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 [4]. Recent experiments on Josephson qubits indicated that charged impurities may also be responsible for noise [5] exhibiting an ohmic power spectrum at GHz-frequencies. Different theoretical models have been proposed aiming to 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, 6, 7, 8]. In particular in Ref. [8] it has been proposed that a noise power spectrum compatible with the observed relaxation of charge-Josephson qubits [2] 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 [5, 10] and non-thermal [7] 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 protocols [13] are available. Note that at experimental temperatures (∼10 mK) quantum impurities may have a significant influence.

In this 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 non-linear dynamics of the impurity is reflected in the qubit behavior. We identify regimes characterized by strong qubit - impurity backaction. Specifically, we discuss 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 Communication.

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 (\( \sigma \)) via \( \mathcal{H}_{QI} = -\frac{\pi}{2} v \sigma_z \tau_z \). This anisotropic coupling has been discussed for charge qubits, where it models the electrostatic interaction [8, 9, 10]. In this case the two physical states (\( \tau_z \to \pm 1 \)) 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 bath [14] (\( \mathcal{H}_B = \sum \omega_\alpha a_\alpha^\dagger a_\alpha \)) 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 \( \omega_c (k_B = 1) \). 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 \( \sigma_z \), therefore the impurity induces pure dephasing [14] with no relaxation of the qubit [10]. This regime is very interesting since energy exchange processes do not blur deco-
herence of the qubit, which is then maximally sensitive to the SBE dynamics. Pure dephasing due to Fano impurities was addressed in [8]; recently the asymptotic dynamics has been studied [13]. 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.

Method and analytic results.— 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 equation (ME) [18]

$$\partial_t \rho(t) = -i[H_0, \rho(t)] - \int_0^\infty dt' \left\{ \frac{i}{2} S(t') \left[ \tau_z, [\tau_z(t'), \rho(t)] \right] + \frac{1}{2} \chi(t') \left[ \tau_z, [\tau_z(t'), \rho(t)]_z \right] \right\},$$

(1)

where $H_0 = H_{QI} + H_I$ is the undamped Hamiltonian. Here, the transform $S(t)$ of the power spectrum and the bath susceptibility $\chi(t) = -i\langle [\hat{X}(t), \hat{X}(0)]_z \rangle$ enter the damping term. We introduce the conditional Hamiltonians of the impurity $H_{\pm} = \frac{1}{2}(\epsilon \pm v)\tau_z - \frac{i}{2} \Delta \tau_x$, (see Fig. [1]) and the eigenvectors of $H_0$, $\{| i \rangle \}$, which are factorized in eigenstates of $\sigma_z$ and of $H_{\pm}$ [15]. The qubit dynamics at pure dephasing is described by the coherences $\langle \sigma_{\pm}(t) \rangle = \text{Tr}[\rho(t) (\sigma_\pm + i\sigma_y) \otimes 1_z]$, and in particular

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

where $\phi = \frac{1}{2}(\theta - \theta_+)$ is a combination of the mixing angles of $H_{\pm}$ (Fig. [1]). Since $\sigma_z$ is conserved, the damping tensor presents only four non vanishing 4 $\times$ 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 $\rho_{ac}, \rho_{bd}$ and $\rho_{ad}, \rho_{bc}$. We quote here the first set of equations $\rho_{ac}, \rho_{bd}$ and $\rho_{ad}, \rho_{bc}$.

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

(2)

where $\delta = \frac{1}{2}(\Omega_+ - \Omega_-)$, Fig. [1] The rates $\Gamma_i$, describing dissipative transitions and pure dephasing processes between the 4-states and the bosonic bath, read

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

(3)

where $\frac{1}{2}(\theta_+ + \theta_-)$. Here $\Gamma_{\pm}(\omega) = 2\pi K \omega [\cosh(\frac{\omega t}{2}) \pm 1]$, are the impurity emission ($+$) and absorption ($-$) rates of energy $\omega$. The elements $\rho_{ad}, \rho_{bc}$ satisfy similar equations with $\delta$ replaced by $\Omega = \frac{1}{2}(\Omega_+ + \Omega_-)$ and rates

$$\Gamma_{3,4} = \alpha_+^2 \Gamma_{\pm}(\Omega_+) + \alpha_-^2 \Gamma_{\pm}(\Omega_-) + \eta_c S(0), \\
\Gamma_{34,43} = \alpha_+ \alpha_- \left( \Gamma_{\pm}(\Omega_+) + \Gamma_{\pm}(\Omega_-) \right), \\
\eta_c = \frac{1}{2} \cos^2 \theta \sin^2 \phi.$$

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

$$\lambda_{1,2} = -\frac{\Gamma_1 + \Gamma_2}{2} \pm \sqrt{\left(\frac{\Gamma_1 - \Gamma_2}{2}\right)^2 + 4\Gamma_{12}\Gamma_{21}},$$

$$\lambda_{3,4} = -\frac{\Gamma_3 + \Gamma_4}{2} \pm \sqrt{\left(\frac{\Gamma_3 - \Gamma_4}{2}\right)^2 + 4\Gamma_{34}\Gamma_{43}}.$$  

(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 $\rho(0) = \rho_c(0) \otimes \rho_I(0)$, represent a realistic scenario. The impurity initial state is thus out of the experimenter control, thus we choose $\rho_c(t) = \frac{1}{2} (1 + p_z \tau_z), p_z$ being the initial average of $\tau_z$. The impurity starts from a totally unpolarized state for $p_z = 0$, from a pure state if $p_z = \pm 1$. This class of initial states guarantees the positivity of the dynamical process ensuing from Eq. (2). With this choice we find

$$\langle \sigma_{-}(t) \rangle = \langle \sigma_{-}(0) \rangle \sum_i A_i e^{\lambda_i t},$$

$$A_{1,2} = \frac{\cos \phi}{2(\lambda_1 - \lambda_2)} \left[ \cos \left[ \lambda_1 - \lambda_2 \pm (\Gamma_{12} + \Gamma_{21}) \right] + p_z \cos (\theta + \theta) \left[ -2i\delta - \Gamma_2 + \Gamma_1 + \Gamma_{12} + \Gamma_{21} \right] \right],$$

$$A_{3,4} = \frac{\sin \phi}{2(\lambda_3 - \lambda_4)} \left[ \sin \left[ \lambda_3 - \lambda_4 \mp (\Gamma_{34} + \Gamma_{43}) \right] + p_z \sin (\theta + \theta) \left[ -2i\delta - \Gamma_4 + \Gamma_3 - \Gamma_{34} + \Gamma_{43} \right] \right].$$

Eqs. (5–6) are the main result of this Communication. They cover the parameters 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 [15] are recovered. Reliability of ME is confirmed by a real-time path-integral calculation.

Discussion of the results.— We focus our analysis on the low-temperature regime $T \ll \Omega_{\pm}$. 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

$$\lambda_1 = i\delta - \eta_s S(0),$$

$$\lambda_2 = -i\delta - \gamma_{\tau+} + \gamma_{\tau+}^0 + \gamma_{\tau-} + \gamma_{\tau-}^0 - \eta_s S(0),$$

$$\lambda_{3,4} = \pm i\Omega - \gamma_{\tau+}^0 - \gamma_{\tau-}^0 - \eta_c S(0),$$

(7)

$$\lambda_3, \lambda_4 = \pm i\Omega - \gamma_{\tau+}^0 - \gamma_{\tau-}^0 - \eta_c S(0).$$
where intra-doublet relaxation rates (see Fig. 4)

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

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

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 $\delta$ approaches $\Omega$, i.e. around $\varepsilon = v$ which identifies a sort of “resonance regime” for our problem.

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, $\Re \{\lambda_1\}$, vanishes, as expected. Only emission processes contribute to the residual rates, and they directly sound out intra-doublet relaxation rates $\gamma_{r\pm}$.

Their behaviors reflect the sensitivity of $\mathcal{H}_\pm$, to noise acting along $v$. While $\gamma_{r\pm}$ decreases with increasing $v$, $\gamma_{0\pm}$ takes a maximum at the resonance point (see Eq. (8)), the “transverse” $\theta_\pm = \pi/2$ noise condition for $\mathcal{H}_\pm$. This implies a non-monotonous dependence of $\Re \{\lambda_2,3\}$ on the coupling $v$, Fig. 2(a). The imaginary parts of $\lambda_1$ and $\lambda_2,3$ interchange characters at resonance (Fig. 2(a) inset) leading to possible hybridization (see below). Increasing $T$ leading correction to the rates come from pure dephasing terms $S(0)$. 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 $\delta$, 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 $\Re \{\lambda_1\}$ for $v < \varepsilon$ and $\Re \{\lambda_3\}$ for $v > \varepsilon$. It is a non-monotonous function of $v$ and a cusp signals crossing of eigenvalues (a similar effect may explain non-monotonic behavior of $|17\rangle$).

At intermediate times, all eigenvalues may be relevant, depending on the weights $A_i$ in Eq. (9). 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, $v \to 0$, $|A_1| \approx 1$ (Fig. 3(a)) implying universal dynamics independent on the initial conditions. The dominant eigenvalue is $\lambda_1$ with $\delta \to 0$ 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 on $p_z$ ($\delta < v < k, \varepsilon > v$). Damping of the oscillations depends on the initial condition, Fig. 3(b) - (d). For instance, at finite $v < \varepsilon$, the decay occurs with $\Re \{\lambda_1\}$ if $p_z = 1$ and with $\Re \{\lambda_2\}$ 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 $v = \varepsilon$, at least two amplitudes are equal, $|A_1| \approx |A_2| (p_z = 1)$ 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 $v = \varepsilon$. The beatings 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 an 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 $\varepsilon > \Delta$, preparation in the pure state $p_z = +1$ makes the impurity close to its ground state
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 $\varepsilon$ and coupling $v$, may provide valuable insights to realistic scenarios where a wide distribution of the parameters has to be considered \[10\]. 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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\[\text{FIG. 5: } |\langle \sigma_-(t) \rangle/\langle \sigma_-(0) \rangle| \text{ for } \varepsilon = 3\Delta, K = 0.1. \text{ Panels (a) and (b): resonant impurity } v = \varepsilon. \text{ (a) } p_z = 0 \text{ at } T = 0 \text{ (black) and } T = 0.5\Delta \text{ (red); (b) } T = 0 \text{ for } p_z = 1 \text{ (orange), } p_z = -1 \text{ (black). Panels (c) and (d): non resonant case } v = \Delta \text{ at } T = 0 \text{ (blue) and at } T = 0.9\Delta \text{ (red). In (c) } p_z = 0, \text{ in (d) } p_z = 1 \text{ top, } p_z = -1 \text{ bottom. Note the weak } T\text{-dependence.}\]

\[\text{FIG. 4: } \text{Re} \left[ \langle \sigma_-(t) \rangle/\langle \sigma_-(0) \rangle \right] \text{ at resonance } \varepsilon = v = 3\Delta \text{ for initial states (a) } p_z = 1: \text{ slow decay with } \text{Re} \left[ \lambda_{1/3} \right], \text{ (b) } p_z = -1: \text{ fast decay with } \text{Re} \left[ \lambda_{2/3} \right]. \text{ Parameters: } T = 0 \text{ (blue), } T = 0.5\Delta \text{ (red), } T = 0.9\Delta \text{ (green), } K = 0.1.\]