Decoherence due to phonons

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A detailed derivation of decoherence due to phonons. We calculate the decoherence time of magnetic cluster qubits by analyzing phonon-assisted transitions out of the two-state subspace. The resulting exponential dependence on spin quantum number S provides a pathway for optimizing qubit lifetimes.

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Qubits are physical systems coupled to their environment, which can cause the qubits to lose their quantum nature. The decoherence time of a quantum computer is the lifetime of coherent quantum states. In the case of MC QC, the interaction of the MC with the crystal structure and phonons may result in a transition out of the two-state subspace previously defined.

In this section, we discuss the dynamics of decoherence, and calculate the lifetime of an MC qubit, focusing on decoherence originating from phonon-assisted transitions out of the two-state qubit subspace. We turn to references [1]–[4] for the detailed description of the spin-phonon interaction.

To begin, we must consider physically what occurs in a single-state excitation facilitated by absorption or emission of a phonon, which is depicted in Figure 1.

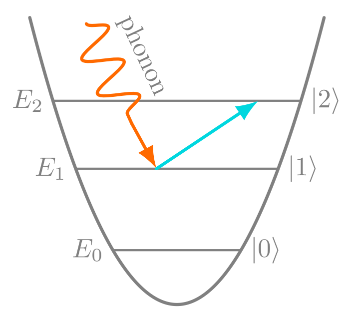

Figure 1: Phonon Stimulated Excitations.

The states of the system, a few of which are shown in Figure 1, have different energy and angular momentum values; therefore, any transition between two states requires angular momentum and energy transfer to or from the qubit. Excitations in the crystal structure will carry in (or out) the required angular momentum and energy difference. These excitations can be described as transverse phonons, denoted as $u(r)$. Phonons cause perturbations on the angles of the crystal axes, which can be written as:

$$\delta\phi(r) = \frac{1}{2}\nabla \times u(r). \tag{1}$$

We can calculate the spin-phonon interaction by perturbing the magnetic anisotropy Hamiltonian with the angles $\delta\phi$ as follows:

$$\begin{aligned} H_{s-ph} &\equiv e^{-iS\cdot\delta\phi}H_A e^{iS\cdot\delta\phi} - H_0 \\ &\simeq (1 - iS\cdot\delta\phi)H_A(1 + iS\cdot\delta\phi) - H_A \\ &= i\delta\phi\cdot[H_A, S], \end{aligned} \tag{2}$$

where high orders in $\delta\phi$ are ignored because $\delta\phi \ll 1$, and the Hamiltonian, H_A, is the anisotropy contribution to the Hamiltonian. The decoherence rate corresponding to the transitions from the subspace to outside the subspace can be calculated utilizing Eq. 2. This is accomplished by calculating the amplitude for the spin-phonon scattering. We define quantum states, $|\Psi_{f,i}\rangle = |\psi_{f,i}\rangle \otimes |\phi_{f,i}\rangle$, where the indices, f and i, refer to the final and initial states. $|\psi_{f,i}\rangle$ and $|\phi_{f,i}\rangle$ are the eigenstates of the spin and phonon Hamiltonians, respectively. Because two adjacent phonon states differ by one phonon quanta, we define the phonon states, $|\phi_f\rangle = |n_{k,\lambda}\rangle$ and $|\phi_i\rangle = |n_{k,\lambda}+1\rangle$, where k is the phonon wavevector, and $\lambda \in \{t_1, t_2, l\}$ show the transverse and longitudinal polarizations of the phonon. A transition from a state to its adjacent state above is given by the amplitude, $\langle\Psi_f|H_{s-ph}|\Psi_i\rangle = \Xi\cdot\Phi$, where $\Xi \equiv -i\hbar w_{fi}\langle\psi_f|S|\psi_i\rangle$ is the spin matrix element, $\hbar w_{fi}$ is the energy gap between the two states, and the phonon matrix elements are given by

$$\Phi \equiv \sqrt{\frac{\hbar}{8MN}}\sum_{k,\lambda}\frac{e^{ik\cdot r}}{\sqrt{w_{k,\lambda}}}[ik\times e_{k,\lambda}]\sqrt{n_{w_{fi}}}. \tag{3}$$

Using Fermi golden rule and the transition amplitude given above, a general transition rate can be defined as:

$$\begin{aligned} \Gamma &= \frac{1}{N}\sum_{k,\lambda}\frac{(k\times e_{k,\lambda})^2}{8M\hbar w_{k,\lambda}}n_{w_{fi}}|\Xi|^2 2\pi\delta(w_{k,\lambda} - w_{fi}) \\ &= \frac{V}{12\pi\hbar}\frac{|\Xi|^2 w_{fi}^3}{Mv_t^5}n_{w_{fi}}, \end{aligned} \tag{4}$$

where $n_{w_{fi}} = \frac{1}{e^{\hbar w_{fi}/k_B T}-1}$ is the phonon occupation number, N is the number of cells in the crystal structure, V is the unit cell volume, M is the mass of the cells, and $w_{k,\lambda} = v_\lambda k$ is the phonon frequency. v_λ, the speed of phonons, can be estimated as $w_{fi}l_c$, where l_c is the lattice constant. The decoherence time, $\tau \equiv \Gamma^{-1}$, must be long enough such that a large number of single-qubit and multi-qubit operations can be executed before the quantum states decohere. The spin matrix element can be computed as $|\Xi|^2 \propto \hbar^2 S^2 w_{fi}^2$, which yields the following expression for the decoherence time:

$$\tau = \tau(S,T) \simeq \frac{12\pi M l_c^2}{S^2}(e^{\frac{\hbar w_{fi}}{k_B T}} - 1), \tag{5}$$

Note that the overall expression depends on the exponential term, which originated from the density of phonons. Since $\hbar w_{fi} \simeq 2KS$, the decoherence time increases exponentially with S. Therefore, by appropriately choosing the values of K and S (i.e., the type of the magnetic cluster), the decoherence time can be made long enough for performing a useful number of operations.

[1] C. Timm and F. Elste, "Spin amplification, reading, and writing in transport through anisotropic magnetic molecules," *Physical Review B*, vol. 73, Dec. 2005, doi: 10.1103/PhysRevB.73.235304.

[2] E. M. Chudnovsky, D. A. Garanin, and R. Schilling, "Universal mechanism of spin relaxation in solids," *Phys. Rev. B*, vol. 72, p. 094426, Sep. 2005, doi: 10.1103/PhysRevB.72.094426. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevB.72.094426

[3] E. M. Chudnovsky and X. Martinez-Hidalgo, "Tunneling with dissipation and decoherence for a large spin," vol. 66, no. 5, p. 054412, Aug. 2002, doi: 10.1103/PhysRevB.66.054412. [Online]. Available: https://arxiv.org/abs/cond-mat/0201184

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