

Characterization of coherent impurity effects in solid-state qubits

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We propose a characterization of the effects of bistable *coherent impurities* in solid-state qubits. We introduce an effective impurity description in terms of a tunable spin-boson environment and solve the dynamics for the qubit coherences. The dominant rate characterizing the asymptotic time limit is identified, and signatures of non-Gaussian behavior of the quantum impurity at intermediate times are pointed out. An alternative perspective considering the qubit as a measurement device for the spin-boson impurity is proposed.

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Coherent nanodevices are inevitably exposed to fluctuations due to the solid-state environment. Well-studied examples are charged impurities and stray flux tubes which are sources of telegraphic noise in a wide class of metallic devices. Large-amplitude low-frequency (mostly $1/f$) noise, ubiquitous in amorphous materials,¹ is also routinely measured in single-electron-tunneling devices.² Noise sources are sets of impurities located in the oxides and in the substrate, each producing a bistable stray polarization. Telegraphic noise has also been observed in semiconductor- and superconductor-based nanocircuits.³ The possible presence of impurities entangled with the device has been suggested in Ref. 4. Recent experiments on Josephson qubits indicated that charged impurities may also be responsible for noise⁵ exhibiting an Ohmic power spectrum at GHz frequencies. Different theoretical models have been proposed aiming at a unified description of broadband noise sources. They share the common idea that the variety of observed features are due to the dynamics of ensembles of bistable impurities.⁵⁻⁸ In particular in Ref. 8 it has been proposed that a noise power spectrum compatible with the observed relaxation of charge-Josephson qubits⁵ can be obtained if sets of *coherent* impurities are considered.

Solid-state noise also determines dephasing. This issue has attracted a great deal of interest in recent years since it has been recognized as a severe hindrance for the implementation of quantum hardware in the solid state. The effect of slow noise due to ensembles of thermal^{9,10} and nonthermal⁷ fluctuators has been addressed. Slow noise explains the non-exponential suppression of coherent oscillations observed when repeated measurements are performed.^{11,12} In addition fluctuations active *during time evolution* represent an unavoidable limitation even when a single-shot measurement scheme or dynamical decoupling protocols¹³ are available. Note that at experimental temperatures (~ 10 mK) quantum impurities may have a significant influence.

In this Rapid Communication we investigate qubit dephasing during time evolution due to coupling to a coherent impurity. The *full* qubit dynamics is solved in the regime where qubit relaxation processes are absent. We show how the coherent and nonlinear dynamics of the impurity is reflected in the qubit behavior. We identify regimes characterized by a strong qubit-impurity back-action. Specifically, we discuss the dependence on the impurity preparation and beating phenomena. An alternative interpretation with the qubit

acting as a measurement device for the impurity is presented at the end of this paper.

Model. We model the impurity as a two-state system, $\mathcal{H}_I = -\frac{1}{2}\varepsilon\tau_z - \frac{1}{2}\Delta\tau_x$, coupled to the qubit (σ) via $\mathcal{H}_{QI} = -\frac{1}{2}v\sigma_z\tau_z$ ($\hbar=1$). This anisotropic coupling has been discussed for charge qubits, where it models the electrostatic interaction.⁸⁻¹⁰ In this case the two physical states ($\tau_z \rightarrow \pm 1$) correspond to a bistable stray polarization of the qubit. They are viewed as the ground states of a double-well deformation potential, the impurity oscillating coherently between them with frequency $\Omega_I = \sqrt{\varepsilon^2 + \Delta^2}$. Dissipative transitions between the minima come from the interaction with a bosonic bath¹⁴ ($\mathcal{H}_B = \sum_\alpha \omega_\alpha a_\alpha^\dagger a_\alpha$) via $\mathcal{H}_{IB} = -\frac{1}{2}\hat{X}\tau_z$. The operator $\hat{X} = \sum_\alpha \lambda_\alpha (a_\alpha + a_\alpha^\dagger)$ is a collective displacement with Ohmic power spectrum $S(\omega) = 2\pi K\omega \coth \frac{\omega}{2T}$ with a high-energy cutoff at ω_c ($k_B=1$).¹⁴ This *spin-boson environment* (SBE) may induce a variety of qubit dynamical behaviors, since its degree of coherence depends on K and on temperature T .¹⁴ For instance, for weak damping, $K \ll 1$ a crossover occurs between a low-“impurity-temperature,” $T \ll \Omega_I$, regime, where the impurity performs damped oscillations, to the regime of incoherent dynamics if $T \gg \Omega_I$ [white noise $S(\omega) \approx 4\pi KT$].¹⁵

We assume that the qubit Hamiltonian conserves σ_z ; therefore, the impurity induces *pure dephasing*¹⁴ with no relaxation of the qubit.¹⁶ This regime is very interesting since energy exchange processes do not blur decoherence of the qubit, which is then maximally sensitive to the SBE dynamics. Pure dephasing due to Fano impurities was addressed in Ref. 9; recently, the asymptotic dynamics has been studied.¹⁷

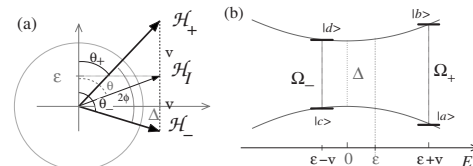


FIG. 1. (a) Impurity Bloch sphere. An isolated impurity \mathcal{H}_I defines the mixing angle $\theta = \arctan \Delta/\varepsilon$; \mathcal{H}_\pm define $\theta_\pm = \arctan \Delta/(\varepsilon \pm v)$. (b) Impurity bands $\pm \sqrt{E^2 + \Delta^2}$: impurity energy splittings depend on the qubit state, $\Omega_\pm = \sqrt{(\varepsilon \pm v)^2 + \Delta^2}$. Eigenstates of \mathcal{H}_0 are $\{|i\rangle\}$, $i=a, b, c, d$. Conservation of σ_z allows only intra-doublet processes $a \leftrightarrow b$, $c \leftrightarrow d$.

This model corresponds to a over-damped impurity (SBE at $K=\frac{1}{2}$); here, we consider $K\ll 1$ where the impurity may behave coherently.

For pure dephasing the qubit Hamiltonian can be gauged away by a proper rotation. In this picture we consider the reduced density matrix $\rho(t)$ describing the entangled qubit-impurity system. For $K\ll 1$ the interaction with the bosonic bath is studied by the Born-Markov master equation¹⁸ (ME)

$$\partial_t \rho(t) = -i[\mathcal{H}_0, \rho(t)] - \int_0^\infty dt' \left\{ \frac{1}{4} S(t') [\tau_z, [\tau_z(t'), \rho(t)]] + \frac{i}{2} \chi(t') [\tau_z, [\tau_z(t'), \rho(t)]_+] \right\}, \quad (1)$$

where $\mathcal{H}_0 = \mathcal{H}_{QI} + \mathcal{H}_I$ is the undamped Hamiltonian. Here, the transform $S(t)$ of the power spectrum and the bath susceptibility $\chi(t) = -i\langle [\hat{X}(t), \hat{X}(0)]_+ \rangle \Theta(t)$ enter the damping term. We introduce the *conditional* Hamiltonians of the impurity $\mathcal{H}_\pm = -\frac{1}{2}(\varepsilon \pm v)\tau_z - \frac{1}{2}\Delta\tau_x$ (see Fig. 1) and the eigenvectors of \mathcal{H}_0 , $\{|i\rangle\}$, which are factorized in eigenstates of σ_z and of \mathcal{H}_\pm .¹⁵ The qubit dynamics at pure dephasing is described by the coherences $\langle \sigma_\pm(t) \rangle = \text{Tr}[\rho(t)(\sigma_x \pm i\sigma_y) \otimes \mathbb{1}_\tau]$, and in particular

$$\langle \sigma_-(t) \rangle = [\rho_{ac}(t) + \rho_{bd}(t)] \cos \phi - [\rho_{ad}(t) - \rho_{bc}(t)] \sin \phi,$$

where $\phi = \frac{1}{2}(\theta_- - \theta_+)$ is a combination of the mixing angles of \mathcal{H}_\pm (Fig. 1). Since σ_z is conserved, the damping tensor presents only four nonvanishing 4×4 diagonal blocks. We focus on the block acting on the terms entering $\langle \sigma_-(t) \rangle$. Performing a partial secular approximation within this block, we get two sets of decoupled equations for ρ_{ac}, ρ_{bd} and ρ_{ad}, ρ_{bc} . We quote here the first set

$$\begin{pmatrix} \dot{\rho}_{ac}(t) \\ \dot{\rho}_{bd}(t) \end{pmatrix} = \begin{pmatrix} i\delta - \Gamma_1 & \Gamma_{12} \\ \Gamma_{21} & -i\delta - \Gamma_2 \end{pmatrix} \begin{pmatrix} \rho_{ac}(t) \\ \rho_{bd}(t) \end{pmatrix}, \quad (2)$$

where $\delta = \frac{1}{2}(\Omega_+ - \Omega_-)$, Fig. 1. The rates Γ_i , describing dissipative transitions and pure dephasing processes between the four states and the bosonic bath, read

$$\begin{aligned} \Gamma_{1,2} &= \alpha_+^2 \Gamma_\mp(\Omega_+) + \alpha_-^2 \Gamma_\mp(\Omega_-) + \eta_s S(0), \\ \Gamma_{12,21} &= \alpha_+ \alpha_- [\Gamma_\pm(\Omega_+) + \Gamma_\pm(\Omega_-)], \\ \alpha_\pm &= \frac{1}{\sqrt{2}} \sin \theta_\pm; \quad \eta_s = \frac{1}{2} \sin^2 \bar{\theta} \sin^2 \phi, \end{aligned} \quad (3)$$

where $\bar{\theta} = \frac{1}{2}(\theta_+ + \theta_-)$. Here $\Gamma_\pm(\omega) = 2\pi K \omega [\coth(\omega/2T) \pm 1]$ are the impurity emission (+) and absorption (-) rates of energy ω . The elements ρ_{ad}, ρ_{bc} satisfy similar equations with δ replaced by $\Omega = \frac{1}{2}(\Omega_+ + \Omega_-)$ and rates

$$\begin{aligned} \Gamma_{3,4} &= \alpha_+^2 \Gamma_\mp(\Omega_+) + \alpha_-^2 \Gamma_\mp(\Omega_-) + \eta_c S(0), \\ \Gamma_{34,43} &= \alpha_+ \alpha_- [\Gamma_\pm(\Omega_+) + \Gamma_\mp(\Omega_-)], \\ \eta_c &= \frac{1}{2} \cos^2 \bar{\theta} \cos^2 \phi. \end{aligned}$$

Diagonalization of Eq. (2) and of the corresponding set for ρ_{ad}, ρ_{bc} yields the eigenvalues

$$\begin{aligned} \lambda_{1,2} &= -\frac{\Gamma_1 + \Gamma_2}{2} \pm \frac{1}{2} \sqrt{(2i\delta + \Gamma_2 - \Gamma_1)^2 + 4\Gamma_{12}\Gamma_{21}}, \\ \lambda_{3,4} &= -\frac{\Gamma_3 + \Gamma_4}{2} \pm \frac{1}{2} \sqrt{(2i\Omega + \Gamma_4 - \Gamma_3)^2 + 4\Gamma_{34}\Gamma_{43}}. \end{aligned} \quad (4)$$

The explicit form of $\langle \sigma_-(t) \rangle$ depends on the initial conditions for $\rho(t)$. Because of the high accuracy of preparation presently achieved in solid-state implementations, factorized qubit-impurity states $\rho(0) = \rho_\sigma(0) \otimes \rho_\tau(0)$ represent a realistic scenario. The impurity initial state is instead out of the experimentalist's control; thus, we choose $\rho_\tau(0) = \frac{1}{2}(\mathbb{1}_\tau + p_z \tau_z)$. The impurity starts from a totally unpolarized state for $p_z = 0$, from a pure state if $p_z = \pm 1$. Additional $p_{x,y} \tau_{x,y}$ terms are not expected to qualitatively effect the qubit dynamics. This class of initial states guarantees the positivity of the dynamical process ensuing from Eq. (1). With this choice we find

$$\begin{aligned} \langle \sigma_-(t) \rangle &= \langle \sigma_-(0) \rangle \sum_i A_i e^{\lambda_i t}, \\ A_{1,2} &= \frac{\cos \phi}{2(\lambda_1 - \lambda_2)} \left\{ \cos \phi [\lambda_1 - \lambda_2 \pm (\Gamma_{12} + \Gamma_{21})] \mp p_z \cos(\theta + \bar{\theta}) \right. \\ &\quad \left. \times [-2i\delta - \Gamma_2 + \Gamma_1 + \Gamma_{12} - \Gamma_{21}] \right\}, \\ A_{3,4} &= \frac{\sin \phi}{2(\lambda_3 - \lambda_4)} \left\{ \sin \phi [\lambda_3 - \lambda_4 \mp (\Gamma_{34} + \Gamma_{43})] \right. \\ &\quad \left. \mp p_z \sin(\theta + \bar{\theta}) [-2i\Omega - \Gamma_4 + \Gamma_3 - \Gamma_{34} + \Gamma_{43}] \right\}. \end{aligned} \quad (5)$$

Equations (4)–(6) are the main result of this paper. They cover the regime where $S(\Omega_\pm) \ll \Omega_\pm$. Single-phonon processes dominate at low T , whereas multiphonon exchanges are paramount at higher T where the white noise results of Ref. 15 are recovered. Reliability of ME is confirmed by a real-time path-integral calculation.

We now focus our analysis on the low- T regime $T \ll \Omega_-$. Here effects of the dissipative processes internal to the SBE on the qubit behavior are clearly identifiable. In this limit energy absorption processes are exponentially suppressed [$\Gamma_-(\Omega_\pm) \approx 0$] and the eigenvalues take the forms

$$\begin{aligned} \lambda_1 &= i\delta - \eta_s S(0), \\ \lambda_2 &= -i\delta - \frac{\gamma_{r+} + \gamma_{r+}^0 + \gamma_{r-} + \gamma_{r-}^0}{4} - \eta_s S(0), \\ \lambda_{3,4} &= \pm i\Omega - \frac{\gamma_{r\mp} + \gamma_{r\mp}^0}{4} - \eta_c S(0), \end{aligned} \quad (7)$$

where intradoublet relaxation rates (see Fig. 1)

$$\gamma_{r\pm} = \frac{1}{2} \sin^2(\theta_\pm) S(\Omega_\pm) = \frac{1}{2} \left(\frac{\Delta}{\Omega_\pm} \right)^2 S(\Omega_\pm) \quad (8)$$

have been introduced ($\gamma_{r\pm}^0$ value at $T=0$). Note that pure dephasing processes $\propto S(0)$ are not a simple sum of intradoublet dephasing terms, $\gamma_{\phi\pm} = \frac{1}{2} \cos^2(\theta_\pm) S(0)$.

In the following we present a selection of illustrative behaviors for $\varepsilon > \Delta$. In this regime the two conditional Hamiltonians \mathcal{H}_\pm may differ significantly and enforce peculiar impurity dynamical behaviors: for example, beatings when δ approaches Ω —i.e., around $\varepsilon = v$, which identifies a sort of “resonance regime” for our problem.

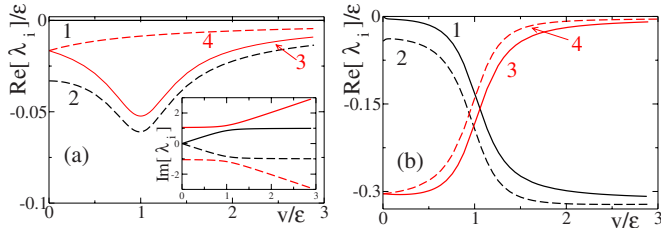


FIG. 2. (Color online) The four rates $\text{Re}[\lambda_i]$ from Eqs. (4) for $K=0.1$, $\varepsilon=3\Delta$. In (a) $T=0$. Inset: imaginary parts (independent on temperature for $T<\Omega_+$). In (b) $T=0.5\Delta$.

We first characterize the asymptotic qubit dynamics, by the T and v dependence of the eigenvalues. At zero temperature the pure dephasing contributions fade away, and one rate $\text{Re}[\lambda_1]$ vanishes, as expected. Only emission processes contribute to the residual rates, and they directly sound out intradoublet relaxation rates $\gamma_{r\pm}^0$. Their behaviors reflect the sensitivity of \mathcal{H}_{\pm} to noise acting along τ_z . While γ_{r+}^0 decreases with increasing v , γ_{r-}^0 takes a maximum at the resonance point [see Eq. (8)], the “transverse” ($\theta_-=\pi/2$) noise condition for \mathcal{H}_- . This implies a nonmonotonous dependence of $\text{Re}[\lambda_{2,3}]$ on the coupling v , Fig. 2(a). The imaginary parts of $\lambda_{1,2}$ and $\lambda_{3,4}$ interchange characters at resonance [Fig. 2(a), inset], leading to possible hybridization (see below). With increasing T the main variation of the rates comes from the pure dephasing terms $\propto S(0)$. As a difference with $T=0$, all the rates are finite and cross around resonance, Fig. 2(b).

These features are crucial for the asymptotic dynamics of $\langle\sigma_-(t)\rangle$, which does not depend on the impurity preparation. We then expect, at $T=0$, undamped oscillations with δ , while at finite T , damped oscillations driven by one or two complex eigenvalues. For example, in the case of Fig. 2(b) the dominant rate is $\text{Re}[\lambda_1]$ for $v<\varepsilon$ and $\text{Re}[\lambda_4]$ for $v>\varepsilon$. It is a

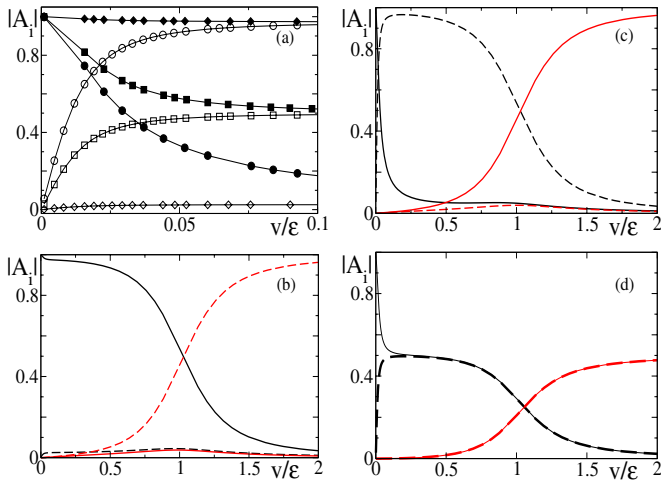


FIG. 3. (Color online) Weights $|A_i|$ of $e^{\lambda_i t}$ from Eq. (6) as a function of v/ε , for $T=0$, $\varepsilon=3\Delta$, and $K=0.1$. (a) Dominant weights for small v : $|A_1|$ (solid symbols), $|A_2|$ (open symbols) for $p_z=0$ (squares), $p_z=-1$ (circles), and $p_z=1$ (diamonds). Effect of impurity preparations: $p_z=1$ (b), $p_z=-1$ (c), and $p_z=0$ (unpolarized state) (d). $|A_1|$ black line, $|A_2|$ black dashed line, $|A_3|$ red (gray line), and $|A_4|$ red (gray line) dashed.

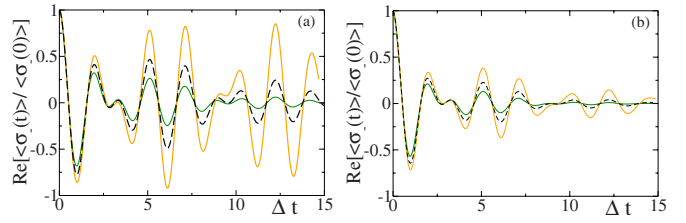


FIG. 4. (Color online) $\text{Re}[\langle\sigma_-(t)\rangle/\langle\sigma_-(0)\rangle]$ at resonance $\varepsilon=v=3\Delta$ for initial states (a) $p_z=1$, slow decay with $\text{Re}[\lambda_{1/4}]$; (b) $p_z=-1$, fast decay with $\text{Re}[\lambda_{2/3}]$. Parameters: $T=0$ orange (light gray line), $T=0.5\Delta$ black dashed line, and $T=0.9\Delta$ green (dark gray line), $K=0.1$.

nonmonotonous function of v and a cusp signals crossing of eigenvalues (a similar effect may explain the nonmonotonic behavior of Ref. 17).

At intermediate times, all eigenvalues may be relevant, depending on the weights A_i in Eq. (6). To substantiate this point, in Fig. 3 we show A_i corresponding to the eigenvalues in Fig. 2(a) for different preparations. Remarkably, the weights very weakly depend on T (not shown); then, the following picture generally holds for $T<\Omega_-$. For extreme weak coupling, $v\rightarrow 0$, $|A_1|\approx 1$ [Fig. 3(a)], implying universal dynamics independent of the initial conditions. The dominant eigenvalue is λ_1 with $\delta\rightarrow 0$ and $\langle\sigma_-(t)\rangle$ decays exponentially with the golden rule rate $\Gamma_{GR}=\frac{v^2}{2}\frac{S(0)}{\varepsilon^2+\Delta^2}\sin^4\theta$. In this regime the impurity acts as a Gaussian reservoir and may be described with linear response theory in the coupling v . Away from this tiny region non-Gaussian effects occur and different impurity preparations result in different time behaviors, giving separate information on the various eigenvalues. Far from resonance, a single frequency shows up in $\langle\sigma_-(t)\rangle$ independently of p_z (δ if $v<\varepsilon$, Ω if $v>\varepsilon$). Damping of the oscillations depends on the initial condition, Figs. 3(b)–3(d). For instance, at finite $v<\varepsilon$, the decay occurs with $\text{Re}[\lambda_1]$ if

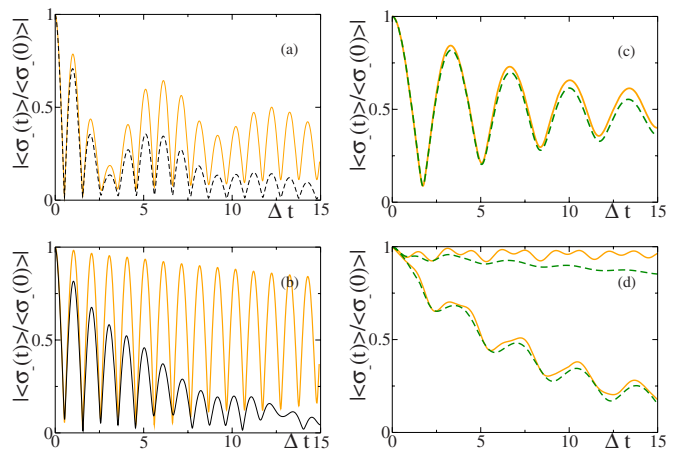


FIG. 5. (Color online) $|\langle\sigma_-(t)\rangle/\langle\sigma_-(0)\rangle|$ for $\varepsilon=3\Delta$, $K=0.1$. Panels (a), (b): resonant impurity $v=\varepsilon$. (a) $p_z=0$ at $T=0$ orange (light gray line), $T=0.5\Delta$ black dashed line; (b) $T=0$ for $p_z=1$ orange (light gray line), $p_z=-1$ black line. Panels (c), (d): nonresonant case $v=\Delta$, $T=0$ orange (light gray line), $T=0.9\Delta$ green (dark gray line) dashed line. In (c) $p_z=0$, in (d) $p_z=1$ top, $p_z=-1$ bottom. Note the weak T dependence.

$p_z=1$ and with $\text{Re}[\lambda_2]$ if $p_z=-1$; both rates are present for unpolarized initial state. This behavior is stable against temperature variations. Beatings *and* T dependence are instead characteristic of the resonant regime. At $v=\epsilon$, at least two amplitudes are equal, $|A_1| \approx |A_4|$ ($p_z=1$) or $|A_2| \approx |A_3|$ ($p_z=-1$). Damped beatings at $\Omega_{\pm}=\Omega \pm \delta$ are possible due to the hybridization of $\Omega \approx \delta$ [Fig. 2(a), inset].

We illustrate these features in Fig. 4 for $v=\epsilon$. The beating visibility is reduced with increasing T , due the onset of the pure dephasing processes. For an unpolarized state, $p_z=0$, $\langle \sigma_-(t) \rangle$ shows a intermediate behavior between the ones at $p_z=\pm 1$ since at resonance all eigenvalues contribute [Fig. 3(d)]. Damping is strongest for $p_z=-1$, weakest for $p_z=1$, and intermediate for $p_z=0$. In fact, for $\epsilon > \Delta$, preparation in the pure state $p_z=+1$ makes the impurity close to its ground state and less damped, while it is close to the excited state when $p_z=-1$ with strongest damping.

In the last part of this paper we present an alternative perspective, considering the qubit as a measuring device for a mesoscopic system described by the SBE. Remarkably, the qubit acts as a detector despite the absence of direct qubit-SBE inelastic transitions.¹⁹ In fact, the pure dephasing coupling amounts to a “dispersive,” quantum nondemolition measurement regime for the qubit. Detection is feasible due to the qubit back-action on the SBE. This point of view is

illustrated in Fig. 5, where the length of the Bloch vector in the \hat{x} - \hat{y} plane, $|\langle \sigma_-(t) \rangle|$, acts as a sensitive detector of the mesoscopic system (“impurity”) preparation. At resonance, the unpolarized state $p_z=0$ is identified by beatings, Fig. 5(a). These almost disappear for pure states, $p_z=\pm 1$, where oscillations at Ω_{\pm} occur, Fig. 5(b). Identification of the impurity preparation far from resonance results instead from different oscillation amplitudes and/or decay rates, Figs. 5(c) and 5(d).

In conclusion, we have identified in time domain non-Gaussian and back-action effects due to a coherent bistable impurity. These may represent a ultimate limitation for solid-state qubits even when single-shot measurement schemes are available. Our analysis, by changing temperature, strain ϵ , and coupling v , may provide valuable insights into realistic scenarios where a wide distribution of the parameters has to be considered.¹⁰ The reported qualitative features are expected to hold true for general impurity preparation. The employed SBE represents a general effective model for complex physical baths awaiting specific microscopic description, as those typical of solid-state nanodevices.

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