Tailoring population inversion in Landau-Zener-Stückelberg interferometry of flux qubits

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We distinguish different mechanisms for population inversion in flux qubits driven by dc+ac magnetic fields. We show that for driving amplitudes such that there are Landau-Zener-Stückelberg interferences, it is possible to have population inversion solely mediated by the environmental bath at long driving times. We study the effect of the resonant frequency \( \Omega_p \) of the measuring circuit, finding different regimes for the asymptotic population of the state of the flux qubit. By tailoring \( \Omega_p \) the degree of population inversion can be controlled. Our studies are based on realistic simulations of the device for the Josephson flux qubit using the Floquet-Born-Markov formalism.

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Population inversion, where the highest populated state is an excited state, is among the most interesting phenomena in maser and laser physics [1]. The usual mechanism to get population inversion requires driven quantum systems with three or more energy levels, since indirect transitions through a third energy level are involved [1–4]. Here, we find that the device for the Josephson flux qubit (DJFQ) can have population inversion even in the case in which only two levels are involved in the driven dynamics. Furthermore when tailoring the structure of the environmental bath different mechanisms for population inversion can arise.

Superconducting circuits with mesoscopic Josephson junctions are used as quantum bits [5] and can behave as artificial atoms [6]. A well studied circuit is the DJFQ [5–8] which, for millikelvin temperatures, exhibits quantized energies levels that are sensitive to an external magnetic field. When driven by a dc+ac magnetic flux, transitions between energy levels at avoided crossings occur, and a rich structure of Landau-Zener-Stückelberg (LZS) interferences [9] combined with multi-photon resonances is observed [10–12]. For large ac amplitudes diamond-like interference patterns are displayed, from which the energy level spectrum has been reconstructed [11]. LZS interferences have also been observed in charge qubits [13], Rydberg atoms [14], ultracold molecular gases [15], optical lattices [16] and single electron spins [17].

The DJFQ consists on a superconducting ring with three Josephson junctions [5] enclosing a magnetic flux \( \Phi = f \Phi_0 \) (\( \Phi_0 = h/2e \)) with phase differences \( \varphi_1, \varphi_2 \) and \( \varphi_3 = -\varphi_1 + \varphi_2 - 2\pi f \). Two of the junctions have coupling energy, \( E_J \), and capacitance, \( C \), and the other has \( E_{f,3} = \alpha E_J \) and \( C_3 = \alpha C \). The hamiltonian is:

\[
H = -2E_C \left( \frac{\partial^2}{\partial \varphi_1^2} + \frac{1}{1+2\alpha} \frac{\partial^2}{\partial \varphi_1^2} \right) + E_J V(\varphi_t, \varphi_1),
\]

with \( \varphi_t = (\varphi_1 + \varphi_2)/2 \), \( \varphi_1 = (\varphi_1 - \varphi_2)/2 \), \( E_C = e^2/2C \) and \( V(\varphi_t, \varphi_1) = 2 + \alpha - 2 \cos \varphi_t \cos \varphi_1 - \alpha \cos (2\pi f + 2\varphi_t) \).

The DJFQ has several discrete levels with eigenenergies \( E_1 \) and eigenstates \( |\Psi_k \rangle \) which depend on \( f, \alpha \) and \( \eta = \sqrt{SE_C/E_J} \). Typical experiments have \( \alpha \approx 0.6 - 0.9 \) and \( \eta \approx 0.1 - 0.6 \) [10–11]. For \( \alpha \geq 1/2 \) and \( |f - 1/2| \ll 1 \), the potential \( V(\varphi_t, \varphi_1) \) has the shape of a double-well with two minima along the \( \varphi_1 \) direction. In this regime the system can be operated as a quantum bit [5, 7, 9] and approximated by a two-level system (TLS) [5, 8]. When driven by a magnetic flux \( f(t) = f_{dc} + f_{ac} \sin(\omega t) \), the hamiltonian is time periodic \( H(t) = \tilde{H}(t + \tau) \), with \( \tau = 2\pi/\omega \). In the Floquet formalism, that allows to treat periodic forces of arbitrary strength and frequency [13, 19–21], the solutions of the Schrödinger equation are of the form \( |\Psi_\beta(t)\rangle = e^{i\epsilon_\beta t/\hbar} |\Phi_\beta(t)\rangle \), where the Floquet states \( |\Phi_\beta(t)\rangle \) satisfy \( |\Phi_\beta(t)\rangle = |\Phi_\beta(t + \tau)\rangle = \sum_k |\Phi_k^\beta\rangle e^{-ik\omega t} \), and are eigenstates of the equation \( \hat{H}(t) - i\hbar \partial/\partial t |\Phi_\beta(t)\rangle = \epsilon_\beta |\Phi_\beta(t)\rangle \), with \( \epsilon_\beta \) the associated quasi-energy.

Experimentally, the system is affected by the electromagnetic environment that introduces decoherence and relaxation processes. A standard theoretical model to study environmental effects is to couple the system with a bath of harmonic oscillators [21–24]. Following [21], we assume that the DJFQ is linearly coupled through \( \varphi_t \) to a bath that has spectral density \( J(\omega) \) and is equilibrium at temperature \( T \). For weak coupling (Born approximation) and fast bath relaxation (Markov approximation), a Floquet-Born-Markov master equation for the reduced density matrix \( \hat{\rho} \) in the Floquet basis,
\[ \rho_{\alpha\beta}(t) = \langle \Phi_\alpha(t) | \hat{\rho}(t) | \Phi_\beta(t) \rangle \], can be obtained \cite{21}:

\[ \frac{d\rho_{\alpha\beta}(t)}{dt} = -\frac{i}{\hbar} (\varepsilon_\alpha - \varepsilon_\beta) \rho_{\alpha\beta}(t) + \sum_{\alpha'\beta'} L_{\alpha'\beta'\alpha\beta} \rho_{\alpha'\beta'}(t). \]  

When the time scale for dissipation is larger than \( \tau \), the transition rates \( L_{\alpha'\beta'\alpha\beta}(t) \) can be averaged over one period \( \tau \) \cite{21}, obtaining \( L_{\alpha'\beta'\alpha\beta} = \sum_k \left\{ (N_{\alpha'\beta',k} + N_{\beta'\alpha',k}) \Gamma_{\alpha'\beta',k} \Gamma_{\beta'\alpha',-k} - \sum_q (\delta_{\beta',\alpha'} N_{\alpha'\beta',k} \Gamma_{\alpha'\beta',k} + \delta_{\alpha',\beta'} N_{\beta'\alpha',k} \Gamma_{\beta'\alpha',k} + \Gamma_{\beta'\alpha',-k}) \right\} \), with \( \Gamma_{\alpha,\beta,q} \equiv \sum_k (\phi_{\alpha}^k \phi_{\beta}^k \hat{q}) \), and \( N_{\alpha,\beta,k} = N_\alpha - \varepsilon_\beta + \hbar \omega \). This formalism has been extensively employed to study relaxation and decoherence for time dependent periodic evolutions in double-well potentials and in TLS \cite{21, 22}.

Here we use it to model the ac driven DJFQ, beyond the TLS approach, considering the full hamiltonian of Eq. \( \[ \] \). We calculate the coefficients \( L_{\alpha'\beta'\alpha\beta} \) using the Floquet states \( | \Phi_k^\alpha \rangle \) and quasienergies \( \varepsilon_\beta \), obtained as in \( \[ \] \), and then we integrate numerically Eq. \( \[ \] \), obtaining \( \rho_{\alpha\beta}(t) \) as a function of \( t \).

![Figure 1: Population \( P_R \) as a function of the driving amplitude \( f_{ac} \) for \( t = 1000\tau \) (continuous line). The dashed line shows the asymptotic \( (t \to \infty) \) average population \( P_R \). The inset shows the dependence of \( P_{R0} \) on \( T \) for a driving amplitude \( f_{ac} = 0.00245 \). The calculations were performed for \( f_{ac} = 0.50151 \), \( \omega = 2\pi/\tau = 0.003E_J/\hbar \) and an ohmic bath with \( \gamma = 0.001 \) at \( T = 20\text{mK} \) (for \( E_2/\hbar \approx 300\text{GHz} \)). Vertical lines separate regimes A, B, C, D described in the text. Black circle: \( f_{ac} \) corresponding to the inset, Fig.2(a) and Fig.3; black square: \( f_{ac} \) corresponding to Fig.2(b).](image)

We start by considering a DJFQ coupled to a bath with an ohmic spectral density \( J(\omega) = \gamma \omega \), which mimics an unstructured electromagnetic environment that in the classical limit leads to white noise. We take \( \gamma = 0.001 \), corresponding to weak dissipation as in \( \[ \] \), and the bath at \( T = 0.0014E_J/\hbar_B \) (~20mK for \( E_J/\hbar \sim 300\text{GHz} \)). The DJFQ parameters are \( \alpha = 0.8 \) and \( \eta = 0.25 \). The static field is taken as \( f_{dc} = 0.50151 \), and for the driving microwave field we choose \( \omega = 0.003E_J/\hbar \sim 900\text{MHz} \) and different amplitudes \( f_{ac} \). The initial condition is the ground state \( |\Psi_0\rangle \) of the static hamiltonian \( H_0 = H(f_{dc}) \).

Experimentally, the probability of having a state of positive or negative persistent current in the flux qubit is measured \cite{8}. The probability of a positive current measurement (“right” side of the double-well potential) can be calculated as \( P_R(t) = \text{Tr}(\Pi_R\hat{\rho}(t)) \), with \( \Pi_R \) the operator that projects wave functions on the \( \varphi_1 \) > 0 subspace \cite{20}. For a static field \( f_{dc} \geq 1/2 \), the ground state has \( P_R \approx 1 \). In Fig.1 we show \( P_R \) vs. \( f_{ac} \) calculated from the numerical solution of Eq. \( \[ \] \) after a driving time \( t = 1000\tau \), which is similar to the time scale of the experiments \cite{11}, finding different regimes. (A) For small \( f_{ac} \), \( P_R \sim 1 \), since the system is slightly perturbed from the ground state. (B) When further increasing \( f_{ac} \), new regimes are found whenever the extreme driving amplitudes \( f_{dc} \pm f_{ac} \) reach an avoided crossing in the energy level spectrum \( \{ E_i(f) \} \). Since the slopes \( dE_i/df \) are proportional to the average loop current of the DJFQ, there is an interference of “positive” and “negative” loop current states (“right” and “left” sides of the double-well potential) at avoided crossings, which results in LZS oscillations \cite{9} in the dependence of \( P_R \) with \( f_{ac} \). The first case is found in Fig.1 when the avoided crossing at \( f = 1/2 \) between the ground state level \( E_0 \) and the first excited level \( E_1 \) is reached, and the transfer of population to the \( E_1 \) level lowers \( P_R \). The DJFQ of \( \[ \] \) has short decoherence times \( (\tau = \sim 1 \sim 10\text{ns}) \) and large relaxation times \( (t_r \sim 100\mu s) \). Due to this time scale separation \( \tau < t_0 < t_r \), a TLS model with classical noise, valid for \( t < t_r \), can explain the experimentally the observed LZS oscillations of \( P_R \) vs. \( f_{ac} \), where the minima correlate with the zeros of Bessel functions \( J_n(\alpha f_{ac}/\omega) \) (a a normalization constant) \cite{10, 11}. The results of Fig.1 for \( t = 1000\tau \) are in agreement with this finding. (C) At higher values of \( f_{ac} \) more than two levels have to be considered. When the avoided level crossing between \( E_1 \) and \( E_2 \) is reached by the driving amplitude the ground level \( E_0 \) is repopulated due to fast \( E_2 \to E_0 \) ‘intrawell’ transitions (the corresponding states have the same sign of the average loop current) and \( P_R \) increases to values near 1 (‘cooling’ effect, see \cite{11}). (D) For \( f_{ac} \) such that the symmetrically located (with respect to \( f = 1/2 \)) avoided crossing between \( E_1 \) and \( E_2 \) is reached, there are new LZS oscillations. Furthermore the levels \( E_0 \) and \( E_2 \) are also involved in the dynamics (since the avoided crossings between \( E_2 \leftrightarrow E_3 \) and \( E_0 \leftrightarrow E_1 \) are traversed by the driving) and a more complex dependence of \( P_R \) with \( f_{ac} \) emerges. In this case, we find population inversion \( (P_R < 1/2) \), which is also observed experimentally in \cite{11}. A multilevel extension of the semiclassical model of \cite{10} can describe this behavior as well \cite{25}.

In Fig.2 we show the explicit time dependence of \( \rho_{\alpha\beta}(t) \) for two different values of \( f_{ac} \). We find that the off-diagonal elements \( \rho_{\alpha\beta} \) go to zero exponentially for large \( t \) [see Fig.2(a) and (b), left axis], with the decay time
corresponding to the decoherence time \( t_\phi \) of the periodically driven case. This shows that the density matrix is diagonal in the Floquet basis after full decoherence \[26\], and the relaxation process is determined by the evolution of the diagonal \( \rho_{\alpha\alpha}(t) \) for \( t > t_\phi \). Thus the asymptotic regime, \( t \gg t_\tau \), can be obtained from the non-trivial solution of \( \sum_\beta L_{\beta\alpha}\alpha\rho_{\beta\beta} = 0 \) after imposing \( d\rho_{\alpha\alpha}/dt = 0 \) in Eq.(2). In this way, we calculate \( \overline{P}_R = \lim_{t\to\infty} \langle P_R(t) \rangle_{\tau} \), averaged over one period \( \tau \), which is shown in Fig.1 (dashed line) as a function of \( f_{ac} \). We see that, while for low and large values of \( f_{ac} \), it follows the finite time asymptotic regime of TLS has been found in \[27–29\] under different approaches. Within the approximation of \[29\] it can be understood as mediated by virtual transitions to bath oscillator states at energies \( E_0 + n\hbar\omega \). Here we find that the asymptotic regime is difficult to reach, since population inversion needs long times \( (t \gg t_\phi) \) to emerge when mediated by the bath. We also find that the inversion effect and the difference between the finite time and asymptotic \( P_R \) are enhanced when decreasing temperature (see inset of Fig.1) \[30\].

(ii) Third-level-mediated population inversion: For higher \( f_{ac} \), the \( E_2 \) and \( E_3 \) levels are involved in the dynamics. In this case, the relaxation of the populations \( P_i \) to the asymptotic regime takes place fast, in a time scale similar to \( t_\phi \). In Fig.2(b) we see that first \( P_0 \) decreases while the populations \( P_1, P_2, P_3 \) increase (through a series of LZS transitions, see \[11, 23\]), until at a later time \( P_2 \) and \( P_3 \) decrease transferring population to \( P_1 \). An asymptotic regime is quickly reached where there is population inversion, \( P_1 > P_0 \), mediated by \( E_2 \) and \( E_3 \), an effect that can be observed even in time scales \( t \gtrsim t_\phi \).
it is possible to fully control the population $P_R$, going from $P_R \sim 1$ to complete population inversion $P_R \sim 0$, with small changes of $\Omega_p$. In the inset of Fig.3 we show in detail the case near the $n = 9$ resonance. (2) **Bath mediated population inversion.** In the opposite limit, $\Omega_p > \Delta_+$, the behavior is similar to the one discussed previously in Fig.2(a), observing population inversion at very long times mediated by the bath (note that for large $\Omega_p$, the spectral density $J_\omega(\omega)$ tends to the ohmic one). (3) **Bath mediated cooling.** In the intermediate regime, $\Delta_- \lesssim \Omega_p \lesssim \Delta_+$, virtual LZS transitions to an effective energy level [22, 31] at $E_0 + \Omega_p < E_1$ predominate. From this effective level it is possible to decay an repopulate the ground state, obtaining $P_R \sim 1$. The resonances at $\Omega_p = n\omega + \epsilon_1 - \epsilon_0$ are still observed. A full picture of the effect of an structured bath can be observed in Fig.4, which shows a map of the asymptotic population $P_R$ as a function of $\Omega_p$ and $f_{ac}$. The above mentioned three different regimes for $\Omega_p < \Delta_-$, $\Delta_- \lesssim \Omega_p \lesssim \Delta_+$ and $\Delta_+ < \Omega_p$ can be distinguished. Also, in Fig.4 we observe the onset of LZS oscillations involving $E_2$ and $E_3$ at higher $f_{ac}$ (corresponding to the second 'diamond' of [11]) where the third level mediated population inversion discussed in Fig.2(b) takes place. Here we see that while the bath-mediated population inversion mechanism appears for $\Omega_p > \Delta_+$, the third-level-mediated population inversion mechanism is almost independent of $\Omega_p$.

![FIG. 4: (color online) Contour map of the stationary population $P_R$ as a function of the driving amplitude $f_{ac}$ and the resonance frequency of the dc SQUID $\Omega_p$ for $T = 20$ mK, $f_{dc} = 0.50151$, $\omega = 0.003$, $\gamma = 0.001$ and $\kappa = 0.001$. The black and green lines represent the positions of $\Delta_+$ and $\Delta_-$. Black circle: $f_{ac}$ corresponding to Fig.2(a) and Fig.3; black square: $f_{ac}$ corresponding to Fig.2(b).](image)

In conclusion, by performing a realistic modeling of the flux qubit we are able to analyze different scenarios for population inversion in strongly driven quantum systems, understanding the parameter regimes for their occurrence. One puzzling situation is that the bath-mediated population inversion expected to happen in LZS oscillations [27, 29] has not been observed in the experiments of [11]. Here we show that this effect is observable only when driving the system for very long times, after full relaxation with the bath degrees of freedom ($t \gg t_\phi$).

The large time scale separation $t_r \gg t_\phi$ present in the device of [11] (due to the very small gap $\Delta = E_1 - E_0$ at $f = 1/2$ [24, 32]) explains that the predicted population inversion is beyond the experimental time window. It will be interesting if experiments could be carried out for longer driving times in this device. Population inversion in LZS oscillations has been observed in another flux qubit device driven at large frequencies [33], and interpreted in [34] as due to quantum noise, (which is consistent with our asymptotic $P_R$ results). Another interesting point we found is the dependence of the LZS oscillations on the frequency $\Omega_p$ of the SQUID detector. The flux qubits fabricated with Nb junctions as in [16, 11] have typically a small gap and thus they are in the regime $\Omega_p > \Delta_+$, where bath-mediated population inversion takes place. The flux qubits fabricated with Al junctions, as in [8, 31], have a large gap and thus they are expected to be in the regime $\Omega_p < \Delta_-$. Amplitude spectroscopy measurements like [11] but carried out in Al flux qubits could give different ‘diamond’ patterns as function of $f_{dc}, f_{ac}$ with resonance and LZS interference effects from the oscillator levels at $E_1 + n\hbar \Omega_p$. In principle, the frequency $\Omega_p$ can be varied (in a small range) by varying the driving current of the SQUID detector [31] or with a variable shunt capacitor. In this case there is room to fully control the population $P_R$ and the degree of population inversion as a function of $\Omega_p$.

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