

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

Cristobal I. Vallejos¹ Ricardo C. Heitzer¹ Jorge O. Sofo^{1,2}

¹Department of Physics, Penn State ²Materials Research Institute, Penn State



Overview

Quantum systems are never completely isolated—they constantly interact with their surroundings (the bath). This coupling, especially through vibrations, can limit the performance of emerging technologies such as quantum sensors. In a purely harmonic bath, where phonons have infinite lifetimes, energy transfer is restricted by a spectral gap. Introducing bath anharmonicities (nonlinear effects) enables phonon scattering processes that allow low-frequency transitions. We study a qubit embedded in a crystal and show how these anharmonic processes influence both its energy dissipation and decoherence.

State of the art: The dynamics of an 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.

Physical Motivation

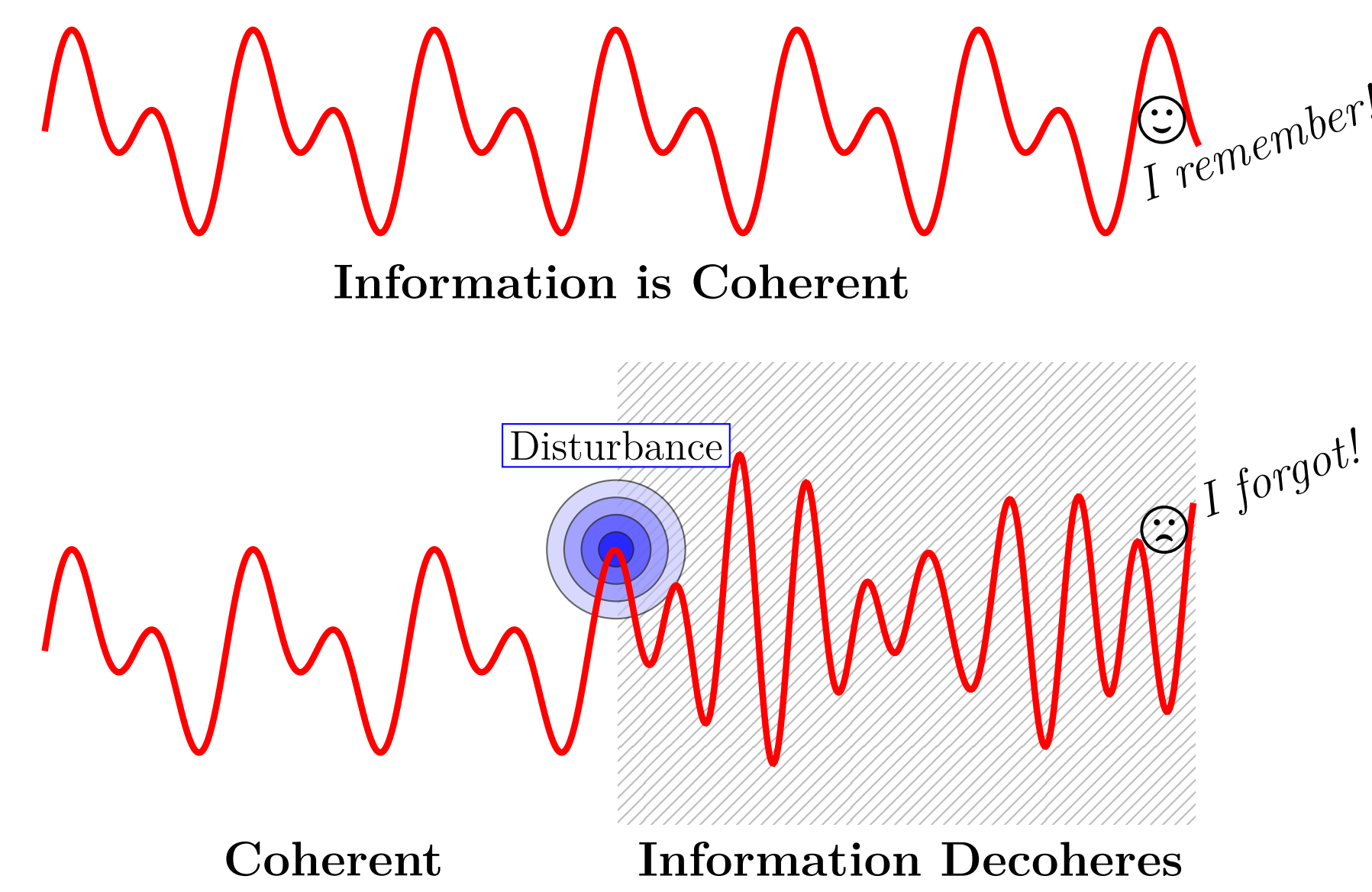


Figure 1. Quantum phase coherence: discernible, repeating pattern (top). Decoherence: loss of a clear pattern (bottom). Environmental disturbance sources: electromagnetic waves (photons), mechanical vibrations (phonons), and temperature fluctuations.

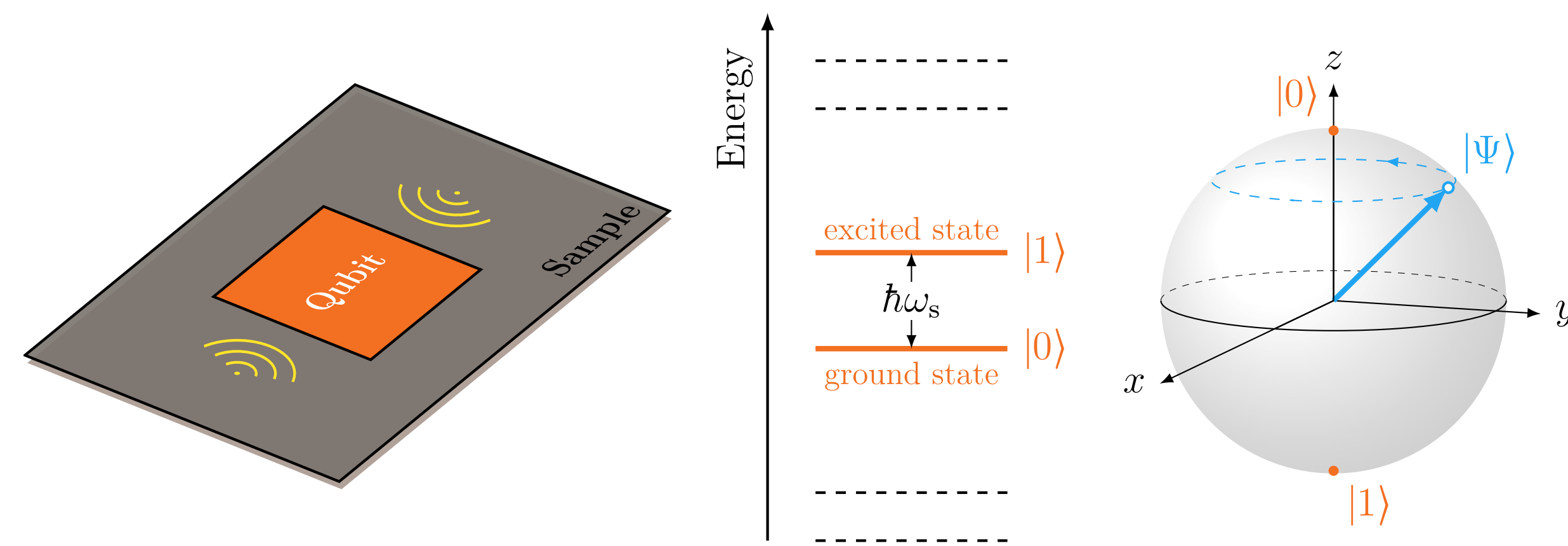


Figure 2. A qubit embedded in a solid affected interacting with lattice vibrations (left). The qubit modeled as a two-level system (middle). Bloch sphere representation of the qubit state and its free time evolution (right).

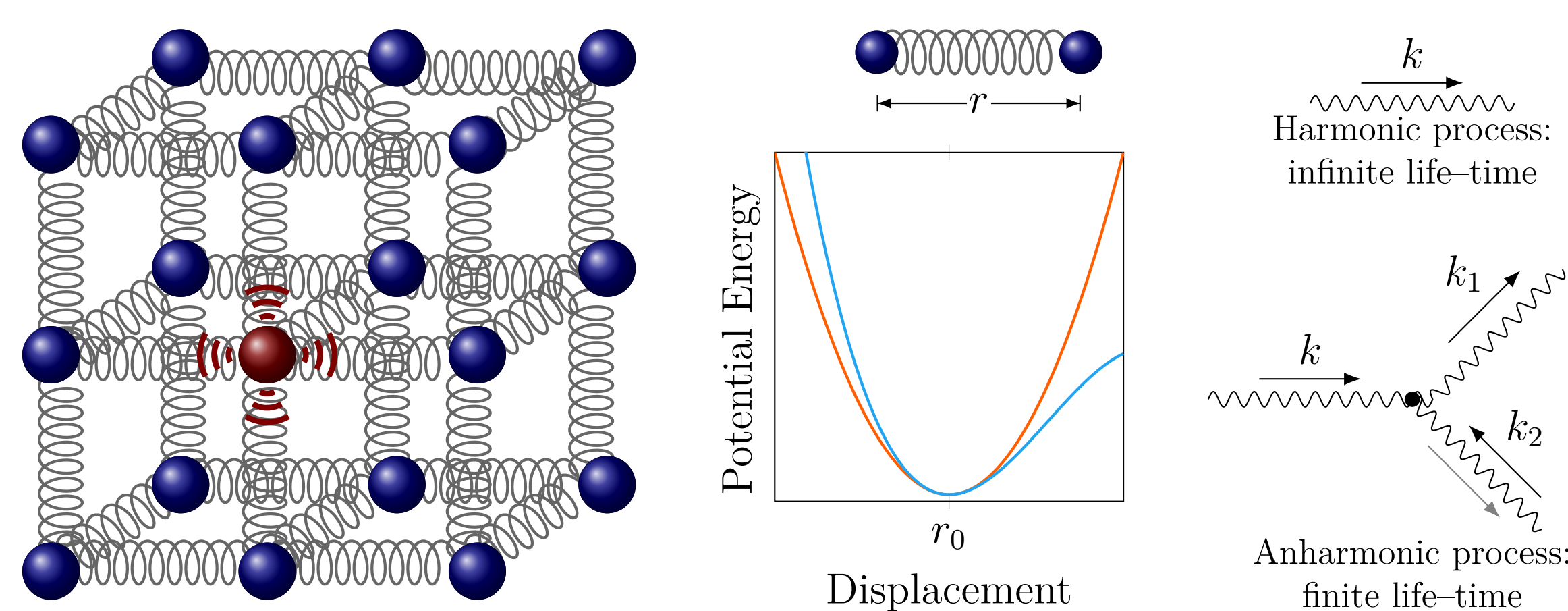


Figure 3. Illustration of lattice vibrations in a three-dimensional solid (left). Interatomic potential energy: harmonic potential vs. anharmonic potential, $U(r) = kr^2/2 - \lambda r^3$ (middle). Diagrams of harmonic and three-phonon anharmonic processes (right).

Theoretical Framework

The Hamiltonian describing the qubit-bath system consists of three parts [2, 3]:

$$\hat{H} = \underbrace{\frac{\hbar\omega_s}{2}\hat{\sigma}_z}_{\text{Qubit}} + \underbrace{\sum_k \left[\frac{\hat{P}_k^2}{2m} + \frac{m\Omega_k^2}{2}\hat{Q}_k^2 \right]}_{\text{Bath}} + \underbrace{\lambda_b \hat{H}_{\text{anharmonic}} + \sum_{k,j} c_{k,j} \hat{\sigma}_j \hat{Q}_k}_{\text{SB Interaction}}. \quad (1)$$

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

$$\frac{d}{dt}\hat{\rho}_s(t) = -\frac{i}{\hbar} \left[\hat{H}_s + \hat{H}_{\text{LS}}, \hat{\rho}_s(t) \right] + \mathcal{D}[\hat{\rho}_s(t)] \quad \text{with} \quad \hat{\rho}_s(t) = \begin{pmatrix} \hat{\rho}_{00}(t) & \hat{\rho}_{01}(t) \\ \hat{\rho}_{10}(t) & \hat{\rho}_{11}(t) \end{pmatrix}. \quad (2)$$

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

The bath influences the qubit through:

1. **Lamb shift:** renormalized frequency $\bar{\omega}_s = \omega_s + \Delta_{\text{LS}}$.
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:

$$J(\omega) = \text{Im} \mathcal{F} \left[\theta(t-t') \left\langle \left\{ \sum_k c_k \hat{Q}_k(t), \sum_{k'} c_{k'} \hat{Q}_{k'}(t') \right\} \right\rangle_{\hat{\rho}_b} \right]. \quad (3)$$

Our Toy Model

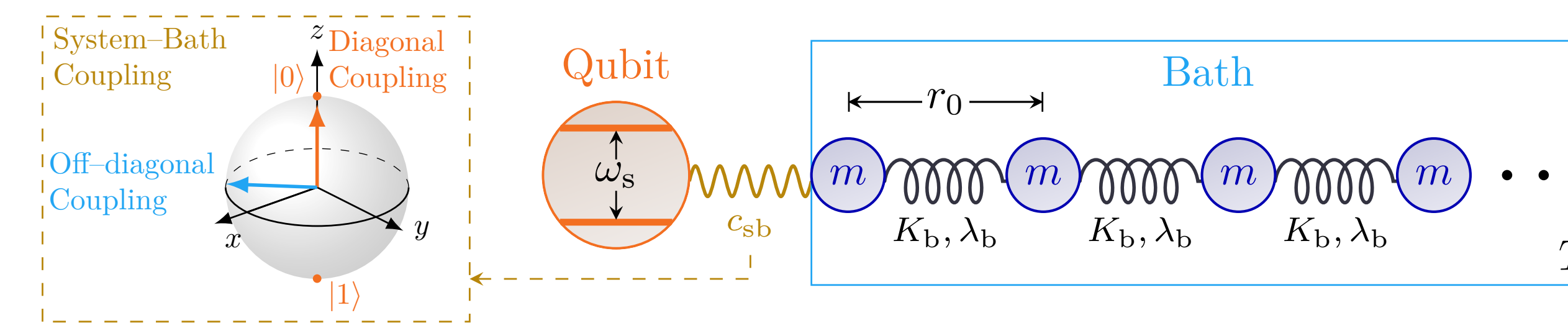


Figure 4. Pictorial representation of a one-dimensional model of a qubit coupled to an anharmonic crystal. The coupling to the qubit states can be either diagonal (affecting populations) or off-diagonal (affecting coherences).

Computational Results

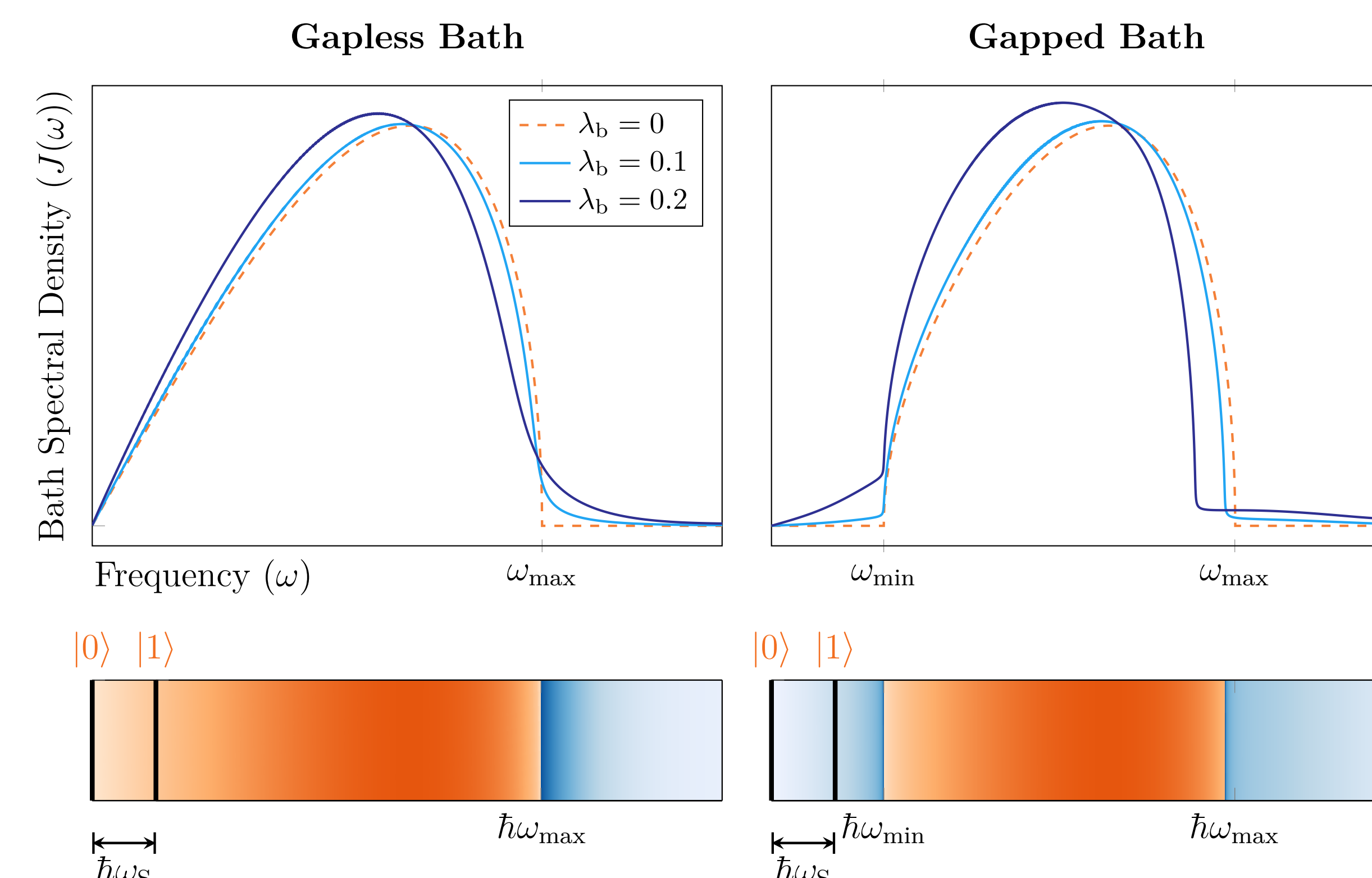


Figure 5. Bath spectral function as a function of frequency for a gapless (top left) and gapped (top right) bath at different values of the anharmonic coupling strength λ_b . Color maps (bottom) show the corresponding spectral densities compared to the qubit energy scale, with harmonic effects in orange tones and anharmonic effects in blue tones.

Interpretation of the Results

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

$$\Gamma_{\text{diag}} = \lim_{\omega \rightarrow 0} \frac{2J(\omega)}{\tanh(\hbar\omega/(2k_B T))} = \frac{4k_B T \gamma}{\hbar} \propto \begin{cases} c_{\text{sb}}^2 T + \mathcal{O}(c_{\text{sb}}^2 \lambda_b^2 T^2) & \text{Gapless Bath} \\ c_{\text{sb}}^2 \lambda_b^2 T^2 & \text{Gapped Bath} \end{cases} \quad (4)$$

Transverse relaxation time: $T_2 = \Gamma_{\text{diag}}^{-1}$ (decoherence).

- For off-diagonal coupling, the amplitude damping rate is:

$$\Gamma_{\text{off-diag}} = \frac{J(\omega_s)}{\tanh(\hbar\omega_s/(2k_B T))}. \quad (5)$$

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

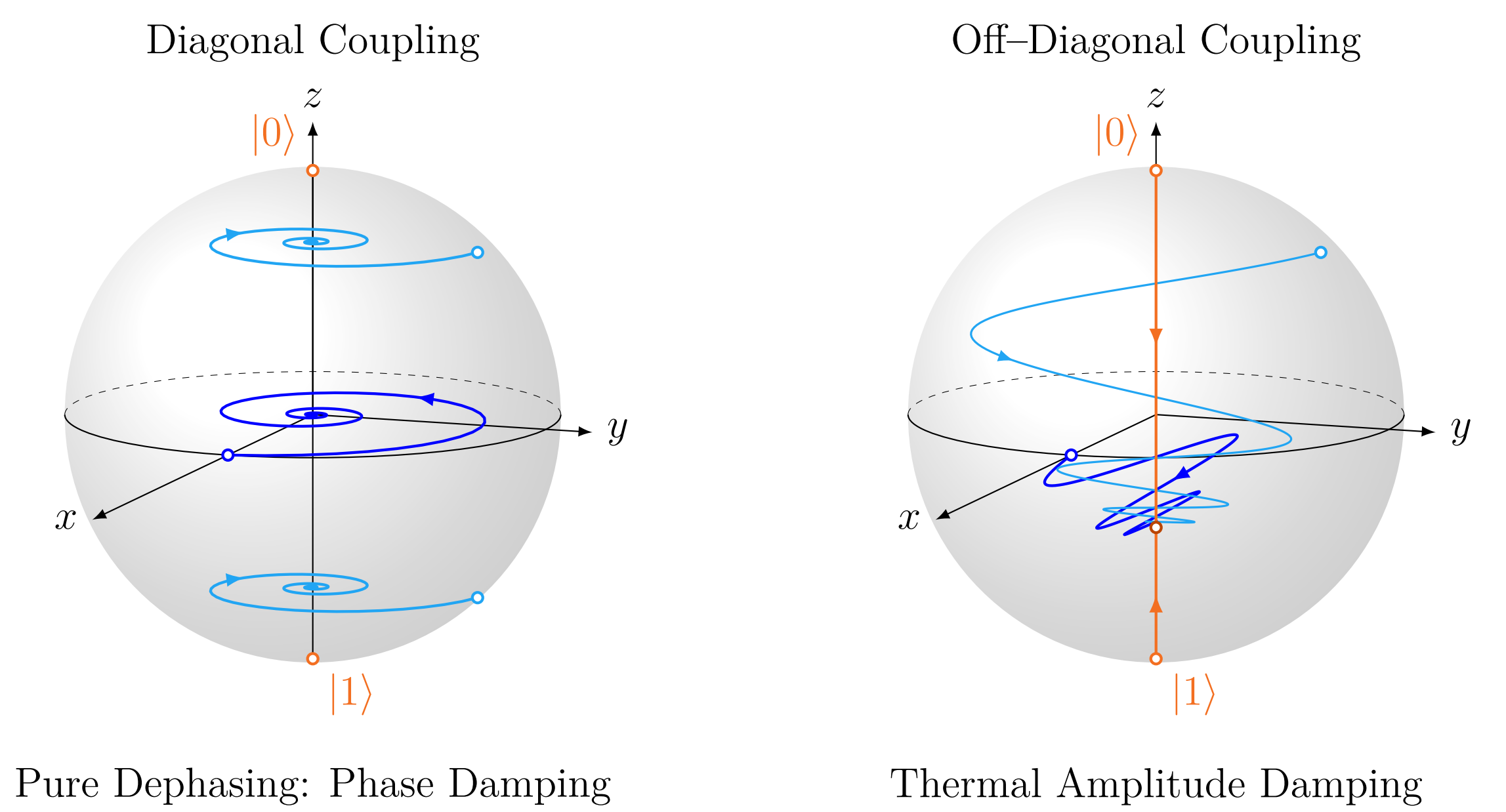


Figure 6. Bloch-sphere trajectories of the qubit for different initial states under diagonal coupling (left) and off-diagonal coupling (right).

Conclusions and Future Work

Conclusions

1. Qubit-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 (see Ricardo's poster).
2. To apply this framework to quantum computing, with the goal of reducing decoherence in qubits embedded in solid materials.

Take-Home Message

Understanding how environmental vibrations affect quantum systems brings us closer to designing materials and devices that preserve quantum coherence—an essential step toward practical quantum technologies.

References

- [1] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press, Jan. 2007.
- [2] H. Grabert and M. Thorwart, *Quantum mechanical response to a driven caldeira-leggett bath*, Physical Review E, 98 (2018), p. 012122.
- [3] S. Lovesey, *Condensed matter physics: Dynamic correlations*, Benjamin/Cummings, 1986.
- [4] C. Meier and D. J. Tannor, *Non-markovian evolution of the density operator in the presence of strong laser fields*, The Journal of Chemical Physics, 111 (1999), p. 3365–3376.
- [5] U. Weiss, *Quantum dissipative systems*, fourth edition, 01 2012.