Computer Physics

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Project 1

In this project I calculate the energy spectrum of $H = H_0 + \lambda V$ where H_0 is the harmonic oscillator and $V = \hbar\omega(\frac{x}{a})^4$ where $a = \sqrt{\frac{\hbar}{m\omega}}$ is the natural length of the system.

This is achieved by adding the matrices of H_0 and V in the basis of the eigenvectors of H_0 and then truncating the basis. We know the matrix representation of $\frac{x}{a}$ in this basis is

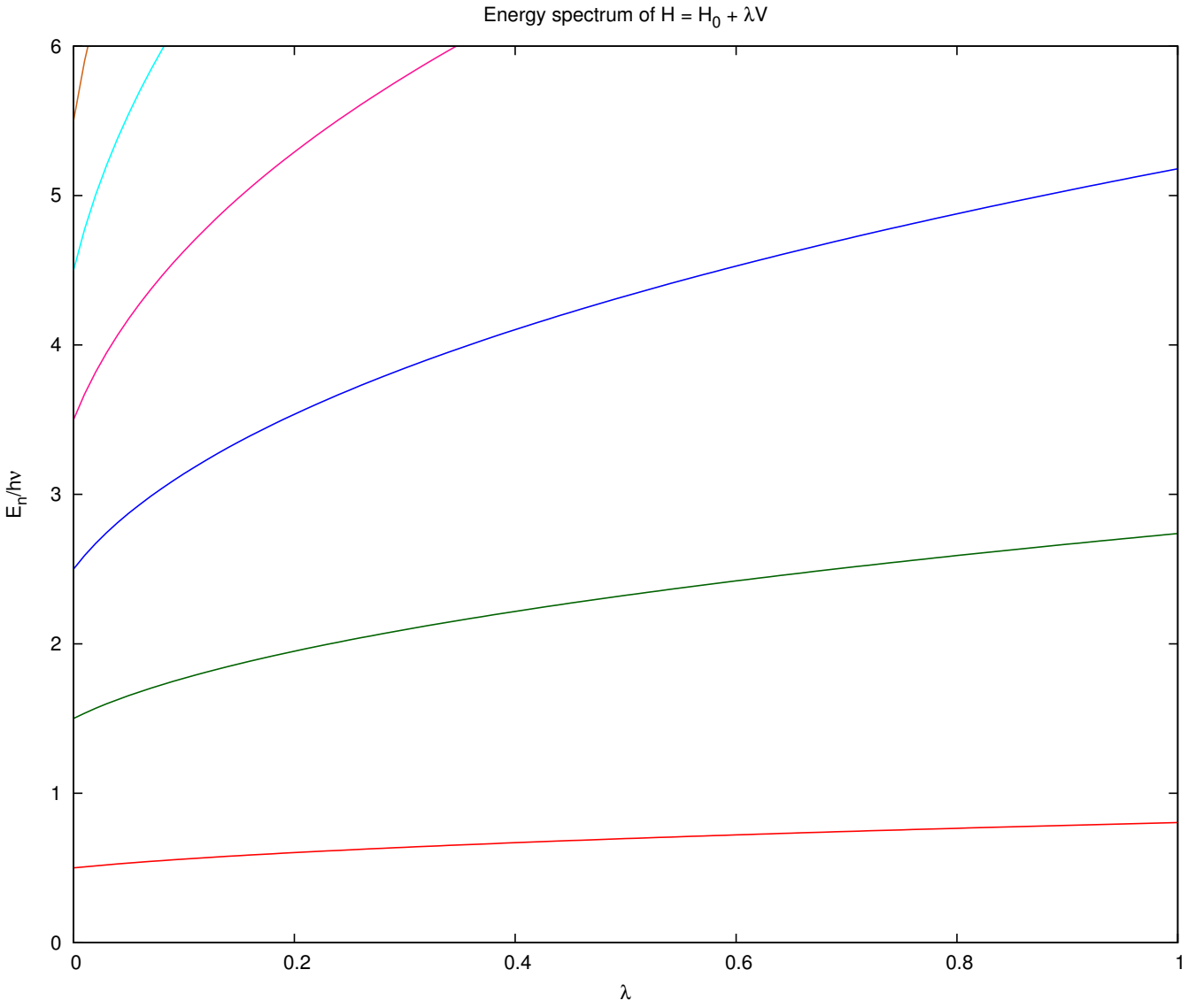
$$\mathbb{x} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

and the matrix for V is simply $\hbar\omega\mathbb{x}^4$. We add this (multiplied by some λ) to

$$H_0 = \hbar\omega \begin{bmatrix} 0.5 & 0 & 0 & 0 & \dots \\ 0 & 1.5 & 0 & 0 & \dots \\ 0 & 0 & 2.5 & 0 & \dots \\ 0 & 0 & 0 & 3.5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

and then truncate. In our case we used a basis of 128 eigenvectors of H_0.

The eigenvalues of the resulting matrix are of course the possible values of energy of the system. The following is a graph of the first six eigenvalues as a function of λ.


Energy spectrum of H = H0 + λV
En/hν
λ
0
1
2
3
4
5
6
0
0.2
0.4
0.6
0.8
1

Project 2

We continue with the harmonic oscillator H_0 but this time we take a look at $H = H_0 + H'(t)$ where $H'(t) = \frac{1}{\sqrt{2}}\hbar\Omega(a^\dagger + a)\theta(t)$ where a is the ladder operator and $\theta(t)$ is the Heaviside step function. We again use the energy basis of the harmonic oscillator. Then the matrix for a is

$$\begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

so the matrix for $a^\dagger + a$ is

$$\begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Now given some initial state of the density operator ρ, for example the ground state of the harmonic oscillator:

$$\rho = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

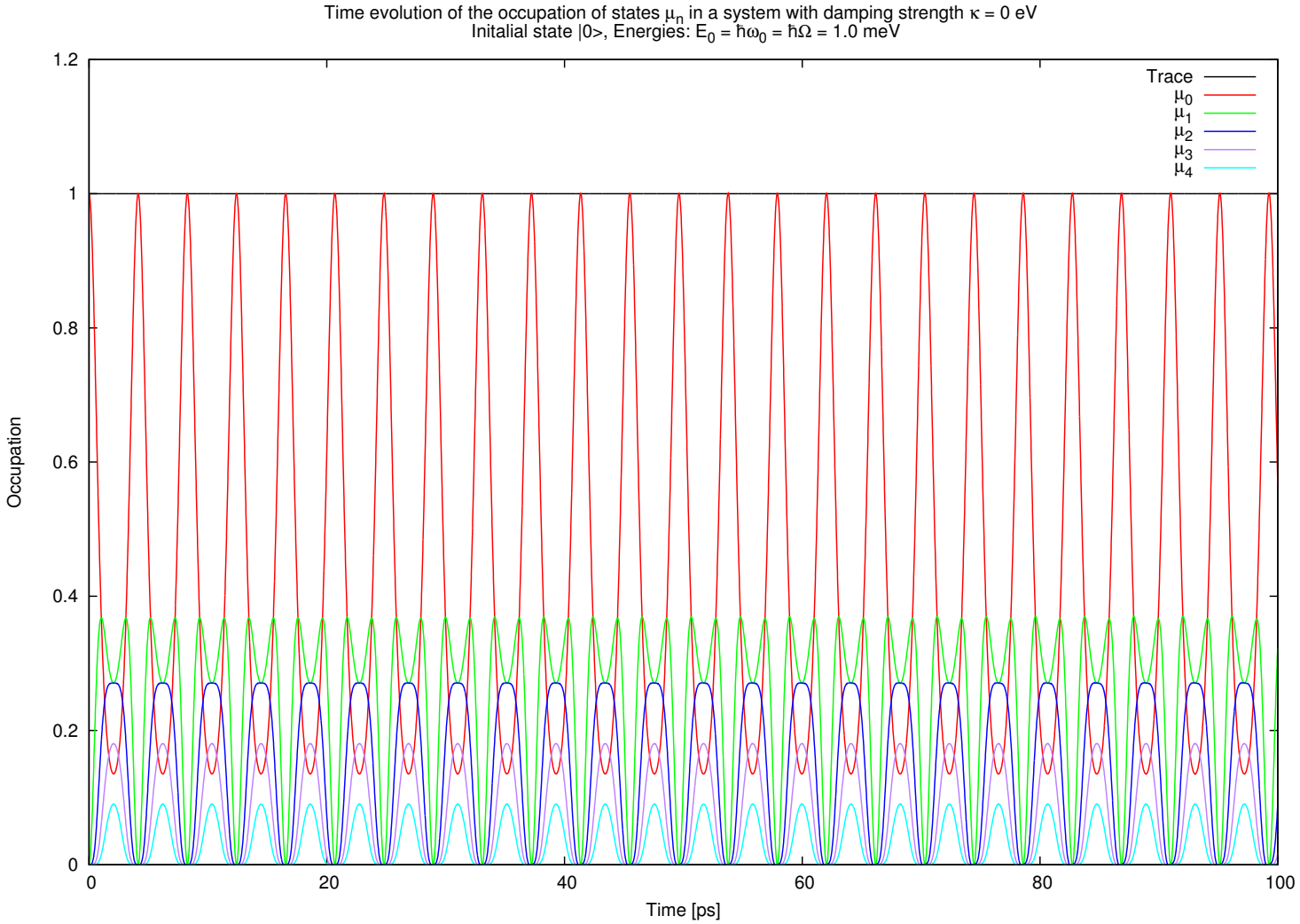
we can add these matrices in a truncated basis (here we use a 16 eigenvector basis) and then calculate the time evolution of the system using the Liouville-von Neumann equation:

$$i\hbar\dot{\rho}(t) = [H(t), \rho(t)] \text{ i.e. } \dot{\rho}(t) = \tfrac{1}{\hbar}\Lambda[\rho(t)],\ \Lambda[\rho(t)] = -i[H(t), \rho(t)]$$

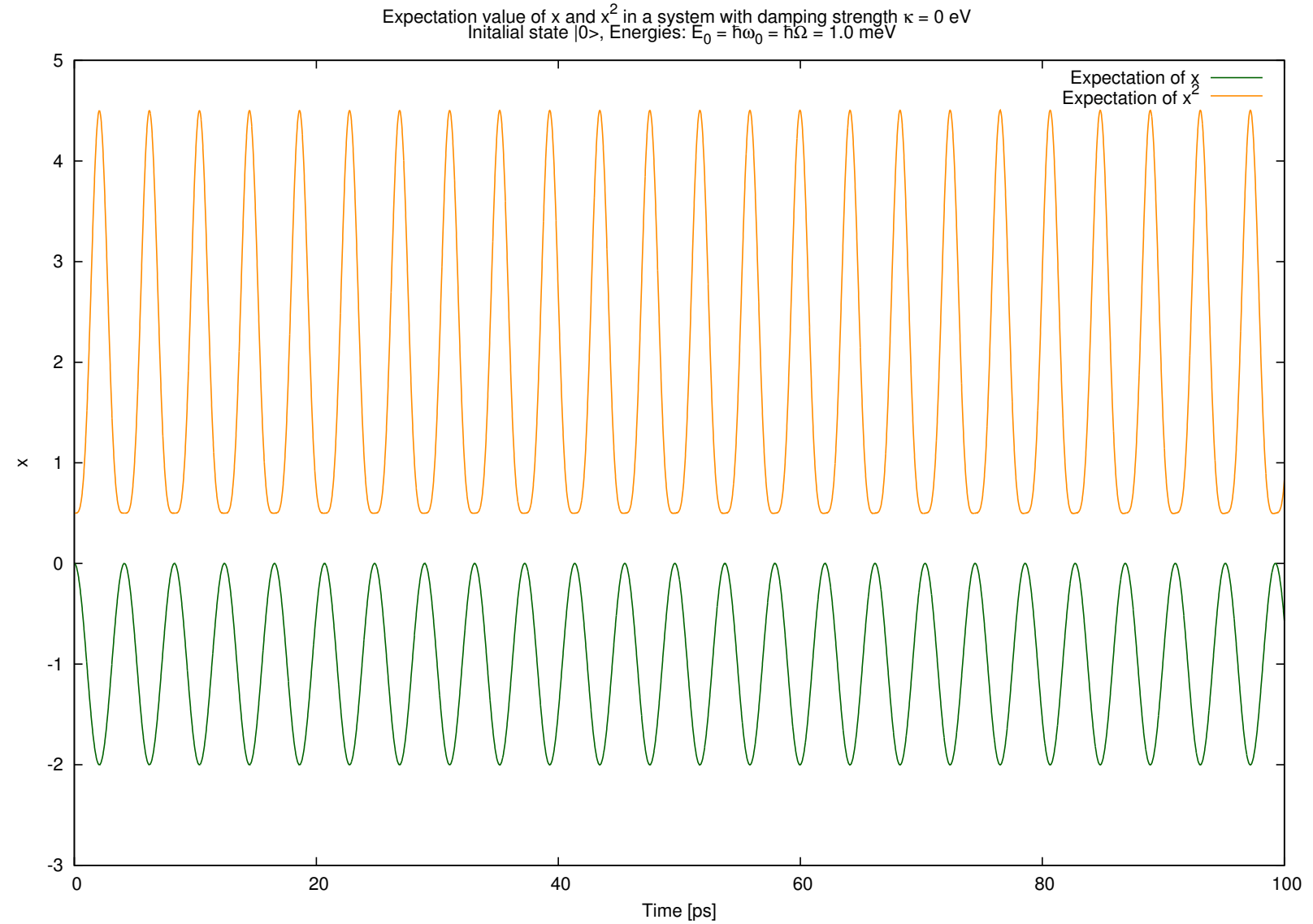
or, more specifically, using iteration of the following Crank-Nicolson approximation of the Liouville-von Neumann equation:

$$\rho(t_{n+1}) = \rho(t_n) + \tfrac{\Delta t}{2\hbar}(\Lambda[\rho(t_n)] + \Lambda[\rho(t_{n+1})])$$

for some timegrid where $t_0 = 0$ and $t_{n+1} = t_n + \Delta t$. Throughout this project we use $\Delta t = 0.01\ ps$. In the graph below we show the time evolution of the occupation of the five lowest states of our system.


Time evolution of the occupation of states μ_n in a system with damping strength κ = 0 eV
Initalial state |0>, Energies: $E_0 = \hbar\omega_0 = \hbar\Omega$ = 1.0 meV
Trace
μ_0
μ_1
μ_2
μ_3
μ_4
Occupation
Time [ps]
0
0.2
0.4
0.6
0.8
1
1.2
0
20
40
60
80
100

Now we find $< x >$ and $< x^2 >$ (actually we'll find $< \frac{x}{a} >$ and $< (\frac{x}{a})^2 >$ where a is the same as in project 1, in all the graphs below where it says x we mean $\frac{x}{a}$) for this same system $H = H_0 + H'(t)$. This is done simply by evaluating the trace of $\rho\mathbb{x}$ (where $\mathbb{x}$ is the same as in project 1) and the trace of $\rho\mathbb{x}^2$. Below is a graph of the expectation values.



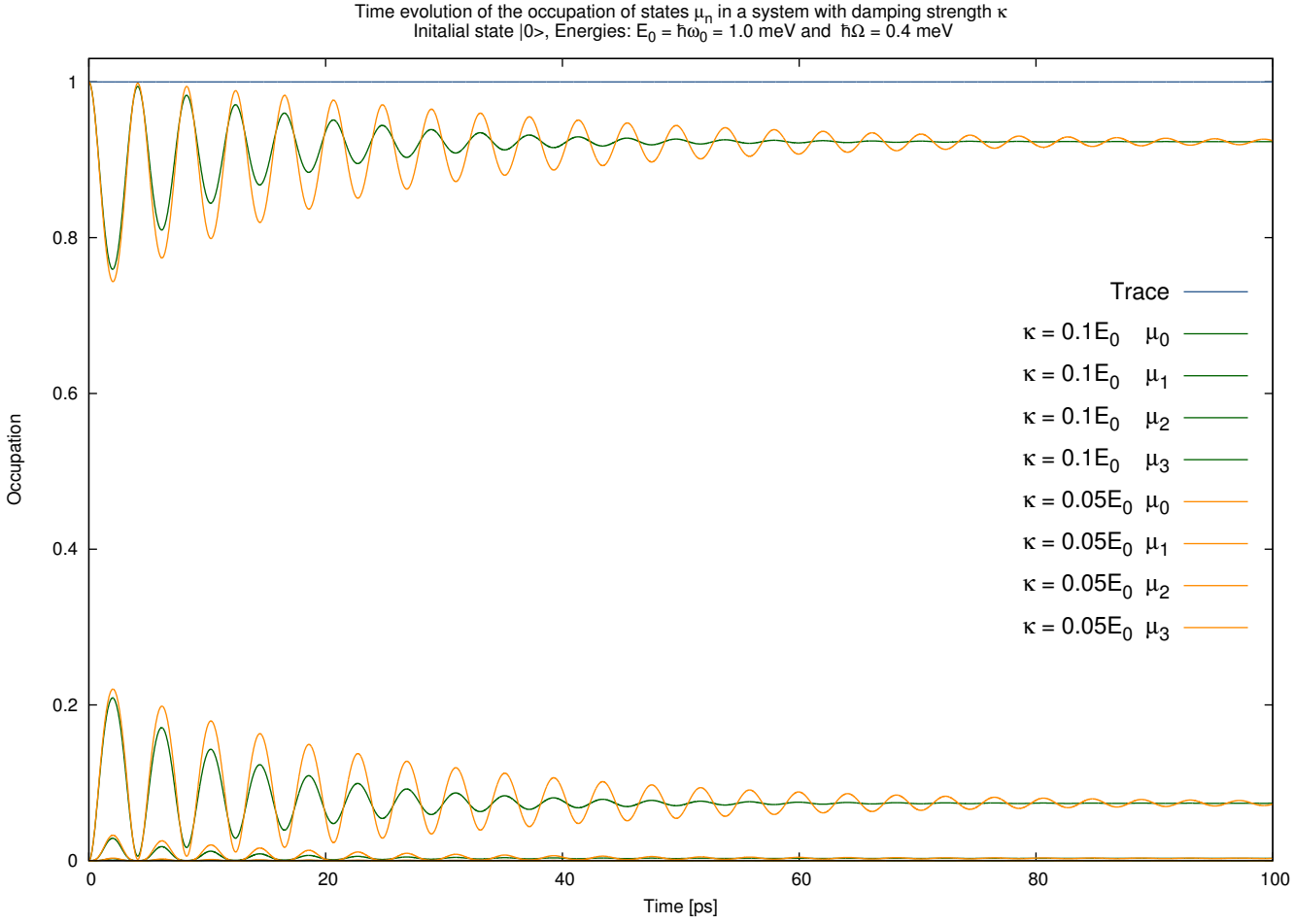
At this point we add dissipation to the model. The Liovulle-von Neumann equation becomes:

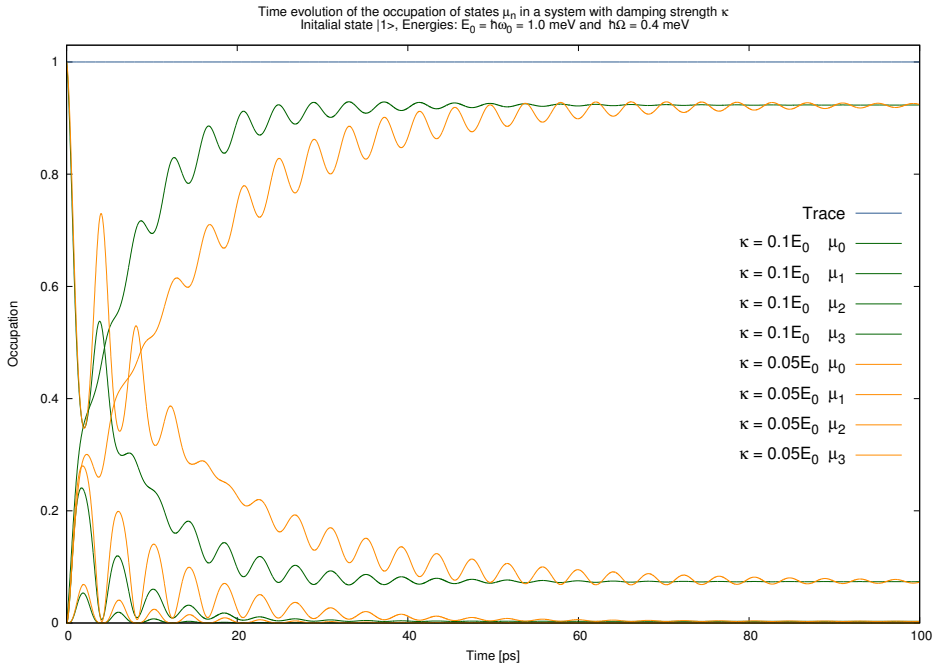
$$i\hbar\dot{\rho}(t) = [H(t), \rho(t)] + i\tfrac{\kappa}{2}\{[a, \rho a^\dagger] + [a\rho, a^\dagger]\}$$

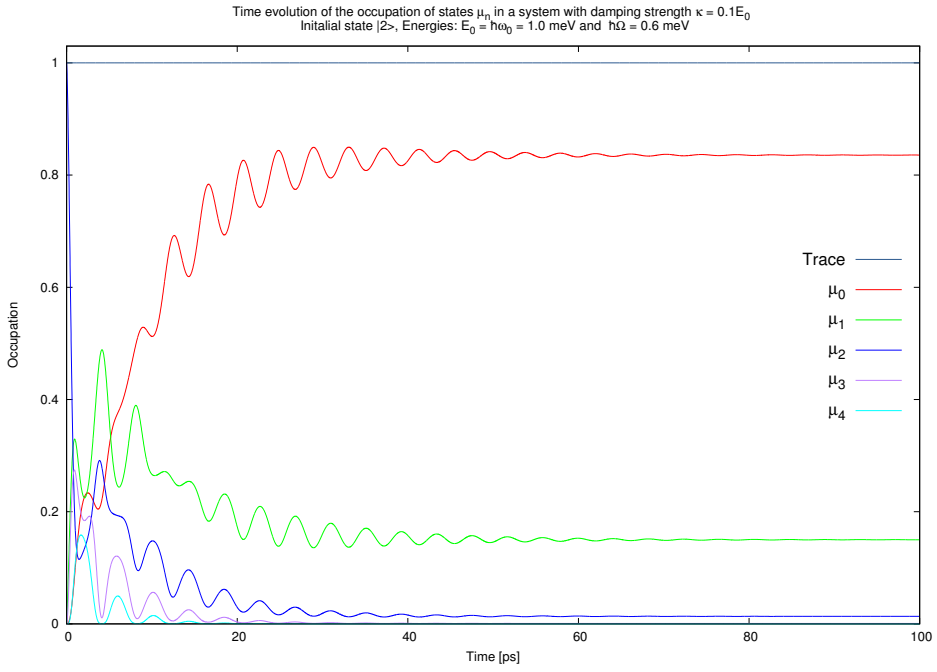
The only change we have to make in our code is to modify Λ, which now becomes

$$\Lambda[\rho(t)] = -i[H(t), \rho(t)] + \tfrac{\kappa}{2}\{[a, \rho(t)a^\dagger] + [a\rho(t), a^\dagger]\}$$

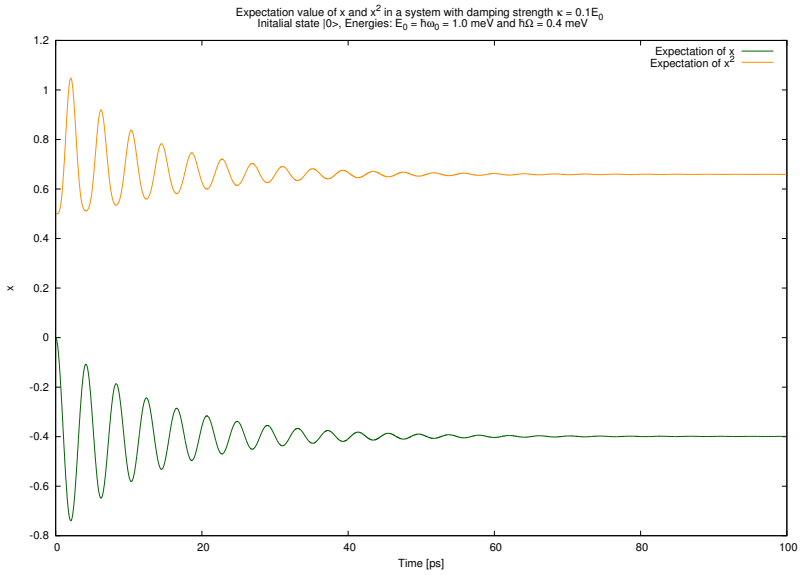
The following are three graphs of the time evolution of the occupation. The first assumes an initial state of $|0>$ and shows the evolution for two different values of κ. The second is the same except it assumes an initial state of $|1>$ and the third assumes an initial state of $|2>$ and only shows one value of κ.

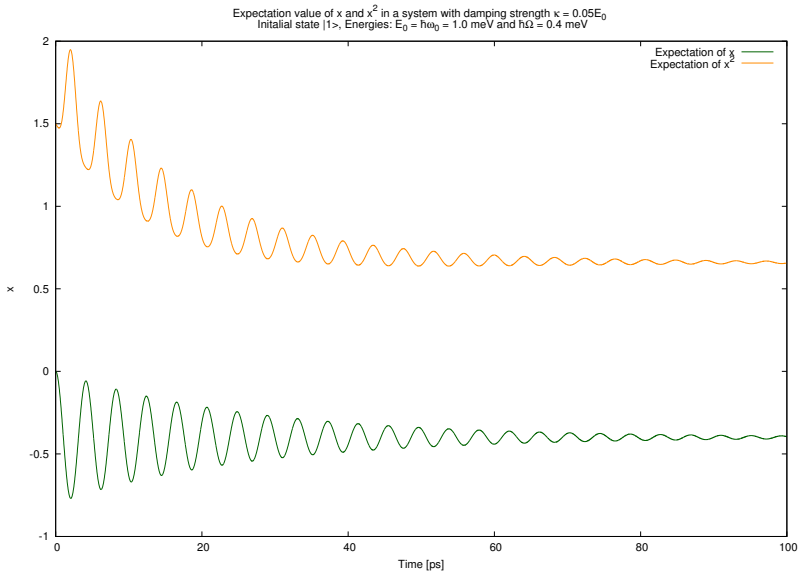



Time evolution of the occupation of states μ_n in a system with damping strength κ
Initalial state |1>, Energies: $E_0 = \hbar\omega_0$ = 1.0 meV and $\hbar\Omega$ = 0.4 meV
Occupation
Time [ps]
Trace
$\kappa = 0.1E_0$ μ_0
$\kappa = 0.1E_0$ μ_1
$\kappa = 0.1E_0$ μ_2
$\kappa = 0.1E_0$ μ_3
$\kappa = 0.05E_0$ μ_0
$\kappa = 0.05E_0$ μ_1
$\kappa = 0.05E_0$ μ_2
$\kappa = 0.05E_0$ μ_3


Time evolution of the occupation of states μ_n in a system with damping strength $\kappa = 0.1E_0$
Initalial state |2>, Energies: $E_0 = \hbar\omega_0$ = 1.0 meV and $\hbar\Omega$ = 0.6 meV
Occupation
Time [ps]
Trace
μ_0
μ_1
μ_2
μ_3
μ_4

And finally here are two graphs of the expectation values $< \frac{x}{a} >$ and $< (\frac{x}{a})^2 >$ using this new model.





Project 3

In this project we find the steady states from project 2 directly by going from Hilbert space to Liouville space. Since the condition for a steady state is

$$\dot{\rho}(t) = 0$$

and the dynamics of our system are governed by

$$i\hbar\dot{\rho}(t) = [H(t), \rho(t)] + i\tfrac{\kappa}{2}\{[a, \rho a^\dagger] + [a\rho, a^\dagger]\}$$

we are looking to solve the equation:

$$[H(t), \rho(t)] + i\frac{\kappa}{2}\{[a, \rho a^\dagger] + [a\rho, a^\dagger]\} = 0. \qquad (\star)$$

By representing the vectorization of a matrix A by $vec(A)$ and utilizing the fact that

$$vec(ABC) = (C^T \otimes A)vec(B)$$

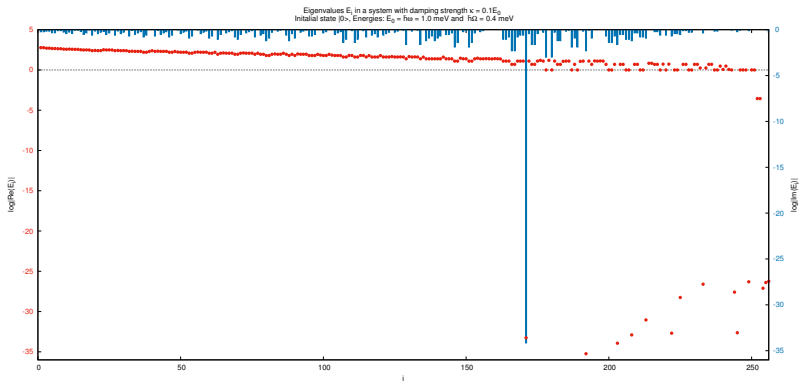
we can rewrite $(\star)$ as the following:

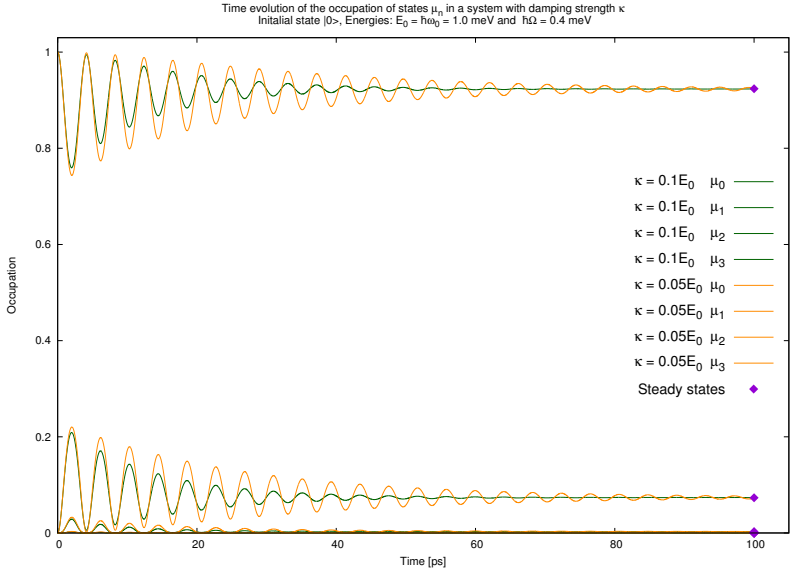
$$\{I \otimes A_- + A_+^T \otimes I + i\kappa((a^\dagger)^T \otimes a)\}vec(\rho) = 0$$

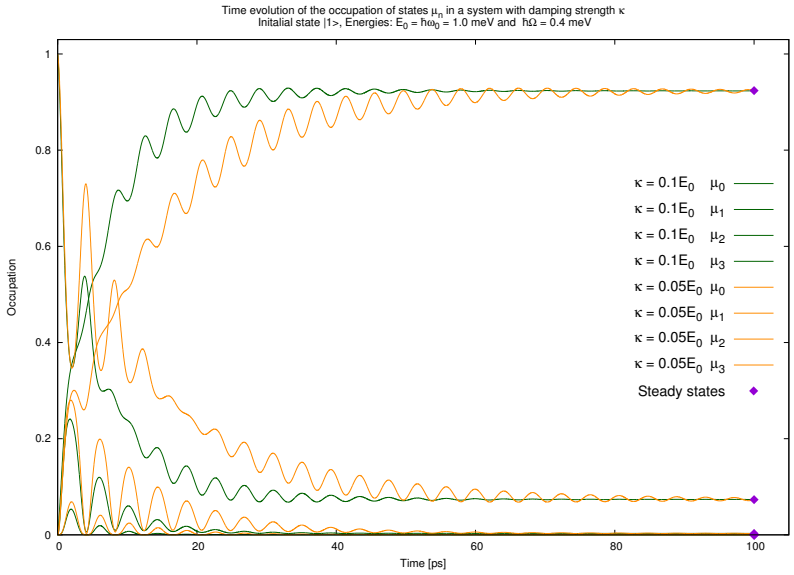
where $A_\pm = H \pm i\frac{\kappa}{2}a^\dagger a$. We start by simply finding all the eigenvalues (and vectors) of

$$I \otimes A_- + A_+^T \otimes I + i\kappa((a^\dagger)^T \otimes a)$$

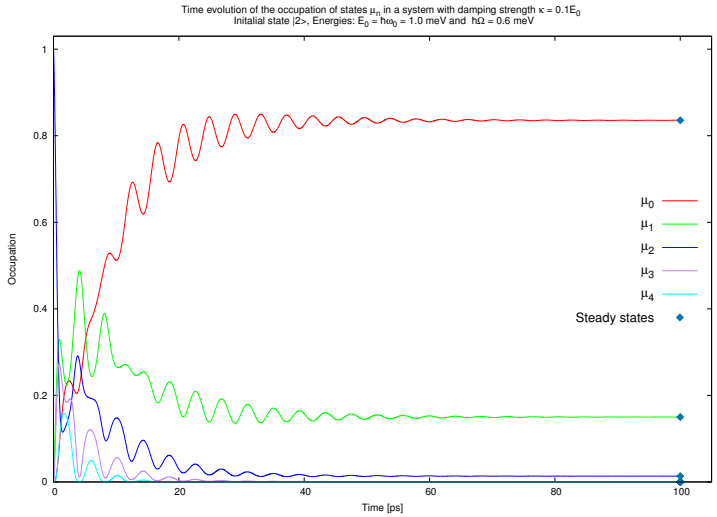
So for example using our usual basis of the first 16 states of H_0 we get 256 eigenvalues, shown in the following plot for $\kappa = 0.2E_0$, initial state $|0>$ and energies $\hbar\omega = 1.0$ meV and $\hbar\Omega = 0.4$ meV.







We see what is clearly a zero just below the 150th eigenvalue (it happens to be E_{141}). Its corresponding eigenvector, $vec(\rho_{ss})$, is a steady state for this system. The diagonal elements of the matrix ρ then tell us the occupation of states of the harmonic oscillator. Above and below we have marked these on our time evolution plot from project 2.



Now we can directly calculate the time evolution of the occupation of states in our system. If we have our left eigenvectors in the matrix U, our right eigenvectors in the matrix V and the eigenvalues themselves in the matrix λ, then the density matrix can be written as

$$\rho(t) = (Ve^{-i\lambda t}U^{\dagger})\rho_0$$

where ρ_0 is the initial state of the system. In the plot below we compare the time evolution calculated directly (this way) and the one obtained in project 2 by time integration. There is no visable difference.