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

Eberly Research Showcase 2025

Cristóbal Vallejos and Jorge O. Sofo

Department of Physics @ The Pennsylvania State University

Physical Motivation

Quantum Phase Decoherence

Two–Level System

Quantum Superposition
$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

How to measure it?

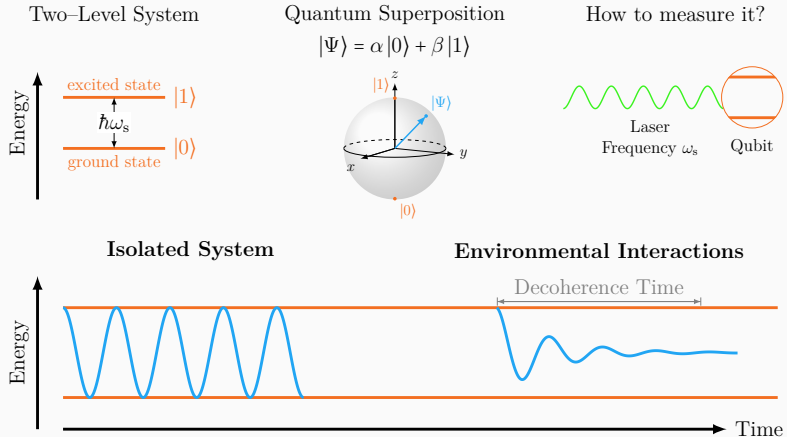**Isolated System**

Environmental Interactions

Figure 1: Quantum phase coherence for a two-level system. Environmental disturbance sources: electromagnetic waves (photons), mechanical vibrations (phonons), and temperature fluctuations.
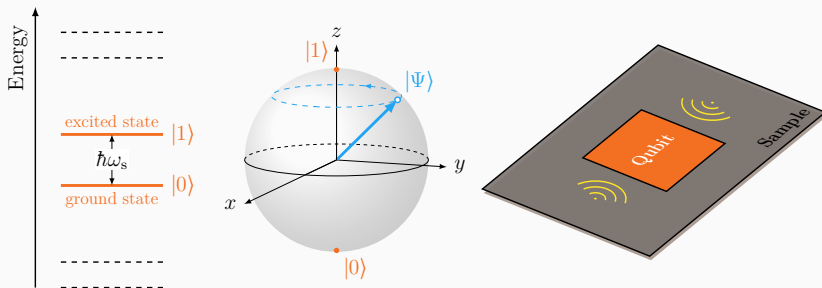
Figure 2: The qubit modeled as a two–level system (left). Bloch sphere representation of the qubit state and its free time evolution (middle). A qubit embedded in a solid affected interacting with lattice vibrations (right).
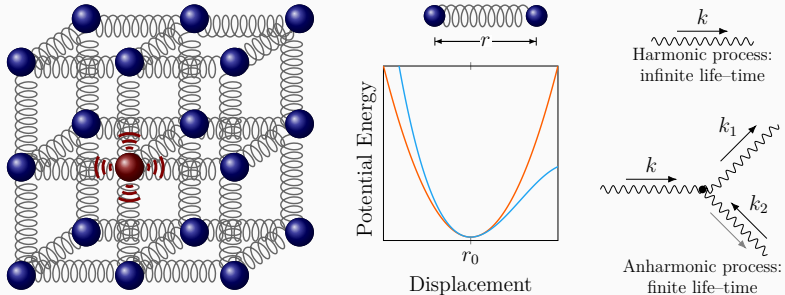
Figure 3: Illustration of lattice vibrations in a three–dimensional solid (left). Interatomic potential energy: harmonic potential (Hooke's law) vs. anharmonic potential, $U(r) = Kr^2/2 - \lambda r^3$ (middle). Diagrams of harmonic and three–phonon anharmonic processes (right).

What Can We Do?

State of the art

- The dynamics of a open quantum system coupled to a **harmonic baths** are well understood [2].

- The properties of **anharmonic solids** have been extensively studied on their own [3].

- **Numerical parameterizations** of anharmonic solids are available [4].

Our Goal

Develop a **microscopic framework** that captures how **anharmonic solid environments** modify the dynamics of **open quantum systems**.
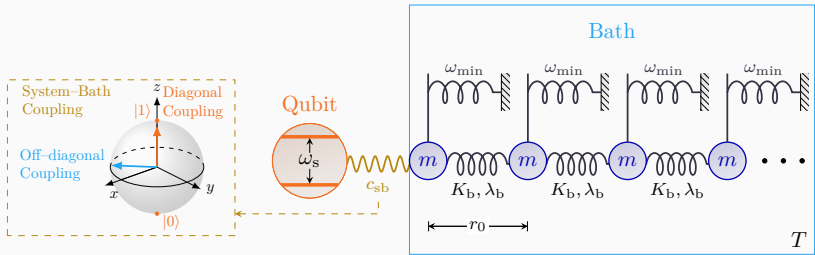
Theoretical Framework

Figure 4: 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.

Assumptions: Weak system–bath coupling and Markovian bath (short memory).

Lindblad Master Equation

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

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

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

- $\hat{\rho}_{\mathsf{s}}(t)$: density matrix of the qubit (populations and coherences).
- $\hat{H}_{\mathsf{s}}$: Hamiltonian (energy) of the qubit.
- $\mathcal{D}[\hat{\rho}_{\mathsf{s}}(t)] = \sum_j \gamma_j \left[\hat{L}_j \hat{\rho}_{\mathsf{s}}(t)\hat{L}_j^\dagger - \frac{1}{2}\left\{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_{\mathsf{s}}(t)\right\}\right]$: dissipative contributions from the bath.

The bath influences the qubit through:

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

The quantities 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.

Computational Results:
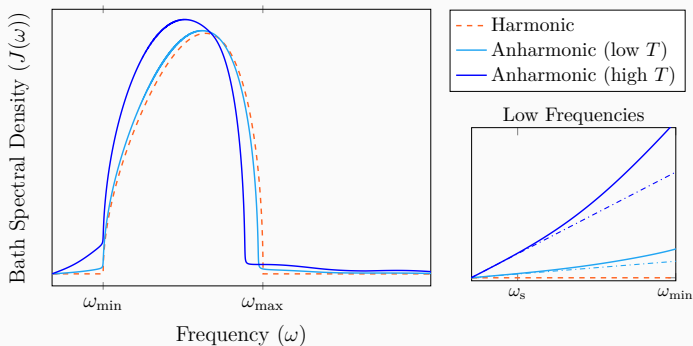# Presentation and Interpretation

Figure 5: Bath spectral function as a function of frequency for a gapped bath in the harmonic (temperature–independent) and anharmonic cases (low and high temperature).

- At low frequencies, the spectral density behaves as

$$J(\omega) = \alpha\omega \quad \text{with} \quad \alpha = \alpha(T, \omega_{\mathsf{min}}, \omega_{\mathsf{max}}, \lambda_{\mathsf{b}}, c_{\mathsf{sb}}).$$

- For **diagonal coupling**, the decoherence time is

$$\frac{1}{T_2} = \lim_{\omega \to 0} \frac{J(\omega)}{\tanh(\hbar\omega/(2k_B T))} = \frac{2k_B T\alpha}{\hbar} \propto c_{\mathsf{sb}}^2 \lambda_{\mathsf{b}}^2 T^2.$$
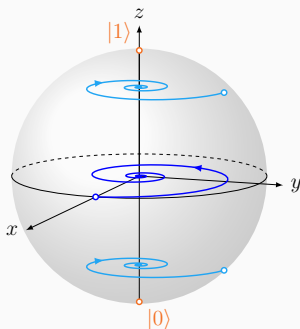
- For **off–diagonal coupling**, the population relaxation time is

$$\frac{1}{T_1} = \frac{J(\omega_{\mathsf{s}})}{2\tanh(\hbar\omega_{\mathsf{s}}/(2k_B T))}.$$
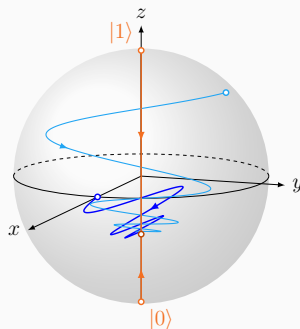
and the coherence relaxation time is $T_2 = 2T_1$.

Figure 6: Bloch–sphere trajectories of the qubit for different initial states under diagonal coupling (left) and off–diagonal coupling (right).

Conclusions and Future Work

Conclusions

1. Qubit–Phonon interaction produces a bath spectral density with a linear low–frequency behavior.
2. Damping coefficients depend on temperature and on anharmonicity of the bath.

Future Work and Applications

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

References

[1] Heinz-Peter Breuer and Francesco Petruccione. **The Theory of Open Quantum Systems.** Oxford University Press, Jan. 2007. ISBN: 978-0-19-921390-0. DOI: 10.1093/acprof:oso/9780199213900.001.0001.

[2] Hermann Grabert and Michael Thorwart. **"Quantum mechanical response to a driven Caldeira-Leggett bath".** en. In: *Physical Review E* 98.1 (July 2018), p. 012122. ISSN: 2470-0045, 2470-0053. DOI: 10.1103/PhysRevE.98.012122.

[3] S.W Lovesey. **Condensed matter physics: Dynamic correlations.** Benjamin/Cummings, 1986.

[4] Christoph Meier and David J. Tannor. **"Non-Markovian evolution of the density operator in the presence of strong laser fields".** In: *The Journal of Chemical Physics* 111.8 (Aug. 1999), pp. 3365–3376. ISSN: 0021-9606. DOI: 10.1063/1.479669.

[5] Ulrich Weiss. **Quantum dissipative systems, fourth edition.** Jan. 2012, pp. 1–566. ISBN: 978-981-4374-91-0. DOI: 10.1142/8334.

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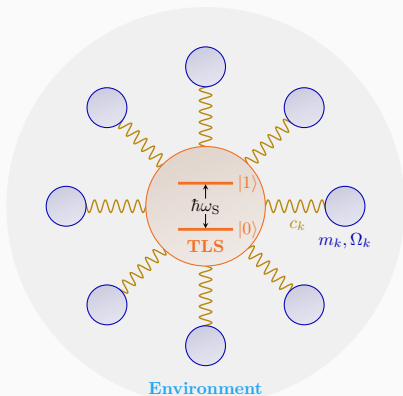

Figure 7: Schematic representation of the standard spin–boson model.

(Weak) Anharmonic Contributions

$$H_{\text{anharmonic}} = - \lambda_{\text{b}} \sum_{k_1, k_2, k_3} V^{(3)}(k_1, k_2, k_3) \hat{Q}_{k_1} \hat{Q}_{k_2} \hat{Q}_{k_3}$$
$$- \sum_{k_1, k_2, k_3, k_4} V^{(4)}(k_1, k_2, k_3, k_4) \hat{Q}_{k_1} \hat{Q}_{k_2} \hat{Q}_{k_3} \hat{Q}_{k_4}$$

where $V^{(3)}(k_1, k_2, k_3)$ are called *cubic force constants*, which include momenta conservation.

Bath Spectral Density

$$J(\omega) = \text{Im} \, \mathcal{F}\left[\theta(t - t') \left\langle \left\{ \sum_k c_k \hat{Q}_k(t), \sum_{k'} c_{k'} \hat{Q}_{k'}(t') \right\} \right\rangle_{\hat{\rho}_{\text{b}}(T)} \right].$$
$$= \frac{\pi}{2} \sum_k \frac{c_k^2}{m_k \Omega_k} \delta(\omega - \Omega_k) \rightarrow \sum_k p_k \frac{\omega}{[(\omega - \Omega_k)^2 + \Gamma_k^2][(\omega + \Omega_k)^2 + \Gamma_k^2]}$$

Supporting Material: Spectral Function

The bath spectral density is given by:

$$J(\omega) = \sum_k c_k^2 \mathcal{A}_k(\omega).$$

where $c_k = c_{\text{SB}} \sin(k)/\sqrt{N}$. See Figure 4. $A_k(\omega)$ is the bath spectral function:

$$\mathcal{A}_k(\omega) = \frac{1}{m} \lim_{\eta \to 0^+} \frac{\Sigma_k''(T,\omega) + 2\omega\eta}{\left(\omega^2 - \Omega_k^2 - \Sigma_k'(T,\omega)\right)^2 + \left(\Sigma_k''(T,\omega) + 2\omega\eta\right)^2},$$

where η is a mathematical regulator introduced for cases in which $\Sigma_k''(T,\omega) = 0$. For the model in Fig. 4, the phonon frequency is $\Omega_k = \sqrt{\omega_m^2 + 4\omega_b^2 \sin^2(k/2)}$, and the self–energy is
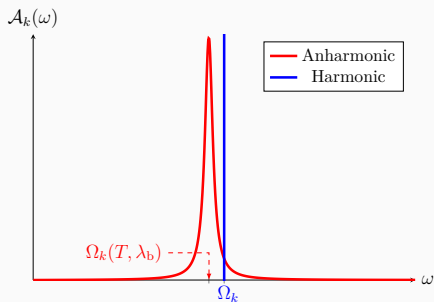
$$\Sigma_k''(T,\omega) = \frac{8\pi\lambda_b^2\omega_R^5}{N} \sum_{k_2} \frac{\sin^2(k/2)\sin^2(k_2/2)\sin^2((k-k_2)/2)}{\Omega_{k-k_2}\Omega_{k_2}}$$

$$\times \left[\begin{array}{l} (1 + n_{k_2}(T) + n_{k-k_2}(T))(\delta(\omega - \Omega_+) - \delta(\omega + \Omega_+)) \\ + (n_{k_2}(T) - n_{k-k_2}(T))(\delta(\omega - \Omega_-) - \delta(\omega + \Omega_-)) \end{array} \right].$$

$$J(\omega) = \sum_k c_k^2 \mathcal{A}_k(\omega)$$

Harmonic case: Dirac deltas.
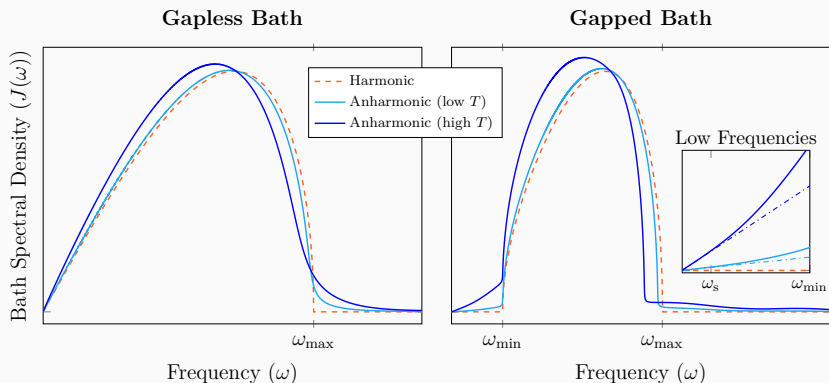
Anharmonic case: Lorentzians.

Figure 8: Bath spectral function as a function of frequency for a gapless (left) and gapped (right) bath for the harmonic and anharmonic case (low and high temperature).

$$\frac{1}{T_2} \propto \begin{cases} c_{sb}^2 T + \mathcal{O}\left(c_{sb}^2 \lambda_b^2 T^2\right) & \text{Gapless Bath} \\ c_{sb}^2 \lambda_b^2 T^2 & \text{Gapped Bath} \end{cases}$$