Spin simulator comprehensive plan

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1 Background theory

1.1 Spin Hamiltonian

Assume we have an array of N_0 quantum dots that are defined in a 2-dimensional electron gas (2DEG) in the xOz coordinate plane. We describe the $\mathrm{N}<\mathrm{N}_0$ electrons located in some of the dots with a density matrix $\rho(t)$. In the lab frame, the system spin Hamiltonian is given by the following expression (SI units are used in the calculations):

$$\mathcal{H}_{\mathrm{L}} = \sum_{j=1}^{N} \underbrace{\frac{g(t)}{2}\mu_{\mathrm{B}}B_0 Z_j}_{\text{Zeeman}} + \sum_{j=1}^{N-1} \underbrace{\frac{J_{j,j+1}(t)}{4}\vec{\sigma}_j \cdot \vec{\sigma}_{j+1}}_{\text{exchange}} + \sum_{j=1}^{N} \underbrace{\mu_{\mathrm{B}}B_{\mathrm{RF}}(t)\left[\cos(\omega_{\mathrm{RF}}t + \phi(t))X_j + \sin(\omega_{\mathrm{RF}}t + \phi(t))Y_j\right]}_{\text{radio frequency field}}, \tag{1.1}$$

where the following parameters are introduced:

- $\mu_{\mathrm{B}} = 5.788\,381\,801 \cdot 10^{-2}\frac{\mathrm{meV}}{\mathrm{T}} = 9.274\,009\,994 \cdot 10^{-24}\frac{\mathrm{J}}{\mathrm{T}}$ is the Bohr magneton;

- B_0 and $B_{\text{RF}}(t)$ are Zeeman field and the envelope of RF field (in tesla), respectively;
- $\omega_{\text{RF}} = 2\pi f_{\text{RF}}$ and $\phi(t)$ are the RF field frequency and phase, respectively.
- $J_{j,j+1}(t)$ is the voltage-controlled parameter of exchange between j^{th} and $(\text{j+1})^{\text{th}}$ dots (in joules);
- $\vec{\sigma}_j = \{X_j, Y_j, Z_j\}$ is the Pauli vector of j^{th} spin;
- $g = 2 + \delta g(t)$ and $g_{\perp,j} = 2 + \delta g_{\perp,j}(t)$ is voltage-controlled in-plane g-factor of j^{th} spin. Out-of-plane g-factor is equated to 2.

Note: each addend in the equation (1.1) is a Kronecker product of N matrices 2×2. To simplify notation, we omit the identity operators in Kronecker products, e.g.:

$$Z_k \equiv \left(\bigotimes_{i=1}^{k-1} \mathbb{1}_i\right) \otimes Z_k \otimes \left(\bigotimes_{i=k+1}^{N} \mathbb{1}_i\right), \quad \text{where} \quad \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.2}$$

We adhere to this convention throughout the document.

The Hamiltonian (1.1) and density matrix ρ are transformed into the rotation frame in the following way:

$$\rho_{\text{R}} \equiv \rho = R\rho_{\text{L}}R^\dagger, \qquad \mathcal{H}_{\text{R}} = R\mathcal{H}_{\text{L}}R^\dagger + i\hbar\dot{R}R^\dagger, \tag{1.3}$$

$$R = \bigotimes_{j=1}^{N} e^{\frac{i}{2}\omega_{\text{RF}}tZ_j} = \bigotimes_{j=1}^{N} \left(\cos\frac{\omega_{\text{RF}}t}{2} + i\sin\frac{\omega_{\text{RF}}t}{2}Z_j\right) = \begin{pmatrix} e^{\frac{i}{2}\omega_{\text{RF}}t} & 0 \\ 0 & e^{-\frac{i}{2}\omega_{\text{RF}}t} \end{pmatrix}^{\otimes N} \tag{1.4}$$

By substituting (1.4) into (1.3) and neglecting fast-oscillating terms, we obtain the Hamiltonian (normalized by $\hbar$) in the rotating wave approximation:

$$\mathscr{H} = \mathcal{H}_{\text{R}}/\hbar = \sum_{j=1}^{N} \left\{ \left[\left(1 + \frac{\delta g_j(t)}{2}\right)\omega - \tilde{\omega} \right] Z_j + \Omega(t)\left(\cos\phi(t)\, X_j + \sin\phi(t)\, Y_j\right) \right\} +$$

$$+ \sum_{j=1}^{N-1} \frac{J_{j,j+1}(t)}{4\hbar} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}, \qquad \text{where} \quad \omega = \frac{\mu_{\text{B}}B_0}{\hbar}, \quad \tilde{\omega} = \frac{\omega_{\text{RF}}}{2} = \pi f_{\text{RF}}, \quad \Omega(t) = \frac{\mu_{\text{B}}B_{\text{RF}}(t)}{\hbar} \tag{1.5}$$

Note: $\hbar = 1.054\,571\,817 \cdot 10^{-34}$ J·s; $\frac{\mu_{\text{B}}}{\hbar} = 8.794\,099\,979 \cdot 10^{10}$ $\frac{\text{rad}}{\text{s·T}}$

1.2 Equation of motion

To simulate the spin system dynamics, we solve the master equation in Lindblad form in the rotation frame:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = i\left[\rho, \mathscr{H}\right] + \sum_{\alpha=1}^{3}\sum_{j=1}^{N} 2L_{\alpha,j}\,\rho\,L_{\alpha,j}^\dagger - \left\{L_{\alpha,j}^\dagger L_{\alpha,j}, \rho\right\}, \tag{1.6}$$

Here, the Lindblad operators are defined as demonstrated below:

$$L_{1,j} = \sqrt{\frac{p_j}{2T_1}}\sigma_{+,j} \qquad L_{2,j} = \sqrt{\frac{1-p_j}{2T_1}}\sigma_{-,j} \qquad L_{3,j} = \frac{Z_j}{2\sqrt{T_2}}, \tag{1.7}$$

where p_j is the statistical probability of finding j^{th} electron in the state $|\uparrow\rangle$; T_1 and T_2 are spin relaxation and dephasing times, respectively. Since Zeeman splitting determines the largest energy scale in the system, we assume Boltzmann distribution for p_j:

$$E_{|\uparrow\rangle} - E_{|\downarrow\rangle} \approx 2\hbar\omega; \qquad p_j \equiv p \approx \frac{1}{\exp\left(\frac{2\hbar\omega}{k_{\mathrm{B}}T}\right) + 1} \quad \left(k_{\mathrm{B}} = 1.380\ 649 \cdot 10^{-23} \frac{J}{K}\right) \tag{1.8}$$

Combining the formulas (1.5),(1.6) and (1.7), we obtain the master equation:

$$\begin{aligned} \frac{\mathrm{d}\rho}{\mathrm{d}t} = F(\rho, t) = i \left[\rho, \sum_{j=1}^{N} \frac{\delta g_j(t)}{2} \omega Z_j + \Omega(t) \left(\cos\phi(t)\ X_j + \sin\phi(t)\ Y_j\right)\right] \\ + i \left[\rho, \sum_{j=1}^{N-1} \frac{J_{j,j+1}(t)}{4\hbar} \vec{\sigma_j} \cdot \vec{\sigma}_{j+1}\right] + i(\omega - \tilde{\omega}) \left[\rho, \sum_{j=1}^{N} Z_j\right] \\ + \sum_{j=1}^{N} \frac{p}{2T_1} \left(2\sigma_{+,j}\, \rho\, \sigma_{-,j} - \{\sigma_{-,j}\, \sigma_{+,j}, \rho\}\right) + \frac{1-p}{2T_1} \left(2\sigma_{-,j}\, \rho\, \sigma_{+,j} - \{\sigma_{+,j}\, \sigma_{-,j}, \rho\}\right) + \frac{1}{2T_2} \left(Z_j \rho Z_j - \rho\right) \end{aligned} \tag{1.9}$$

2 Implementation

2.1 Basic functionality

The main function in the spin simulator module solves the Cauchy problem for the master equation (2.1). Its mandatory input parameters include:

- System parameters: number of electrons N, temperature T;
- Material parameters (T_1, T_2)
- Time-independent parameters of magnetic fields: B_0, f_{RF};
- The simulation duration t_{max} and time step Δt;
- Time-dependent parameters: RF pulse sequence envelope $B_{\mathrm{RF}}(t)$, deviation g-factor $\delta g_j(t)$, $\phi(t)$;

Among the optional parameters, we note (additional functionality is discussed in the sec. 3):

- Additional quantities to be calculated during the simulation;
- Sequence of interrupts that represent measurements or loads of new electrons.

Using the obvious identities:

$$\sigma_{+,j}\sigma_{-,j} = 2 \cdot \mathbb{1} + 2Z_j, \qquad [\sigma_{+,j}, \sigma_{-,j}] = 4Z_j,$$

the equation (1.9) could be rewritten in the following way to optimize its numerical evaluation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = F(\rho,t) = i\left[\rho,\ \frac{\omega}{2}\sum_{k=1}^{N}\delta g_k(t)Z_k + B_{\mathrm{RF}}(t)\left(\cos\phi(t)\ \frac{\mu_{\mathrm{B}}}{\hbar}\sum_{k=1}^{N}X_k + \sin\phi(t)\ \frac{\mu_{\mathrm{B}}}{\hbar}\sum_{k=1}^{N}Y_k\right)\right]$$
$$+\left[\rho,\sum_{k=1}^{N-1}\frac{i\vec{\sigma}_k\cdot\vec{\sigma}_{k+1}}{4\hbar}J_{k,k+1}(t)\right] + \left[\rho, i(\omega-\tilde{\omega})\sum_{k=1}^{N}Z_k\right] + \frac{1}{2T_2}\sum_{k=1}^{N}Z_k\rho Z_k$$
$$+\frac{p}{T_1}\sum_{k=1}^{N}\sigma_{+,k}\,\rho\,\sigma_{-,k} + \frac{1-p}{T_1}\sum_{k=1}^{N}\sigma_{-,k}\,\rho\,\sigma_{+,k} + \frac{2p-1}{T_1}\sum_{k=1}^{N}Z_k - \left(\frac{2}{T_1}+\frac{1}{2T_2}\right)N\rho \quad (2.1)$$

At the beginning, an auxillary function construct an array of time-independent Pauli matrices $(X_k, Y_k, Z_k, \sigma_{\pm,k})$ and the expressions highlighted in (2.1) for $k \in [1,n], n \in [1,N_0]$. The reason why we calculate the matrices for different values of n is that the number of electrons in the system is not fixed, i.e. the electrons could be measured or loaded. The function that constructs the right-hand side of (2.1) at each point of time retrieves the values of pre-calculated matrice and weights them by time-dependent parameters $B_{\mathrm{RF}}(t)$, $\delta g_k(t)$,$J_{k,k+1}(t)$, etc. This significantly speeds up the computation since Kronecker products are not recalculated at each iteration.

2.2 Computation: 4$^{\text{th}}$ order Runge-Kutta method

Such Python libraries as SciPy (as well as less popular ones) do not contain functions that solve initial value problems for complex *matrix* functions like ρ (only for complex vector functions at most). Thus, we implement the Runge-Kutta algorithm for the equation (2.1) ourselves, even though the notation is essentially identical to the textbook algorithm for scalar/vector functions. Namely, given the initial value problem:

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = F(\rho,t), \qquad \rho(0) = \rho_0,$$

we write the approximate value of ρ at the $(n+1)^{\text{st}}$ time step:

$$\rho_{n+1} = \rho_n + \frac{1}{6}\Delta t\left(k_1 + k_2 + k_3 + k_4\right), \quad (2.2)$$

$$k_1 = F\left(\rho_n, n\,\Delta t\right), \qquad k_2 = F\left(\rho_n + \frac{\Delta t}{2}k_1, \left(n+\frac{1}{2}\right)\Delta t\right),$$
$$k_3 = F\left(\rho_n + \frac{\Delta t}{2}k_2, \left(n+\frac{1}{2}\right)\Delta t\right), \qquad k_4 = F\left(\rho_n + \Delta t k_3, (n+1)\,\Delta t\right).$$

The time step Δt is determined by the largest energy scale of the system:

$$\Delta t = 2\pi\cdot 10^{-4}\cdot\max\left\{\frac{\hbar}{J_{j,j+1}}, (\omega-\omega_{\mathrm{RF}})^{-1}, \left(\frac{\delta g_j}{2}\omega\right)^{-1}, \Omega^{-1}\right\} \text{ at } t=0.$$

The error of the method is $O(\Delta t^4)$.

3 Scope

The basic task of the spin simulator is to evaluate the system density matrix at a particular point of time $\rho(t_n) = \rho(n\,\Delta t)$. The individual matrices $\rho(t_i),\ i < N$ are overwritten at each step of the calculation in order not to congest memory. Nevertheless, the method could return the temporal dynamics of such system parameters as fidelity and ... **(Brandon, please prepare a list of the parameters we might in principle want to monitor)**. We could also dynamically change the number of electrons in the system.

3.1 Control of system parameters

Question 8: what is the proper way to define fidelity?

1. The "standard" definition given e.g. in [2]: $\mathscr{F}(\rho,\rho') = \left(\mathrm{Tr}\sqrt{\rho^{\frac{1}{2}}\rho'\rho^{\frac{1}{2}}}\right)^2$. It's unclear to me, though, which matrix (ρ or ρ') is expected and which one is simulated.
2. The definition I found in the work of students that Jonathan shared with me: $\mathscr{F}(\rho,\rho') = \mathrm{Tr}\,(\rho_{sim}\rho_{exp})$.
3. Probably, not a very realistic option, but we could run the second simulation in parallel and obtain $\rho_{exp}(t)$ in case of no Lindblad operators ($T_1 = T_2 \to \infty$).

But in the cases 1 and 2, how do we define the expected matrix in a general way? I presume, we need a helper module that builds the total operator U for the quantum circuit so that $\rho_{exp} = U\rho U^\dagger$, correct? Also, will this result of 1 or 2 be virtually the same as in the case 3?

3.2 Measurements

The implementation of the measurement of the k^{th} qubit is straightforward. The operators are redefined as follows:

$$\rho \leftarrow \mathrm{Tr}_k\,(\rho)\,, \quad \mathscr{H} \leftarrow \frac{1}{2}\mathrm{Tr}_k\,(\mathscr{H})\,, \quad L_{\alpha,j\neq k} \leftarrow \frac{1}{2}\mathrm{Tr}_k\,(L_{\alpha,j\neq k}) \tag{3.1}$$

and N is replaced by $\mathrm{N}-1$. Here, Tr_k denotes a partial trace with respect to k^{th} spin. The factor $\frac{1}{2}$ appears because X, Y, Z are traceless, and $\mathrm{Tr}\,(\mathbb{1}) = 2$. Note that the Hamiltonian transforms as a whole, whereas the Lindblad operators need to be redefined individually. Therefore, in practice it is easier to recalculate each $L_{\alpha,j}$ individually with the formula (1.7) for $j = \overline{1, \mathrm{N}-1}$.

3.3 Loading new qubits

In the general case (when the electrons are loaded into the dots in an arbitrary sequence) the math is nontrivial. It is relatively simple in case we populate the neighboring QDs one by one from left to right or vice versa. For instance, when we load electrons left-to-right, the matrices

for N qubits need to be changed thus:

$$\rho \leftarrow \rho \otimes \rho_{\mathrm{N}+1}, \qquad \mathscr{H} \leftarrow \mathscr{H} + \left[\left(1 + \frac{\delta g_{\mathrm{N}+1}(t)}{2}\right)\omega - \tilde{\omega}\right] Z_{\mathrm{N}+1} + \\ + \left(1 + \frac{\delta g_{\perp,j}(t)}{2}\right)\Omega(t)\left(\cos\phi(t)\ X_{\mathrm{N}+1} + \sin\phi(t)\ Y_{\mathrm{N}+1}\right) + \frac{J_{\mathrm{N},\mathrm{N}+1}(t)}{4\hbar}\vec{\sigma_{\mathrm{N}}} \cdot \vec{\sigma}_{\mathrm{N}+1} \tag{3.2}$$

and N is replaced by $\mathrm{N}+1$. The Lindblad operators redefinition is entirely analogous to the one from subsec. 3.2 with the formula (1.7).

> Question 9: I have an idea how to realize the more general case (i.e. load to an arbitrarily chosen QD) with the aid of a graph that contains the system charge configuration. But is this at all necessary? I might be wrong, but according to [1], it seems to me that it actually *is* necessary to properly simulate a four-node plaquette. Please let me know, and I'll prepare (or not) the detailed explanation based on your answer.

4 Tests

The code will incorporate the features discussed above step by step. It will be tested on several physical systems, especially one and two-qubit ones. The current plan is for now:

- Rabi oscillations of a single qubit
- SWAP and $\sqrt{\mathrm{SWAP}}$ exhange gates of two qubits
- some simple two-qubit algorithm like Deutsch-Josza

The details of these simulations are coming.

References

[1] B. Buonacorsi, Z. Cai, E. B. Ramirez, K. S. Willick, S. M. Walker, J. Li, B. D. Shaw, X. Xu, S. C. Benjamin, and J. Baugh, "Network architecture for a topological quantum computer in silicon," *Quantum Science and Technology*, vol. 4, p. 025003, Jan 2019.

[2] R. Cabrera and W. Baylis, "Average fidelity in n-qubit systems," *Physics Letters A*, vol. 368, no. 1, pp. 25 – 28, 2007.