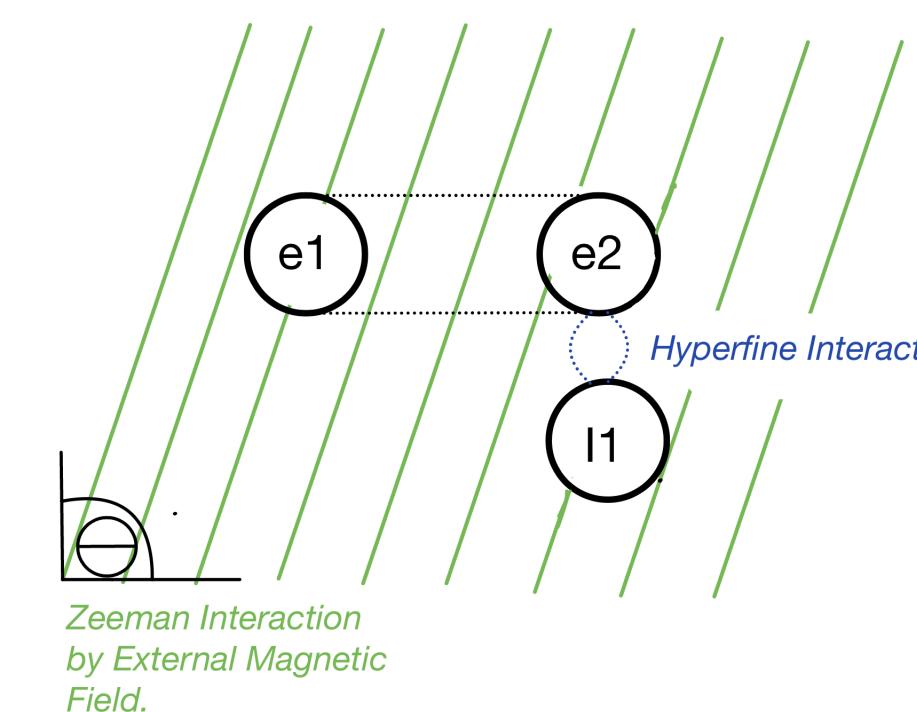


Fig. 5: Spin System Schematic.

A model spin system simulation protocol using hybrid quantum machine learning

- Initialize the quantum circuit into the singlet state via an X-gate and Hadamard gate on q0, X-gate on q1, and a CNOT gate on q0 and q1.
- Evolve the circuit by the parametrized rotations via the input vector.
- Measure the Circuit to obtain the final singlet yields.
- Optimize the input rotations via the Scipy gradient descent optimizer and SPSA noisy optimizer.
- Iteratively perform steps 2-5 until the optimization reaches its step limit or the objective function is effectively minimized (<0.001).

Accurate spin system simulation on NISQ device using variational circuit with SPSA

For our iterative minimization procedure, we used the SciPy gradient-based optimizer and the gradient-free Simultaneous Perturbation Stochastic Approximation. The initial parameters that were chosen for the SPSA protocol were calculated using the standard deviation of the yields from the quantum device, thus encoding the noise of the device into our optimization procedure. As the Scipy results did not approach the expected singlet yield, we only show the results for the yields obtained via SPSA optimization. Due to the noisy nature of quantum computation, the same input rotation vector will produce different outputs, thus we sample each rotation 5 times and plot each of the yields, the average yield, and the yield closest to the Lindblad yield, shown as the 'Best results', as well as the Lindblad yield shown as 'classic results'. Our protocol enables us to simulate a spin system Hamiltonian on a NISQ device by encoding the relevant interactions as rotation gates and learning the rotations that evolve the system to its final state.

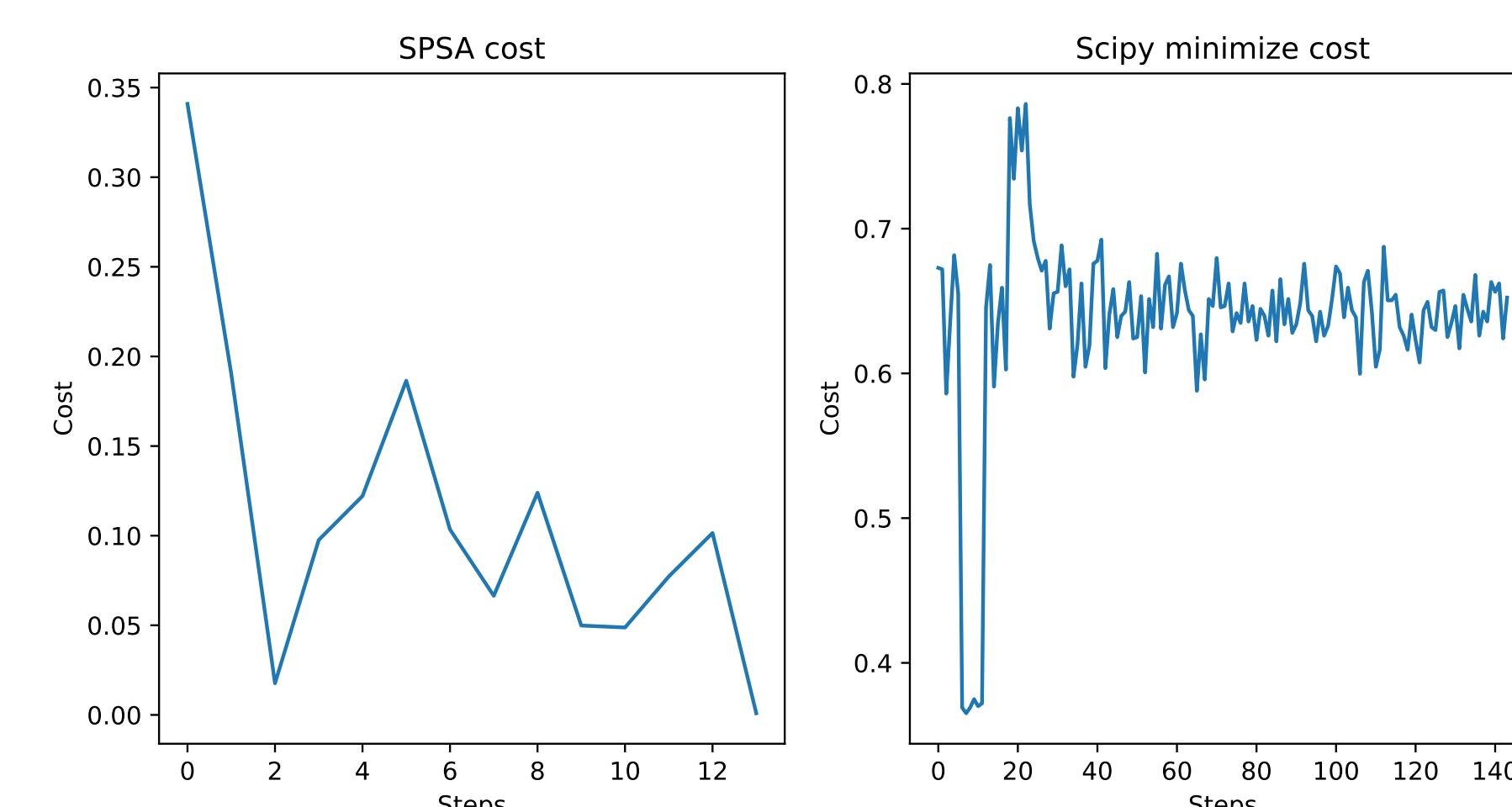


Fig. 6: Cost comparison of SPSA vs Scipy Optimization for a final singlet population value.

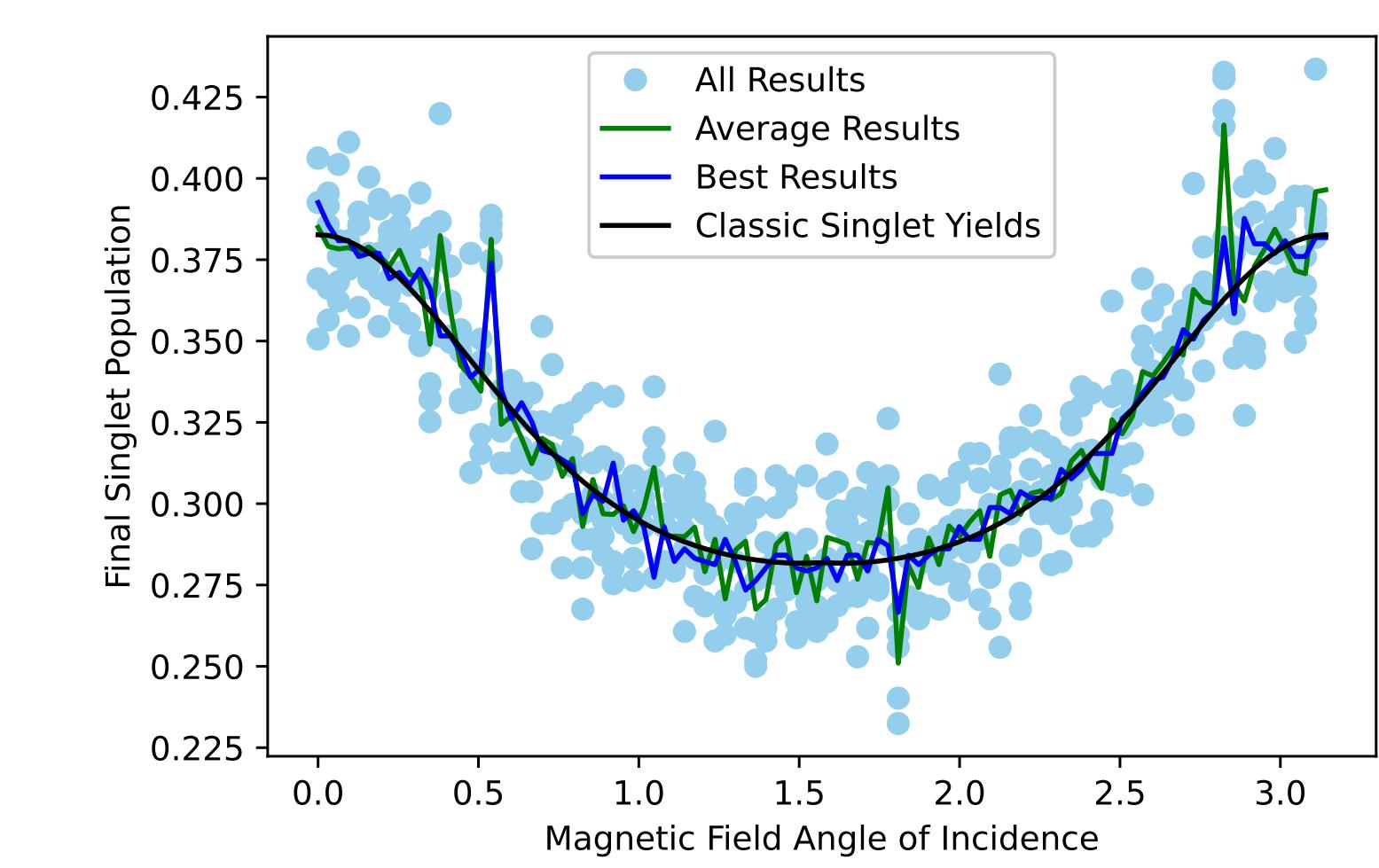


Fig. 7: Results from hybrid Quantum method using the noisy SPSA minimization procedure.

We see that for a NISQ device, a noisy gradient-free optimizer can more accurately arrive at the lowest cost, better deal with local minima, and perform the minimization procedure in a fewer amount of steps. So far we used the 3 spin system radical pair mechanism as our model, as we can simulate the final state of the system classically, however our protocol provides a tool that can potentially allow simulation of more complex spin systems as they scale in size.