Supplementary Information (SI) for Digital Discovery.

Supplemental Information: Mapping Bloch-Redfield dynamics into a unitary gate-based quantum algorithm

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I. DERIVATION OF ROTATION GATE ANGLES

The angles of each rotation gate in our circuit are derived from $e^{\mathcal{R}_d t}$ whose diagonal entries are,

$$\begin{aligned} x_1 &= e^0 = 1 \\ x_2 &= e^{(-2a-2b)t} \\ x_3 &= e^{(-a-b-c)t} \\ x_4 &= e^{(-a-b+c)t}, \end{aligned} \tag{1}$$

with a, b, and c defined in the main text. To implement $e^{\mathcal{R}_d t}$ on the circuit we dilate using,

$$\begin{aligned} x_{1\pm} &= 1 \pm i\sqrt{\frac{1-1}{1}} = 1 \\ x_{2\pm} &= e^{(-2a-2b)t} \pm ie^{(-2a-2b)t}\sqrt{\frac{1-e^{(-2a-2b)t}}{\|e^{(-2a-2b)t}\|}} \\ x_{3\pm} &= e^{(-a-b-c)t} \pm ie^{(-a-b-c)t}\sqrt{\frac{1-e^{(-a-b-c)t}}{\|e^{(-a-b-c)t}\|}} \\ x_{4\pm} &= e^{(-a-b+c)t} \pm ie^{(-a-b+c)t}\sqrt{\frac{1-e^{(-a-b+c)t}}{\|e^{(-a-b+c)t}\|}} \end{aligned} \tag{2}$$

which are the entries of $e^{\tilde{\mathcal{R}}_d t}$. We then decompose $e^{\tilde{\mathcal{R}}_d t}$ into $R(\theta)_z$ gates, with angles defined in the main text in terms of α_i. For this diagonal operator,

$$\begin{aligned} \alpha_1 &= \arctan(x_{1\pm}) \\ \alpha_2 &= \arctan(x_{2\pm}) \\ \alpha_3 &= \arctan(x_{3\pm}) \\ \alpha_4 &= \arctan(x_{4\pm}) \end{aligned} \tag{3}$$

Due to Qiskit's conventions, we multiply each α_i by 2 before inserting them into the R_z gates.

II. METHOD FOR GENERAL SYSTEM-ENVIRONMENT COUPLING

The Redfield tensor for the most general system-environment operator $\hat{s} = \chi\hat{\sigma}_x + \beta\hat{\sigma}_y + \gamma\hat{\sigma}_z + \delta\mathbb{1}$ can be derived as,

$$\mathcal{R} = \begin{bmatrix} \mathcal{R}_{11} & \mathcal{R}_{12} & \mathcal{R}_{12}^* & \mathcal{R}_{14} \\ \mathcal{R}_{21} & \mathcal{R}_{22} & \mathcal{R}_{23} & \mathcal{R}_{24} \\ \mathcal{R}_{21}^* & \mathcal{R}_{23}^* & \mathcal{R}_{22}^* & \mathcal{R}_{24}^* \\ -\mathcal{R}_{11} & -\mathcal{R}_{12} & -\mathcal{R}_{12}^* & -\mathcal{R}_{14} \end{bmatrix},$$

where the matrix elements of $\mathcal{R}$ are,

$$\mathcal{R}_{11} = -2b\left(\chi^2+\beta^2\right) \tag{4}$$

$$\mathcal{R}_{12} = 2d\gamma\left(\chi-i\beta\right) \tag{5}$$

$$\mathcal{R}_{21} = 2b\gamma\left(\chi-i\beta\right) \tag{6}$$

$$\mathcal{R}_{14} = 2a\left(\chi^2+\beta^2\right) \tag{7}$$

$$\mathcal{R}_{22} = -a\chi^2-a\beta^2-\chi^2 b-b\beta^2-4d\gamma^2-i\epsilon \tag{8}$$

$$\mathcal{R}_{23} = (a+b)\left(\chi+i\beta\right)\left(\chi+i\beta\right) \tag{9}$$

$$\mathcal{R}_{24} = -2a\gamma\left(\chi+i\beta\right). \tag{10}$$

The characteristic polynomial $P(y)$ of $\mathcal{R}$ is

$$\begin{aligned}P(y) = {} & 8a^2\chi^3\beta\epsilon+8a\chi^3b\beta\epsilon-8a^2\chi\beta^3\epsilon+8a\chi b\beta^3\epsilon \\ & +2a\chi^2\epsilon^2+2\chi^2b\epsilon^2-2a\beta^2\epsilon^2+2b\beta^2\epsilon^2+16a\chi\beta d\epsilon\gamma^2 \\ & +(4a^2\chi^4+8a\chi^4b+4\chi^4b^2-8a^2\chi^2\beta^2+8\chi^2b^2\beta^2+4a^2\beta^4-8ab\beta^4+4b^2\beta^4 \\ & +4a\chi\beta\epsilon+\epsilon^2+16a\chi^2d\gamma^2+16\chi^2bd\gamma^2-16a\beta^2d\gamma^2+16b\beta^2d\gamma^2+16d^2\gamma^4)y \\ & +(4a\chi^2+4\chi^2b-4a\beta^2+4b\beta^2+8d\gamma^2)y^2+y^3,\end{aligned}$$

whose roots are $\{0, y_1, y_2, y_3\}$.

The eigenvectors of $\mathcal{R}$ can also be represented through system-environment parameters and the eigenvalues of $\mathcal{R}$ as,

$$K = \begin{pmatrix} K_{11} & K_{12} & K_{12}^* & 1 \\ -1 & K_{2,2} & K_{3,2} & 1 \\ -1 & K_{2,3} & K_{3,3} & 1 \\ -1 & K_{2,4} & K_{3,4} & 1 \end{pmatrix} \tag{11}$$

where the matrix elements of K are defined as,

$$K_{11} = \frac{8a\chi\beta d\gamma^2+a(\chi-\beta)(\chi+\beta)(4a\chi\beta+\epsilon)}{b\left(\chi^2+\beta^2\right)\left(4a\chi\beta+\epsilon\right)} \tag{12}$$

$$K_{12} = \frac{4ia\beta\chi\gamma}{(\beta+i\chi)(4a\beta\chi+\epsilon)} \tag{13}$$

$$K_{2,k+1} = \frac{\frac{\epsilon\left(b\left(\beta^2+\chi^2\right)-a(\beta-i\chi)^2\right)}{(\beta+i\chi)(2\beta^2(a-b)-2\chi^2(a+b)-4d\gamma^2+i\epsilon-y_k)}+i\beta(a-b)-\chi(a+b)+\frac{y_k}{-\chi+i\beta}}{2d\gamma} \tag{14}$$

$$K_{3,k+1} = \frac{\left(\chi(a+b)+i\beta(a-b)\right)\left(2\beta^2(a-b)-2\chi^2(a+b)-4d\gamma^2-y_k\right)}{2d\gamma\left(2\beta^2(b-a)+2\chi^2(a+b)+4d\gamma^2-i\epsilon+y_k\right)} \tag{15}$$

with $k \in \{1, 2, 3\}$.

III. IONQ ARIA-1 HARDWARE SPECIFICATIONS

Demonstrations of the Redfield quantum algorithm were performed on IonQ's Aria-1 quantum device, which is a 21 qubit quantum platform with state preparation and measurement (SPAM) error of 0.39%, corresponding to 99.61% measurement fidelity. The 1-qubit and 2-qubit gate errors are 0.05% and 0.4% respectively, with respective gate speeds of 135μs and 600 μs. Furthermore, the respective T_1 and T_2 times are 10-100 s and $\sim$1000ms [1].

IV. RAW DATA FROM FIGURES

[1] IonQ Aria: Practical Performance, accessed March 2025.

	IonQ Aria-1 Populations		Exact Populations	
Time (μs)	Ground State	Excited State	Ground State	Excited State
0.000	0.012	0.988	0.000	1.000
0.065	0.053	0.947	0.042	0.958
0.142	0.091	0.909	0.090	0.910
0.235	0.144	0.856	0.142	0.858
0.347	0.200	0.800	0.198	0.802
0.481	0.264	0.736	0.258	0.742
0.642	0.307	0.693	0.319	0.681
0.835	0.367	0.633	0.381	0.619
1.066	0.440	0.560	0.440	0.560
1.344	0.472	0.528	0.495	0.505
1.678	0.529	0.471	0.543	0.457
2.078	0.576	0.424	0.583	0.417
2.558	0.580	0.420	0.614	0.386
3.134	0.608	0.392	0.635	0.365
3.826	0.613	0.387	0.649	0.351
4.655	0.617	0.383	0.656	0.344
5.651	0.631	0.369	0.660	0.340
6.846	0.631	0.369	0.661	0.339
8.279	0.701	0.299	0.662	0.338
10.000	0.654	0.346	0.662	0.338

TABLE I. Ground and excited state populations for Figure 2 in the main text. Data from IonQ Aria-1 device and the exact classical solution.

	Ground State Population					Excited State Population				
Time (μs)	10K	25K	100K	200K	300K	10K	25K	100K	200K	300K
0.000	0.004	0.008	0.015	0.003	0.008	0.996	0.992	0.985	0.997	0.992
0.065	0.022	0.052	0.156	0.245	0.322	0.978	0.948	0.844	0.755	0.678
0.142	0.053	0.077	0.268	0.410	0.447	0.947	0.923	0.732	0.590	0.553
0.235	0.055	0.165	0.369	0.470	0.500	0.945	0.835	0.631	0.530	0.500
0.347	0.116	0.191	0.442	0.501	0.503	0.884	0.809	0.558	0.499	0.497
0.481	0.149	0.271	0.504	0.532	0.511	0.851	0.729	0.496	0.468	0.489
0.642	0.208	0.325	0.496	0.520	0.513	0.792	0.675	0.504	0.480	0.487
0.835	0.251	0.378	0.533	0.530	0.503	0.749	0.622	0.467	0.470	0.497
1.066	0.295	0.432	0.537	0.508	0.520	0.705	0.568	0.463	0.492	0.480
1.344	0.348	0.485	0.533	0.513	0.496	0.652	0.515	0.467	0.487	0.504
1.678	0.392	0.545	0.541	0.521	0.494	0.608	0.455	0.459	0.479	0.506
2.078	0.476	0.584	0.541	0.520	0.512	0.524	0.416	0.459	0.480	0.488
2.558	0.529	0.611	0.553	0.530	0.505	0.471	0.389	0.447	0.470	0.495
3.134	0.598	0.619	0.540	0.515	0.526	0.402	0.381	0.460	0.485	0.474
3.826	0.635	0.635	0.551	0.522	0.520	0.365	0.365	0.449	0.478	0.480
4.655	0.718	0.653	0.550	0.532	0.519	0.282	0.347	0.450	0.468	0.481
5.651	0.760	0.675	0.547	0.515	0.516	0.240	0.325	0.453	0.485	0.484
6.846	0.777	0.655	0.546	0.514	0.516	0.223	0.345	0.454	0.486	0.484
8.279	0.814	0.672	0.538	0.509	0.522	0.186	0.328	0.462	0.491	0.478
10.000	0.832	0.642	0.538	0.517	0.505	0.168	0.358	0.462	0.483	0.495

TABLE II. Ground and excited state populations for various temperatures using the noisy simulator as described in the main text. Data corresponds to Figure 3.

	Ground State Population					Excited State Population				
Time (μs)	10K	25K	100K	200K	300K	10K	25K	100K	200K	300K
0.000	0.000	0.000	0.000	0.000	0.000	1.000	1.000	1.000	1.000	1.000
0.065	0.020	0.042	0.146	0.249	0.323	0.980	0.958	0.854	0.751	0.677
0.142	0.044	0.090	0.270	0.396	0.455	0.956	0.910	0.730	0.604	0.545
0.235	0.072	0.142	0.368	0.472	0.500	0.928	0.858	0.632	0.528	0.500
0.347	0.104	0.198	0.441	0.505	0.511	0.896	0.802	0.559	0.495	0.489
0.481	0.141	0.258	0.489	0.517	0.514	0.859	0.742	0.511	0.483	0.486
0.642	0.183	0.319	0.518	0.520	0.514	0.817	0.681	0.482	0.480	0.486
0.835	0.229	0.381	0.532	0.521	0.514	0.771	0.619	0.468	0.479	0.486
1.066	0.281	0.440	0.539	0.521	0.514	0.719	0.560	0.461	0.479	0.486
1.344	0.337	0.495	0.541	0.521	0.514	0.663	0.505	0.459	0.479	0.486
1.678	0.398	0.543	0.542	0.521	0.514	0.602	0.457	0.458	0.479	0.486
2.078	0.460	0.583	0.542	0.521	0.514	0.540	0.417	0.458	0.479	0.486
2.558	0.524	0.614	0.542	0.521	0.514	0.476	0.386	0.458	0.479	0.486
3.134	0.587	0.635	0.542	0.521	0.514	0.413	0.365	0.458	0.479	0.486
3.826	0.646	0.649	0.542	0.521	0.514	0.354	0.351	0.458	0.479	0.486
4.655	0.699	0.656	0.542	0.521	0.514	0.301	0.344	0.458	0.479	0.486
5.651	0.744	0.660	0.542	0.521	0.514	0.256	0.340	0.458	0.479	0.486
6.846	0.780	0.661	0.542	0.521	0.514	0.220	0.339	0.458	0.479	0.486
8.279	0.807	0.662	0.542	0.521	0.514	0.193	0.338	0.458	0.479	0.486
10.000	0.824	0.662	0.542	0.521	0.514	0.176	0.338	0.458	0.479	0.486

TABLE III. Ground and excited state populations for various temperatures from exact solution as described in the main text. Data corresponds to Figure 3.

	Ground State Population			Excited State Population		
Time (μs)	0.1T	1T	5T	0.1T	1T	5T
0.000	0.001	0.008	0.032	0.999	0.992	0.968
0.065	0.045	0.052	0.070	0.955	0.948	0.930
0.142	0.084	0.077	0.155	0.916	0.923	0.845
0.235	0.129	0.165	0.243	0.871	0.835	0.757
0.347	0.184	0.191	0.368	0.816	0.809	0.632
0.481	0.249	0.271	0.443	0.751	0.729	0.557
0.642	0.289	0.325	0.506	0.711	0.675	0.494
0.835	0.342	0.378	0.630	0.658	0.622	0.370
1.066	0.384	0.432	0.708	0.616	0.568	0.292
1.344	0.434	0.485	0.779	0.566	0.515	0.221
1.678	0.462	0.545	0.831	0.538	0.455	0.169
2.078	0.475	0.584	0.908	0.525	0.416	0.092
2.558	0.494	0.611	0.943	0.506	0.389	0.057
3.134	0.506	0.619	0.929	0.494	0.381	0.071
3.826	0.502	0.635	0.957	0.498	0.365	0.043
4.655	0.518	0.653	0.963	0.482	0.347	0.037
5.651	0.512	0.675	0.965	0.488	0.325	0.035
6.846	0.528	0.655	0.971	0.472	0.345	0.029
8.279	0.533	0.672	0.965	0.467	0.328	0.035
10.000	0.517	0.642	0.974	0.483	0.358	0.026

TABLE IV. Ground and excited state populations for various magnetic fields using the noisy simulator as described in the main text. Data corresponds to Figure 4.

	Ground State Population			Excited State Population		
Time (μs)	0.1T	1T	5T	0.1T	1T	5T
0.000	0.000	0.000	0.000	1.000	1.000	1.000
0.065	0.041	0.042	0.073	0.959	0.958	0.927
0.142	0.085	0.090	0.154	0.915	0.910	0.846
0.235	0.133	0.142	0.241	0.867	0.858	0.759
0.347	0.184	0.198	0.333	0.816	0.802	0.667
0.481	0.236	0.258	0.429	0.764	0.742	0.571
0.642	0.288	0.319	0.524	0.712	0.681	0.476
0.835	0.337	0.381	0.617	0.663	0.619	0.383
1.066	0.383	0.440	0.703	0.617	0.560	0.297
1.344	0.423	0.495	0.779	0.577	0.505	0.221
1.678	0.455	0.543	0.841	0.545	0.457	0.159
2.078	0.480	0.583	0.890	0.520	0.417	0.110
2.558	0.497	0.614	0.924	0.503	0.386	0.076
3.134	0.507	0.635	0.945	0.493	0.365	0.055
3.826	0.513	0.649	0.957	0.487	0.351	0.043
4.655	0.515	0.656	0.963	0.485	0.344	0.037
5.651	0.516	0.660	0.965	0.484	0.340	0.035
6.846	0.517	0.661	0.966	0.483	0.339	0.034
8.279	0.517	0.662	0.966	0.483	0.338	0.034
10.000	0.517	0.662	0.966	0.483	0.338	0.034

TABLE V. Ground and excited state populations for various magnetic fields from exact solution as described in the main text. Data corresponds to Figure 4.

Time (μs)	$\langle Z \rangle$ Simulator	$\langle Z \rangle$ Exact
0.000	-0.710	-1.000
0.065	-0.703	-0.915
0.142	-0.706	-0.820
0.235	-0.586	-0.716
0.347	-0.587	-0.604
0.481	-0.432	-0.485
0.642	-0.336	-0.362
0.835	-0.249	-0.239
1.066	-0.170	-0.120
1.344	-0.080	-0.010
1.678	0.097	0.087
2.078	0.187	0.167
2.558	0.192	0.228
3.134	0.222	0.270
3.826	0.263	0.297
4.655	0.310	0.312
5.651	0.294	0.320
6.846	0.339	0.322
8.279	0.277	0.323
10.000	0.293	0.324

TABLE VI. Total magnetization ($\langle Z \rangle$) from the simulator and exact solutions. Data corresponds to Figure 5.