Dissipation and Decoherence in Quantum Systems: The Role of Anharmonic Environments

Eberly Research Showcase 2025

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Outline

1. Physical Motivation

2. Theoretical Framework

3. Computational Results: Presentation and Interpretation

4. Conclusions and Future Work

Physical Motivation

Quantum Decoherence

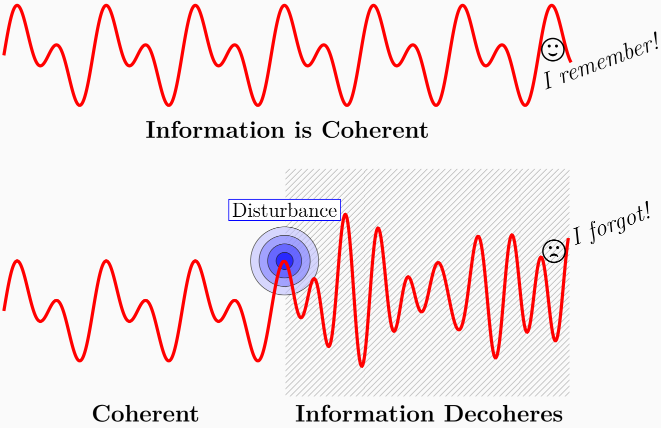

Figure 1: Quantum phase coherence: discernible, repeating pattern (top). Decoherence: loss of a clear pattern (bottom). Environmental disturbance sources: electromagnetic waves (photons), mechanical vibrations (phonons), and temperature fluctuations.

Qubit: Two–Level Quantum System

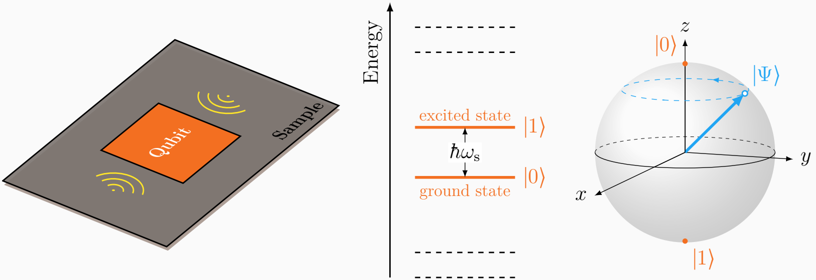

Figure 2: A qubit embedded in a solid affected interacting with lattice vibrations (left). The qubit modeled as a two–level system (middle). Bloch sphere representation of the qubit state and its free time evolution (right).

Anharmonic Solid

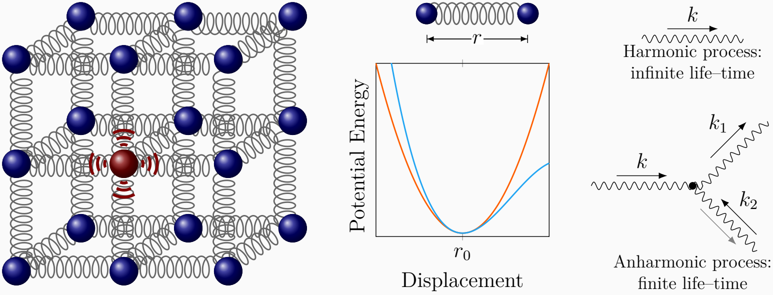

Figure 3: Illustration of lattice vibrations in a three–dimensional solid (left). Interatomic potential energy: harmonic potential vs. anharmonic potential, $U(r) = Kr^2/2 - \lambda r^3$ (middle). Diagrams of harmonic and three–phonon anharmonic processes (right).

What Can We Do?

State of the art: The dynamics of a open quantum system coupled to a bosonic harmonic bath are well understood [2]. The properties of anharmonic baths have been extensively studied on their own [3]. Numerical parametrizations for such baths are available [4].

Our Goal: To develop a microscopic framework that captures how anharmonic environments modify the dynamics of open quantum systems.

Theoretical Framework

Model Hamiltonian

$$\hat{H} = \underbrace{\frac{\hbar\omega_s}{2}\hat{\sigma}_z}_{\textbf{Qubit}} + \underbrace{\sum_k \left[\frac{\hat{P}_k^2}{2m} + \frac{m\Omega_k^2}{2}\hat{Q}_k^2\right] + \lambda_b \overbrace{\hat{H}_{\text{anharmonic}}}^{\sim \hat{Q}_{k_1}\hat{Q}_{k_2}\hat{Q}_{k_3}}}_{\textbf{Bath}} + \underbrace{\sum_{k,j} c_{k,j}\hat{\sigma}_j\hat{Q}_k}_{\textbf{SB Interaction}}$$

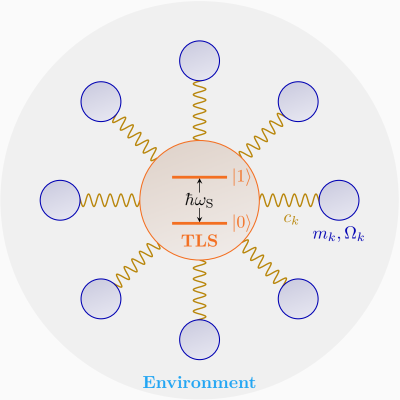

Figure 4: Schematic representation of the standard spin–boson model.

Lindblad Master Equation

The reduced dynamics of the qubit is governed by the Lindblad equation [1, 5]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathsf{s}}(t) = -\frac{i}{\hbar}\left[\hat{H}_{\mathsf{s}} + \hat{H}_{\mathsf{LS}}, \hat{\rho}_{\mathsf{s}}(t)\right] + \mathcal{D}[\hat{\rho}_{\mathsf{s}}(t)]$$

$$\text{with} \quad \hat{\rho}_{\mathsf{s}}(t) = \begin{pmatrix} \hat{\rho}_{00}(t) & \hat{\rho}_{01}(t) \\ \hat{\rho}_{10}(t) & \hat{\rho}_{11}(t) \end{pmatrix}.$$

- $\hat{\rho}_{\mathsf{s}}(t)$: qubit density matrix (populations and coherences).
- $\mathcal{D}[\hat{\rho}_{\mathsf{s}}(t)] = \sum_j \left[\hat{L}_j \hat{\rho}_{\mathsf{s}}(t)\hat{L}_j^\dagger - \frac{1}{2}\left\{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_{\mathsf{s}}(t)\right\}\right]$: dissipative contributions from the bath.
- **Assumptions:** Weak system–bath coupling and Markovian bath (short memory).

Bath Spectral Density

The bath influences the qubit through:

1. **Lamb shift:** renormalized frequency $\bar{\omega}_\mathsf{s} = \omega_\mathsf{s} + \Delta_\mathsf{LS}$.
2. **Relaxation times:** exponential decays e^{-t/T_1} (populations) and e^{-t/T_2} (coherences).

Δ, T_1, and T_2 depend on the qubit splitting frequency ω_s and on the bath spectral density $J(\omega)$, which encodes temperature, characteristic bath frequencies, anharmonicities, and system–bath coupling:

$$J(\omega) = \operatorname{Im} \mathcal{F}\left[\theta(t - t')\left\langle \left\{ \sum_k c_k \hat{Q}_k(t), \sum_{k'} c_{k'} \hat{Q}_{k'}(t') \right\} \right\rangle_{\hat{\rho}_\mathsf{b}} \right].$$

Our Toy Model

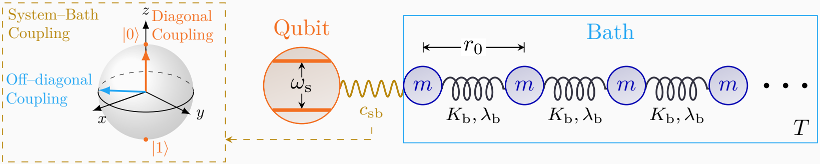

Figure 5: Pictorial representation of a one–dimensional model of a qubit coupled to an anharmonic crystal. The coupling to the qubit states can be either diagonal or off–diagonal.

Computational Results:
Presentation and Interpretation

Computational Results

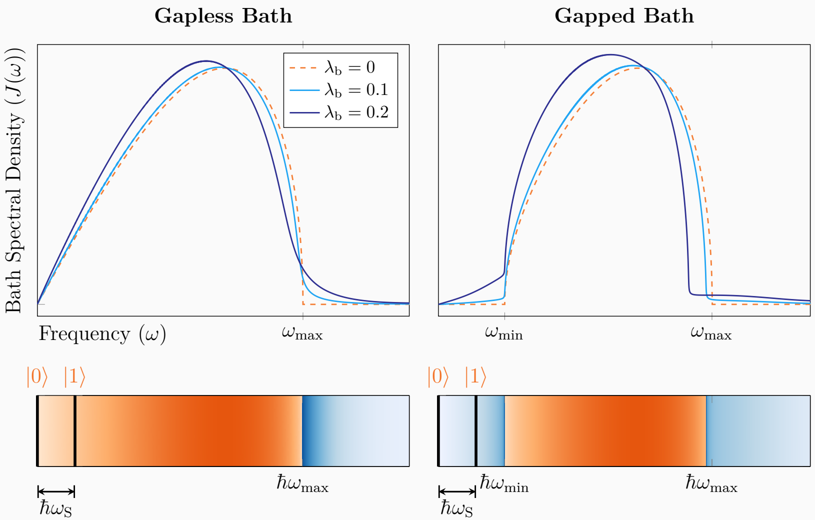

Figure 6: Bath spectral function as a function of frequency for a gapless (top left) and gapped (top right) bath at different values of the anharmonic coupling strength λ_b. Comparisson with the qubit energy scale (bottom).

Computational Results: Interpretation I

- The introduction of anharmonicites enhances the low–frequency regime of the bath.
- At low frequencies, $J(\omega) = \gamma\omega$ with $\gamma = \gamma(T, \omega_{\text{min}}, \omega_{\text{max}}, \lambda_{\text{b}}, c_{\text{sb}})$.
- For diagonal coupling, the phasing damping rate is:

$$\Gamma_{\text{diag}} = \lim_{\omega \to 0} \frac{2J(\omega)}{\tanh(\hbar\omega/(2k_B T))} = \frac{4k_B T\gamma}{\hbar}$$

$$\propto \begin{cases} c_{\text{sb}}^2 T + \mathcal{O}\left(c_{\text{sb}}^2 \lambda_{\text{b}}^2 T^2\right) & \text{Gapless Bath} \\ c_{\text{sb}}^2 \lambda_{\text{b}}^2 T^2 & \text{Gapped Bath} \end{cases}$$

  Transverse relaxation time: $T_2 = \Gamma_{\text{diag}}^{-1}$ (decoherence).
- For off–diagonal coupling, the amplitude damping rate is:

$$\Gamma_{\text{off–diag}} = \frac{J(\omega_{\text{s}})}{\tanh(\hbar\omega_{\text{s}}/(2k_B T))} .$$

  Longitudinal relaxation time: $T_1 = \Gamma_{\text{off–diag}}^{-1}$ (population redistribution), and transverse relaxation time $T_2 = 2\Gamma_{\text{off–diag}}^{-1}$.

Computational Results: Interpretation II

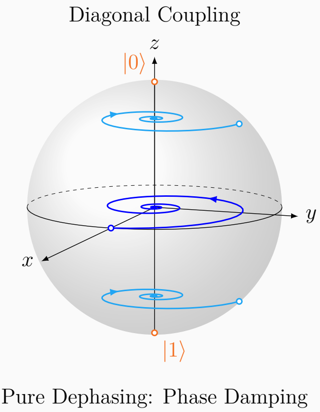

Figure 7: Bloch–sphere trajectories of the qubit for different initial states under diagonal coupling (left) and off–diagonal coupling (right).

Conclusions and Future Work

Conclusions and Future Work

Conclusions

1. Qubit–bath interaction produces a bath spectral density with linear low–frequency behavior.
2. Damping coefficients depend on temperature and bath anharmonicities: linear with temperature for gapless baths, quadratic for gapped baths.

Future Work and Applications

1. To extend the formalism to physically realizable systems, such as nitrogen–vacancy (NV) centers in diamond.
2. To apply this framework to quantum computing, with the goal of reducing decoherence in qubits embedded in solid materials.

References

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