

# Stochastic Simulation of a Two-Level Quantum System

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## 1 Introduction

In this paper we will study and numerically simulate a damped and driven two-level system. The Hamiltonian of the system is:

$$\hat{H} = \varepsilon(\hat{\sigma}_- e^{i\omega t} + \hat{\sigma}_+ e^{-i\omega t}) + \omega \hat{\sigma}_+ \hat{\sigma}_-$$

The constant  $\varepsilon$  controls the strength of the driving force and  $\omega$  controls the speed at which the system oscillates. We can then couple the system to a reservoir, resulting in an evolution of the state which is irreversible and hence cannot be represented by a Hamiltonian. Instead, we must describe the evolution in terms of the master equation:

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}] + \gamma \mathcal{D}[\hat{\sigma}_-] \hat{\rho}$$

where  $\gamma$  controls the strength of the damping of the system caused by interaction with the reservoir. An example of a physical system that could be modelled with this equation is a two-level atom which is being driven by a laser, and where the damping represents the spontaneous emission of photons by the atom.

In this paper we shall use quantum trajectories to stochastically simulate the two-level system. We shall unravel the master equation in terms of the operator  $\hat{\sigma}_-$ , which gives us the SDE:

$$|d\psi\rangle = \left( -\frac{i}{\hbar} \hat{H} + \frac{\gamma^2}{2} (\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle - \hat{\sigma}_+ \hat{\sigma}_-) \right) dt |\psi\rangle + \left( \frac{\hat{\sigma}_-}{\sqrt{\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle}} - \hat{1} \right) dN |\psi\rangle$$

where  $dN$  is a Poissonian process with  $\mathbb{E}(dN) = \gamma^2 \langle \hat{\sigma}_+ \hat{\sigma}_- \rangle$  and where  $|\psi\rangle$  denotes the state of the system. This equation can be physically interpreted as the evolution of the system conditioned on measuring excitations in the reservoir. The jump process represents a positive measurement, as when this occurs the system must have emitted a photon and hence is in the ground state.

## 2 Stochastic Simulation of the System

In vector notation, we can write the state of the system as:

$$|\psi\rangle = a|e\rangle + b|g\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

where  $a$  is the component of the system in the excited state and  $b$  is the component in the ground state. In this representation, the raising and lowering operators are:

$$\hat{\sigma}_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \hat{\sigma}_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

and hence, the average excitation of the system is given by  $\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle = |a|^2$ . After a bit of algebraic manipulation we find that:

$$\begin{pmatrix} da \\ db \end{pmatrix} = \left[ -\begin{pmatrix} i\omega - \frac{\gamma^2}{2}|a|^2 & i\varepsilon e^{-i\omega t} \\ i\varepsilon e^{i\omega t} & 0 \end{pmatrix} + \frac{\gamma^2|a|^2}{2} \mathbb{I} \right] dt \begin{pmatrix} a \\ b \end{pmatrix} + dN \left( \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} a \\ b \end{pmatrix} \right)$$

(as the phase of a quantum state is nonphysical, when the system collapses to ground state we can assume it is the state  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ ). However, directly numerically integrating this equation is not numerically stable, as if numerical errors result in an  $|a|^2 > 1$ , then the  $\frac{\gamma^2|a|^2}{2} \mathbb{I}$  term results in superexponential growth. This problem can be remedied by noticing that all the  $\frac{\gamma^2|a|^2}{2} \mathbb{I}$  term does is scale the vector, and as the norm of the state is always 1 anyway, we can integrate:

$$\begin{pmatrix} da \\ db \end{pmatrix} = \begin{pmatrix} -i\omega - \frac{\gamma^2}{2}|a|^2 & -i\varepsilon e^{-i\omega t} \\ -i\varepsilon e^{i\omega t} & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} dt - dN \begin{pmatrix} a \\ b-1 \end{pmatrix}$$

and then calculate average excitation by dividing  $|a|^2$  through by  $\sqrt{|a|^2 + |b|^2}$ . This is particularly useful, as we can simulate a jump process by randomly choosing a number between 0 and 1, and then triggering the jump

when the norm becomes smaller than this. As the change in norm is  $-\gamma^2|a|^2$ .

There are many different numerical process that can be used to integrate the differential equation. Originally, Euler's method was used to integrate the equations, however, this did not converge very well. Instead, a fourth order Runge-Kutta (RK4) method was used. XMDS code for this is included as an appendix. While when integrating deterministic equations the RK4 method converges as the fourth power of step size, over the steps where the jump process occurred the convergence was only correct to first order. This was a result of the fact that regardless of when the jump occurred, the system was always calculated to be in the unexcited state at the end of the step. Because of, the convergence properties of the RK3 method when used for our stochastic simulation were worse than fourth order. Although this problem was not remedied in our simulations, it could be solved by taking smaller step sizes just before each jump occurs.

The average excitation over time of the system calculated using the RK4 method is graphed in *Figure 1*. The calculations were performed for  $\omega = \varepsilon = \gamma = 1$  and  $t \in [0, 10]$  with the system beginning in the excited state at  $t = 0$ . The step size was 0.005 and 1000000 paths were used.

There are two errors associated with the numerical calculations. The first is due to the stochastic nature of the simulation, which is due to the limited sample size of paths taken, and the second is due to using Runge-Kutta method to calculate numerically integrate the SDE. XMDS can calculate the random error using the variation in the range of average excitations, and can estimate the Runge-Kutta method error by repeating calculations with half the step size and then comparing the results. Both these errors are too small to be seen on *Figure 1*, however, they are plotted in *Figure 2*. As can be seen on the diagram, the two errors are of roughly the same size and they are mostly smaller than 0.001.

Usually, stochastic methods are used because it is too difficult to directly integrate the master equation. However, for our two-level system, the density matrix is of the form:

$$\hat{\rho} = \begin{pmatrix} p & q \\ q^* & 1-p \end{pmatrix}$$

where  $p$  is real and  $q$  is complex. Using the master equation, we find that the evolution of the values is given by:

$$\begin{aligned} \frac{dp}{dt} &= -2\varepsilon \text{Im}(qe^{i\omega t}) - \gamma p \\ \frac{dq}{dt} &= -i\omega q - i\omega(1-2p)\varepsilon e^{-i\omega t} - \frac{\gamma q}{2} \end{aligned}$$

We can now XMDS to numerically integrate these equation using the 9th order Runge-Kutta method with step

size  $h = 0.002$ . The numerical error can be computed by repeating the calculation with half the step size, and this results in error estimates of the order of  $10^{-16}$ , errors which likely originate because of finite machine precision. Hence we can take these computed values as very close to the actual average excitation. For this reason we can take the absolute difference between the stochastic method and this method as a good estimate of the actual error in the stochastic method.

In *Figure 3*, the absolute value of the difference between the two methods is plotted, along with the estimated error computed for the stochastic method. The total error was estimated by simply adding the absolute values of the stochastic and numeric errors. In we can see that our estimate of the error is a very good approximator of the actual error size.

### 3 Calculating the Equilibrium Average Excitation

In this section we will consider a slight generalisation of the two-level system. When we detect an excitation in the reservoir, we can apply feedback to the system by unitarily transforming the system. We shall calculate the effect of such feedback on the average excitation in the limit as  $t \rightarrow \infty$ .

The most general SDE describing the evolution of the state with feedback is given by:

$$\begin{aligned} |d\psi\rangle &= \left( -\frac{i}{\hbar} \hat{H} + \frac{\gamma}{2} (\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle - \hat{\sigma}_+ \hat{\sigma}_-) \right) dt |\psi\rangle \\ &+ \left( \frac{\hat{U} \hat{\sigma}_-}{\sqrt{\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle}} - \hat{1} \right) dN |\psi\rangle \end{aligned}$$

where  $\hat{U}$  is the unitary operation applied after each detection of an excitation. We can reduce this SDE reduces to the master equation:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \gamma \mathcal{D}[\hat{U} \hat{\sigma}_-] \hat{\rho}$$

The general form of the density matrix is:

$$\rho = \begin{pmatrix} p & q \\ q^* & 1-p \end{pmatrix}$$

where  $p$  is real, and the most general form of  $\hat{U} \hat{\sigma}_-$  is:

$$\hat{U} \hat{\sigma}_- = \begin{pmatrix} \alpha & 0 \\ \beta & 0 \end{pmatrix}$$

where  $\alpha$  and  $\beta$  are complex numbers satisfying  $|\alpha|^2 + |\beta|^2 = 1$ . We can then expand out the master equation to find differential equations for  $p$  and  $q$ :

$$\frac{dp}{dt} = -i\varepsilon(q^* e^{-i\omega t} - q e^{i\omega t}) - \gamma |\beta|^2 p$$

$$\frac{dq}{dt} = -i\omega q - i\omega(1-2p)\varepsilon e^{-i\omega t} + \gamma\left(\alpha\beta^*p - \frac{q}{2}\right)$$

Let  $\alpha\beta^* = A$  and  $|\beta|^2 = B$ ; the differential equations then become:

$$\frac{dp}{dt} = -i\varepsilon(q^*e^{-i\omega t} - qe^{i\omega t}) - \gamma Bp$$

$$\frac{dq}{dt} = -i\omega q - i\omega(1-2p)\varepsilon e^{-i\omega t} + \gamma\left(Ap - \frac{q}{2}\right)$$

By calculating  $\text{Tr}(\hat{\rho}\hat{\sigma}_+\hat{\sigma}_-)$ , we find that the average excitation is given by  $p$ . Therefore, in order to find the average excitation of the system in the limit as  $t \rightarrow \infty$ , we must have  $\dot{p} = 0$ . Assume that in this limit,  $q = \Omega e^{-i\omega t}$  for some constant  $\Omega$ , and also rewrite  $A$  as  $A = Ce^{-i\omega t}$ . We now have the equations:

$$\begin{aligned} 0 &= -i\varepsilon(\Omega^* - \Omega) - \gamma Bp \\ -i\omega\Omega e^{-i\omega t} &= -i\omega\Omega e^{-i\omega t} - i\omega(1-2p)\varepsilon e^{-i\omega t} \\ &+ \gamma\left(Ce^{-i\omega t}p - \frac{\Omega}{2}e^{-i\omega t}\right) \end{aligned}$$

Rearranging the first equations gives:

$$p = -\frac{2\varepsilon\text{Im}(\Omega)}{\gamma B}$$

We can then manipulate the second equation:

$$\frac{i2\omega\varepsilon(1-2p)}{\gamma} = 2Cp - \Omega$$

and by taking the imaginary components of both sides, we find that:

$$\text{Im}(\Omega) = \frac{2p\text{Im}(C) - 2\omega\varepsilon(1-2p)}{\gamma}$$

Combining the two equations now gives:

$$p = \frac{4\varepsilon^2\omega(1-2p) - 4p\varepsilon\text{Im}(C)}{\gamma^2 B}$$

and rearranging this equation to isolate  $p$  gives:

$$\begin{aligned} p &= \frac{4\varepsilon^2\omega}{8\varepsilon^2\omega + 4\varepsilon\text{Im}(C) + \gamma^2 B} \\ &= \frac{1}{2 + \frac{\text{Im}(C)}{\varepsilon\omega} + \frac{\gamma^2 B}{4\varepsilon^2\omega}} \end{aligned}$$

We have thus found the average excitation of the system when it is in the steady state.

From this equation we can deduce a few interesting properties of the system. In the case where no unitary transformation is applied, we have:

$$\hat{U}\hat{\sigma}_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

which gives us  $B = 1$ ,  $C = 0$ . In this case the equilibrium excitation is:

$$p = \frac{1}{2 + \frac{\gamma^2}{4\varepsilon^2\omega}} < \frac{1}{2}$$

Instead, if we always transformed the system into the excited state after a measurement, we would have:

$$\hat{U}\hat{\sigma}_- = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and in this case  $B = C = 0$ . We then have:

$$p = \frac{1}{2}$$

which is greater than if we applied no feedback. Curiously, in this case the average excitation is independent of the constants of the system.

## 4 Optimising the Average Excitation

We saw at the end of the last section that by transforming the system into the excited state after measurements, we can increase the average excitation to  $\frac{1}{2}$ . This is not the optimal excitation that we can achieve, and the aim of this section is to find the optimal excitation. We shall assume that  $\text{Im}(C)$  and  $B$  are constant, although this is without loss of generality in the case of a constant  $p$ .

First examine the restrictions placed on  $B$  and  $\text{Im}(C)$ . As:

$$\alpha\beta^* = Ce^{-i\omega t} \quad |\beta|^2 = B$$

we can note that  $B > 0$ . We also have the restriction that  $|\alpha|^2 + |\beta|^2 = 1$ , which when combined with the above expressions allows us to deduce that:

$$|C|^2 + B^2 = B$$

and hence:

$$\text{Im}(C)^2 \leq B - B^2$$

To optimise  $p$ , we wish for  $\text{Im}(C)$  to be as large and negative as possible, and according to the above inequality, this means that:

$$\text{Im}(C) = -\sqrt{B - B^2}$$

We now have a formula for  $p$  in terms of  $B$ :

$$p(B) = \frac{1}{2 - \frac{\sqrt{B - B^2}}{\varepsilon\omega} + \frac{\gamma^2 B}{4\varepsilon^2\omega}}$$

which we can solve by setting  $\frac{dp}{dB} = 0$ . In practise it is easier to minimise  $p^{-1}$ , and then calculate:

$$\frac{d}{dB} \left[ 2 - \frac{\sqrt{B - B^2}}{\varepsilon\omega} + \frac{\gamma^2 B}{4\varepsilon^2\omega} \right] = 0$$

and hence:

$$\frac{\gamma^2}{2\varepsilon} = \frac{1 - 2B}{\sqrt{B - B^2}}$$

This equation can be rearranged into a quadratic, and then solve to find:

$$B = \frac{1}{2} - \frac{1}{2} \frac{\gamma^2}{\sqrt{\gamma^4 + 16\varepsilon^2}}$$

and:

$$\text{Im}(C) = \frac{-2\varepsilon}{\sqrt{\gamma^4 + 16\varepsilon^2}}$$

Once the optimal values of  $B$  and  $C$  have been calculated, we can find a unitary operator giving use these values:

$$\hat{U} = \begin{pmatrix} i\sqrt{B} & e^{-i\omega t} \frac{\text{Im}(C)}{\sqrt{B}} \\ -e^{i\omega t} \frac{\text{Im}(C)}{\sqrt{B}} & -i\sqrt{B} \end{pmatrix}$$

To find the optimal unitary operator in the case of  $\omega = \gamma = \varepsilon = 1$ , we can calculate:

$$B = \frac{1}{2} - \frac{1}{2\sqrt{17}}, \quad \text{Im}(C) = \frac{-2}{\sqrt{17}}$$

To achieve optimal excitation, we can therefore apply the unitary operator:

$$\hat{U} = \begin{pmatrix} 0.6154i & -0.7323e^{-i\omega t} \\ 0.7323e^{i\omega t} & -0.6154i \end{pmatrix}$$

The evolution of this system is shown in Figure 4. The system was stochastically simulated with method used in Section 2, and the errors associated with this method are too small to be seen on the graph.

## 5 Optimising Excitation with Arbitrary Unitary Operators

In this section we shall show that if we can apply an unitary operator arbitrarily and also know the system state at all times, then the average excitation can be kept arbitrarily close to 1.

Let us assume that  $|\psi(0)\rangle$  is the excited state. In the situation where the Poissonian process does not trigger on the interval  $t \in [0, \varepsilon]$  for some  $\varepsilon > 0$ , then we know that the system must be in the state  $|\psi(\varepsilon)\rangle$ . This allows us to construct a family of unitary operators  $\hat{U}_\varepsilon$  with the property that:

$$\hat{U}_\varepsilon |\psi(\varepsilon)\rangle = |\psi(0)\rangle$$

In order to keep the system arbitrarily close to the excited state, we could, every time we detect an excitation in the reservoir, apply a unitary operator to shift the state back to the excited state, and then apply  $\hat{U}_\varepsilon$  at intervals of  $\varepsilon$ . By making  $\varepsilon$  sufficiently small, we can force

the system to be arbitrarily close to the excited state. For this method to work we only need to know the exact state of the system at a single point in time, along with the results of all the measurements of excitations of the reservoir.

## 6 Conclusion

We investigated the behaviour of a damped and driven two-level system. Through the use of a stochastic unravelling we were able to simulate the system through the use of a jump process and were able to use this to calculate the average excitation of the system. By comparing this to a direct integration of the master equation, we were able to verify that the method worked and that the estimated errors were of a similar size to the actual error in the method.

The equilibrium average excitation for the system was then investigated, and a formula was derived that could be used to calculate this quantity. Applying feedback after a jump process could then be used to modify the equilibrium excitation, and we showed how to optimise the equilibrium excitation through feedback. Finally it was shown that if a unitary operator could be applied arbitrarily, then the system could be kept arbitrarily close to the excited state.

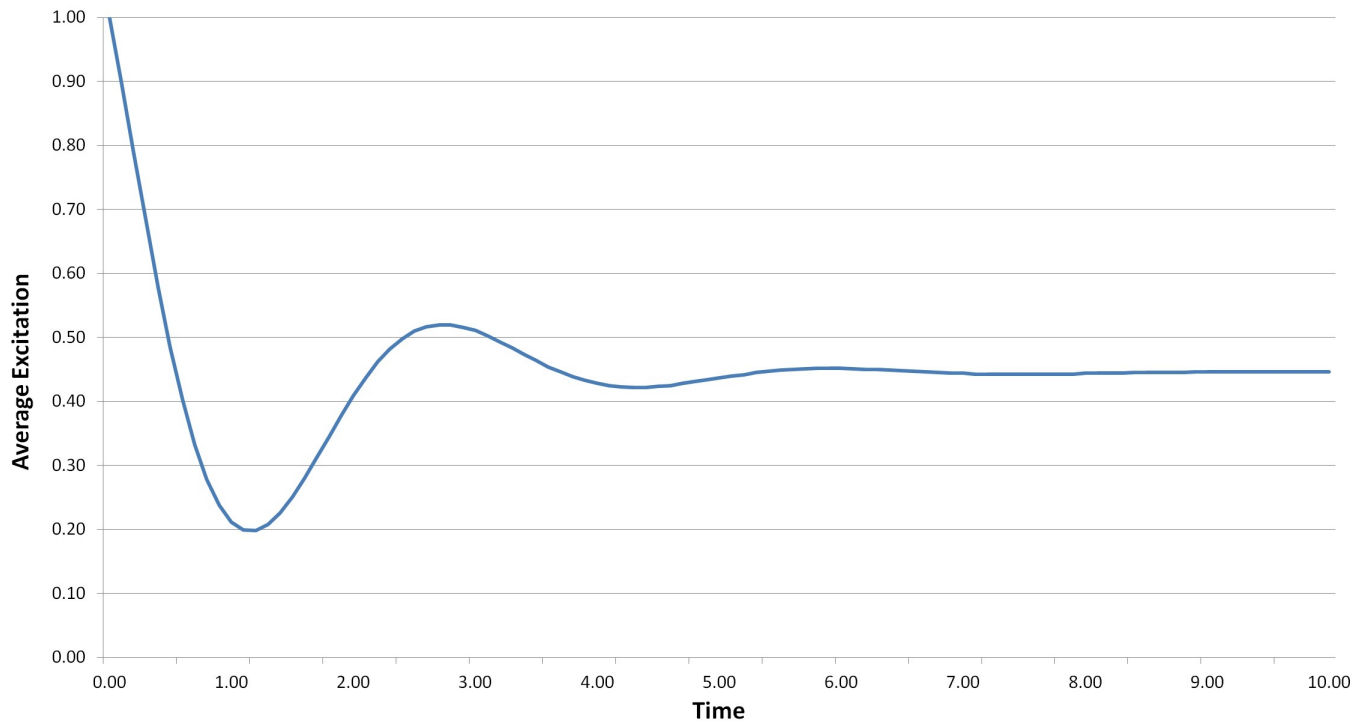


Figure 1: Average Excitation over Time

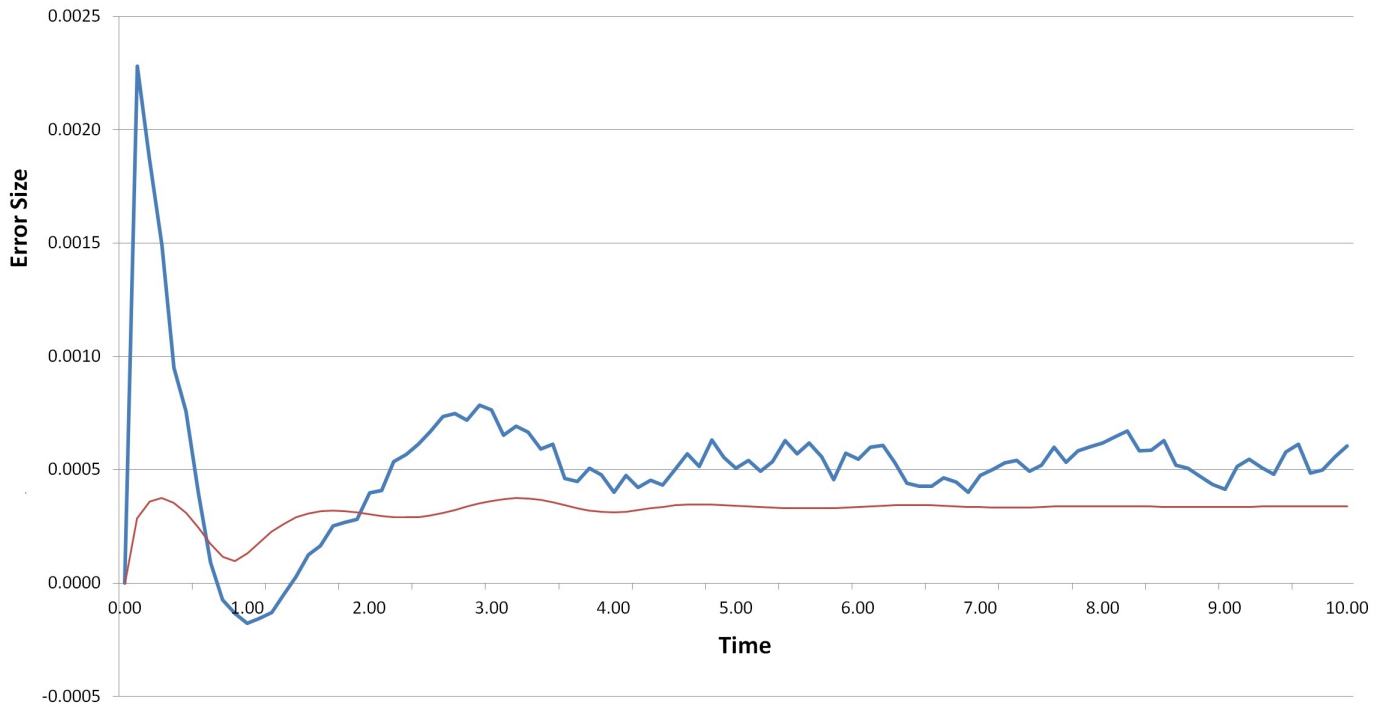


Figure 2: Error in Average Excitation over Time

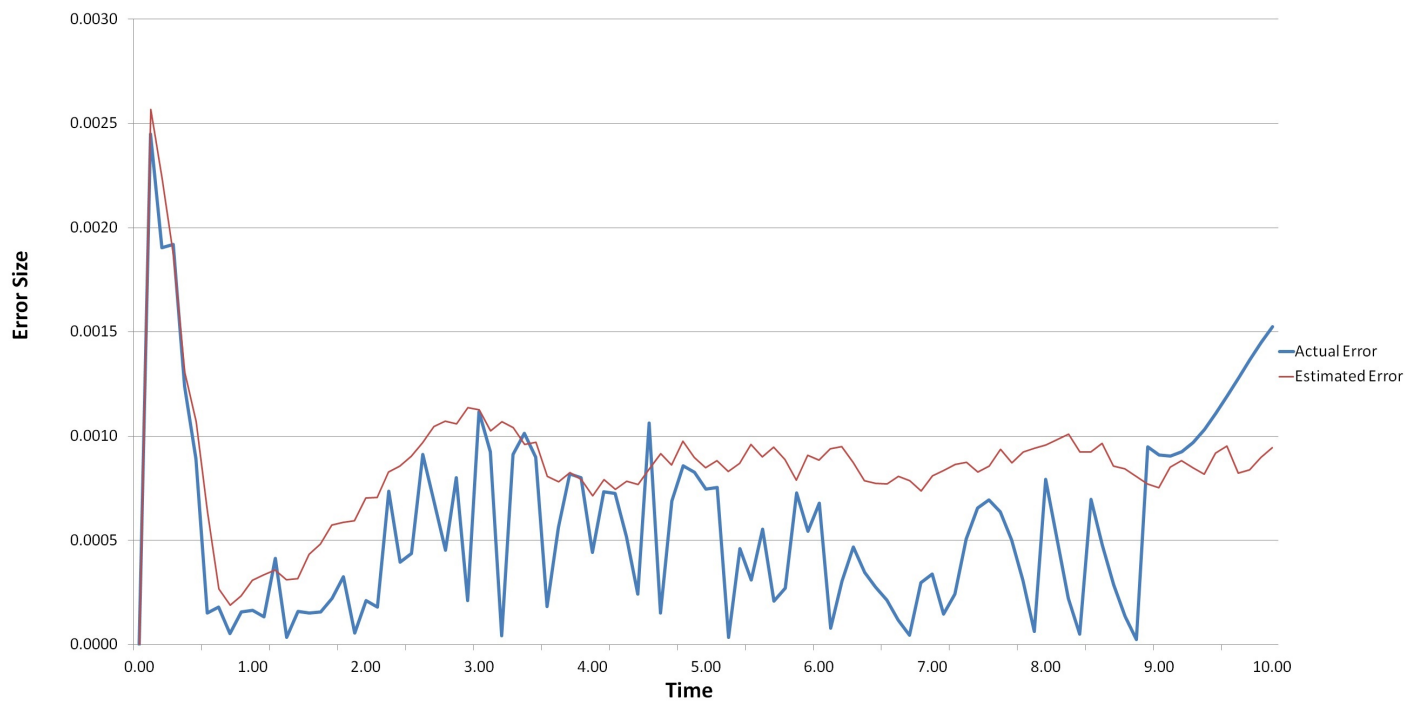


Figure 3: Difference Between Stochastic Method and Integration of Master Equation

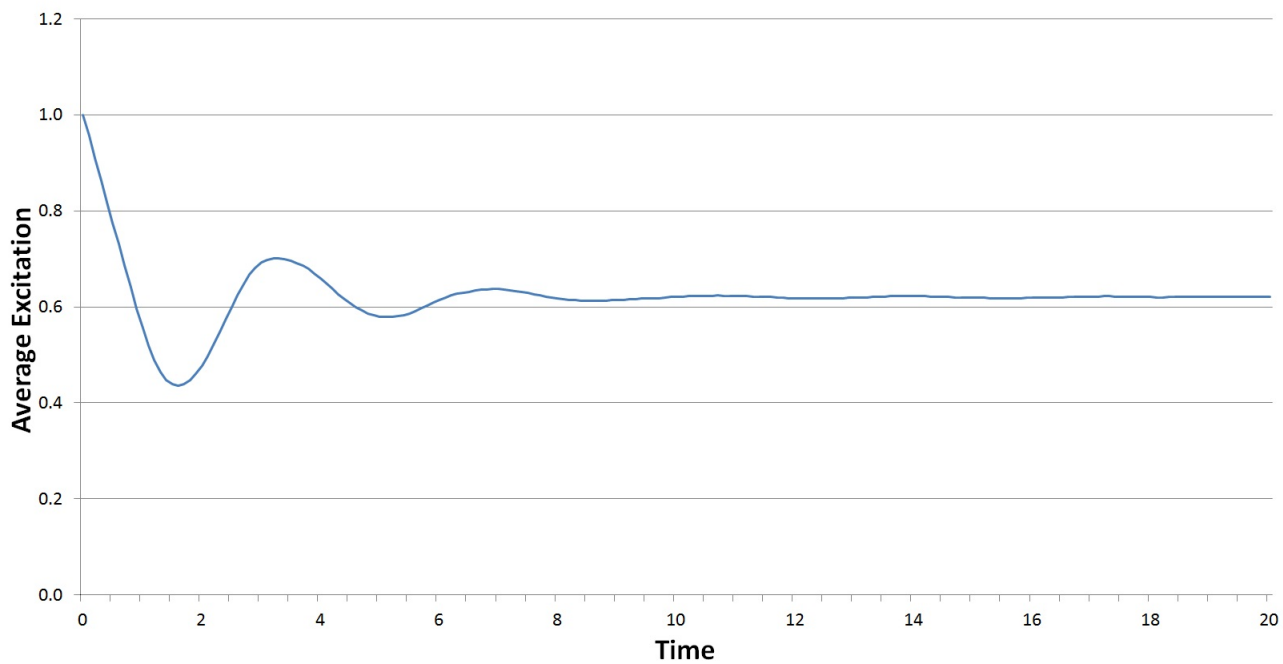


Figure 4: Average Excitation over time for System with Optimal Feedback

## 7 Appendix: XMDS Code

The code below uses the stochastic method to calculate the average excitation of the two-level system.

```
<?xml version="1.0" encoding="UTF-8"?>
<simulation xmds-version="2">
  <name>Stochastic Method</name>

  <author>Damon Binder</author>

  <driver name="multi-path" paths="1000000" />

  <features>
    <error_check />
    <validation kind="run-time" />
    <benchmark />
    <globals>
      <![CDATA[
        real epsilon = 1;
        real omega = 1;
        real kappa = 1;
        real jumpNorm = 0;
      ]]>
    </globals>
  </features>

  <geometry>
    <propagation_dimension> t </propagation_dimension>
  </geometry>

  <vector name="state" type="complex">
    <components>
      a b
    </components>
    <initialisation>
      <![CDATA[
        a = 1.0;
        b = 0.0;
      ]]>
    </initialisation>
  </vector>

  <noise_vector name="uniformNoise" kind="uniform" type="real" method="dsfmt" seed="314 159 276">
    <components>jumpnext</components>
  </noise_vector>

  <computed_vector name="normVec" dimensions="" type="real">
    <components> norm2 </components>
    <evaluation>
      <dependencies>state</dependencies>
      <![CDATA[
        norm2 = mod2(a)+mod2(b);
      ]]>
    </evaluation>
  </computed_vector>
</simulation>
```

```

</computed_vector>

<sequence>
  <filter>
    <dependencies> uniformNoise</dependencies>
    <![CDATA[
      jumpNorm = jumpnext;
    ]]>
  </filter>

  <integrate algorithm="RK4" interval="10.0" steps="2000" tolerance="1e-4">
    <samples>100</samples>
    <operators>
      <integration_vectors>state</integration_vectors>
      <![CDATA[
        da_dt = -kappa^2*0.5*a-i*a*omega-i*epsilon*b*exp(-i*omega*t);
        db_dt = -i*epsilon*a/exp(-i*omega*t);
      ]]>
    </operators>
    <filters>
      <filter>
        <dependencies>normVec</dependencies>
        <![CDATA[
          if (norm2<jumpNorm) { jumpy(); };
        ]]>
      </filter>
    </filters>
  </integrate>

  <filter name="jumpy">
    <dependencies>state uniformNoise</dependencies>
    <![CDATA[
      a = 0;
      b = 1;
      jumpNorm = jumpnext;
    ]]>
  </filter>

</sequence>

<output format="ascii" filename="Stoch2.xsil">
  <sampling_group initial_sample="yes">
    <moments>aR</moments>
    <dependencies>state normVec</dependencies>
    <![CDATA[
      aR = mod2(a)/norm2;
    ]]>
  </sampling_group>
</output>
</simulation>

```



This code uses the 9th order Runge-Kutta method to directly integrate the master equation.

```
<?xml version="1.0" encoding="UTF-8"?>
<simulation xmds-version="2">
  <name>Master Equation</name>

  <author> Damon Binder</author>

  <features>
    <globals>
      <![CDATA[
        real omega = 1;
        real epsilon =1;
        real kappa = 1;
      ]]>
    </globals>
    <error_check />
  </features>

  <geometry>
    <propagation_dimension> t </propagation_dimension>
  </geometry>

  <vector name="state" type="complex">
    <components>
      p q
    </components>
    <initialisation>
      <![CDATA[
        p=1;
        q=0;
      ]]>
    </initialisation>
  </vector>

  <sequence>
    <integrate algorithm="ARK89" interval="10" tolerance="1e-7" steps="500">
      <samples>100</samples>
      <operators>
        <integration_vectors>state</integration_vectors>
        <![CDATA[
          dp_dt = -2*epsilon*Im(q*exp(i*omega*t))-kappa*p;
          dq_dt = -i*omega*q-i*omega*(1-2*p)*epsilon*exp(- i*omega*t)-kappa*q/2;
        ]]>
      </operators>
    </integrate>
  </sequence>

  <output format="ascii" filename="Master Equation.xsil">
    <sampling_group initial_sample="yes">
      <moments>pR</moments>
      <dependencies>state</dependencies>
      <![CDATA[
        pR = p.Re();
      ]]>
    </sampling_group>
  </output>
</simulation>
```

```
    ]]>
  </sampling_group>
</output>
</simulation>
```