2. project

We continue with the harmonic oscillator

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 , \qquad [x, p] = i\hbar$$

or

$$H_0 = \hbar\omega\left\{a^\dagger a + \frac{1}{2}\right\}$$

in the book of Griffiths

$a^\dagger = a_+$ We use the more

$a = a_-$ standard notation

here

At $t=0$ it finds itself all of a sudden in an external „static" electricfield

$$H(t) = H_0 + H'(t)$$

with

Heaviside step function

$$H'(t) = \hbar\Omega\left\{a^\dagger + a\right\}\Theta(t)$$

In http://hartree.raunvis.hi.is/~vidar/Nam/IaSF/22F.pdf you can find an exact analytical solution for the state $|\Psi(t)\rangle$

Here we want to use numerical methods to find information about the time evolution of the system. We want to use a method that allows us later to add new terms to this model. We will solve the Liouville-von Neumann equation

$$i\hbar \dot{\rho}(t) = [H(t), \rho(t)]$$

for the density or probability operator $\rho(t)$. When we have $\rho(t)$ it's diagonal elements give us the occupation of the states of the H.O. The mean value of its location is for example

$$\langle x \rangle = tr\{x\rho\} = \sum_n \langle n | x\rho | n \rangle$$

$$= \sum_{nm} \langle n | x | m \rangle \langle m | \rho | n \rangle$$

the trace of the matrices of x and ρ multiplied.

Usually the best solution method is to find the unitary time-evolution operator $T(t)$

$$\rho(t) = T(t)\,\rho(0)\,T^{+}(t)$$

substitution into L-v N-equation then gives

$$i\hbar\,\dot{T}(t) = H(t)\,T(t)$$

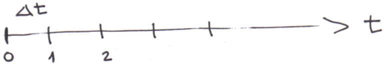
$$-i\hbar\,\dot{T}^{+}(t) = T^{+}(t)\,H(t)$$

but we want later to add terms that might not lead to unitary evolution, so we solve directly the L-v N-eq.

$$i\hbar\,\dot{\rho}(t) = [H(t), \rho(t)] = \underbrace{+i\Lambda[\rho(t)]}$$

Λ is a functional of $\rho(t)$

by introducing a time grid



and use the Crank-Nicolson method that is good for hermitian operators. The time grid suggests 2 equations

$$① \quad \left\{ \rho(t_{n+1}) - \rho(t_n) \right] \simeq \frac{\Delta t}{\hbar} \Lambda \left[\rho(t_n) \right]$$

$$② \quad \left\{ \rho(t_n) - \rho(t_{n-1}) \right\} \simeq \frac{\Delta t}{\hbar} \Lambda \left[\rho(t_n) \right]$$

forward and backward time steps

$$① \rightarrow \rho(t_{n+1}) \simeq \left\{ \rho(t_n) + \frac{\Delta t}{\hbar} \Lambda \left[\rho(t_n) \right] \right\}$$

$$② \rightarrow \left\{ \rho(t_{n+1}) - \rho(t_n) \right\} \simeq \frac{\Delta t}{\hbar} \Lambda \left[\rho(t_{n+1}) \right]$$

$$\hookrightarrow \left\{ \rho(t_{n+1}) - \frac{\Delta t}{\hbar} \Lambda \left[\rho(t_{n+1}) \right] \right\} \simeq \rho(t_n)$$

Við leggjum saman jöfnurnar og deilum með 2

$$\to \underbrace{\left\{\rho(t_{n+1}) - \frac{\Delta t}{2\hbar}\Lambda\left[\rho(t_{n+1})\right]\right\}}_{\text{framtíð}} = \underbrace{\left\{\rho(t_n) + \frac{\Delta t}{2\hbar}\Lambda\left[\rho(t_n)\right]\right\}}_{\text{nútíð}}$$

known

and interprete as

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

unknown

want to find

We scale time $\frac{\Delta t}{\hbar}$ appropriately by comparison to $\hbar\omega$ and select small steps. We need to <u>iterate</u> the equation in <u>each time step</u>

a) Find the time-evolution of the occupation of few lowest states. Check accuracy with respect to $\frac{\hbar\Omega}{\hbar\omega}$

b) Find $\langle x\rangle(t)$, $\langle x^2\rangle(t)$.

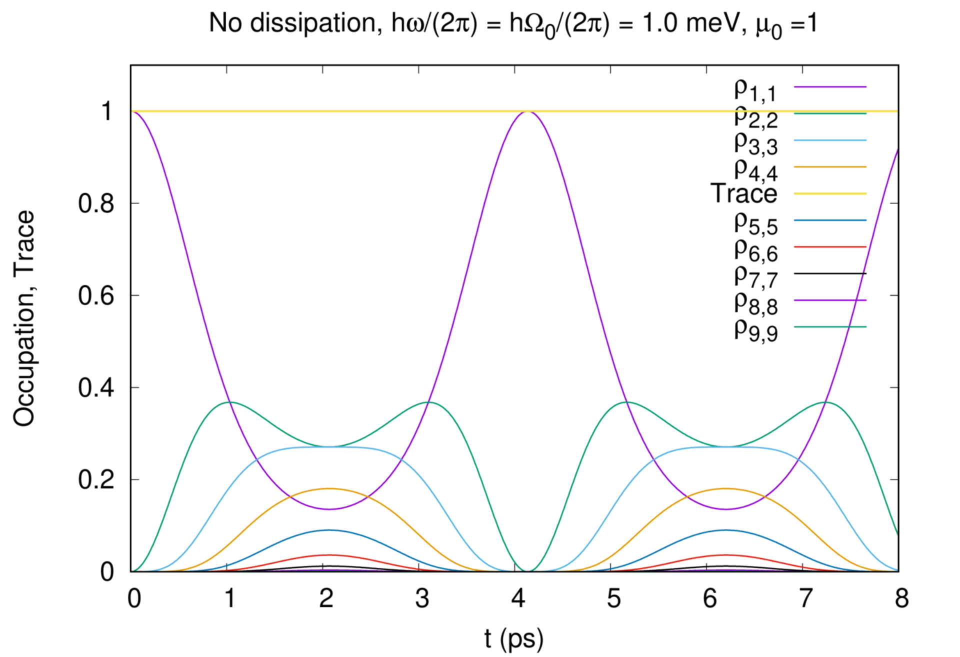
I add here a graph for a).

Because we are working with the L-vN-equation it is possible to add dissipation to our model.
We use a common method for the H.O., see for example

L.S. Bishop, E. Ginossar, and S.M. Girvin, PRL 105, 100505 (2010)

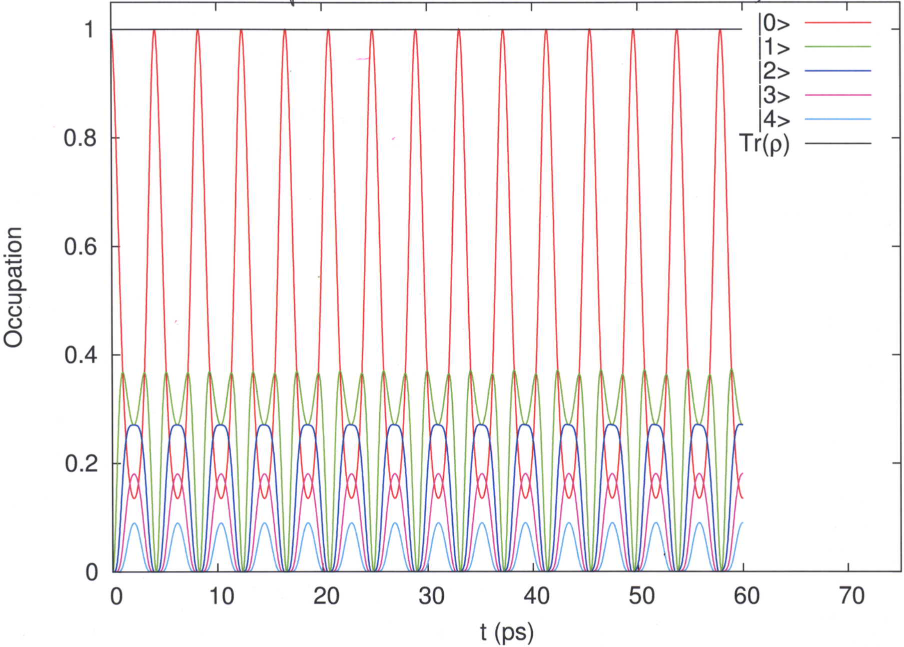
$$i\hbar\dot{\rho} = [H,\rho] - i\frac{\kappa}{2}\left\{[a\rho,a^{+}] + [a,\rho a^{+}]\right\}$$

This damping is caused by coupling to an external reservoir at a high temperature
κ is the damping strength



No dissipation, hω/(2π) = hΩ0/(2π) = 1.0 meV, μ0 =1
Occupation, Trace
t (ps)
ρ1,1
ρ2,2
ρ3,3
ρ4,4
Trace
ρ5,5
ρ6,6
ρ7,7
ρ8,8
ρ9,9

No dissipation $\hbar\omega = \hbar\Omega = 1\,\mathrm{meV}$, $\alpha f = 16$



c) Find the time-evolution of the occupation like in a)

d) Find again $\langle x \rangle (t)$ and $\langle x^2 \rangle (t)$

The dissipation only changes $\mathcal{L}[\rho(t)]$ in the model.

Here are some results

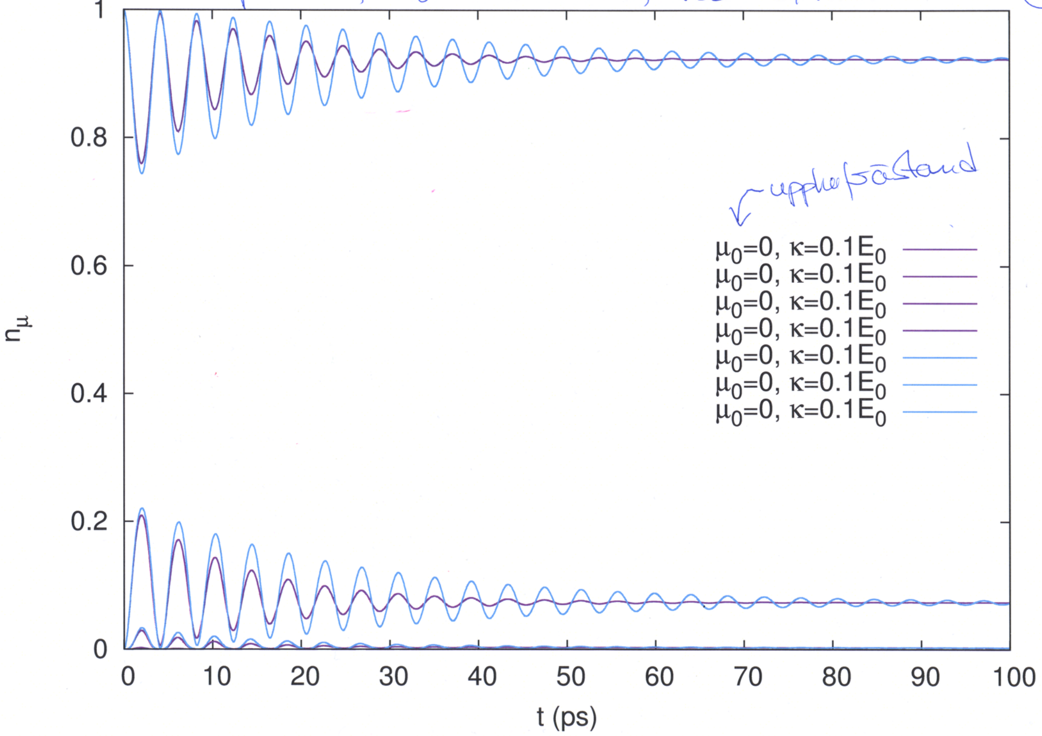
e) Find the Rény-2 entropy

$$S(t) = -k_B \ln\{\mathrm{Tr}(\rho^2)\}$$

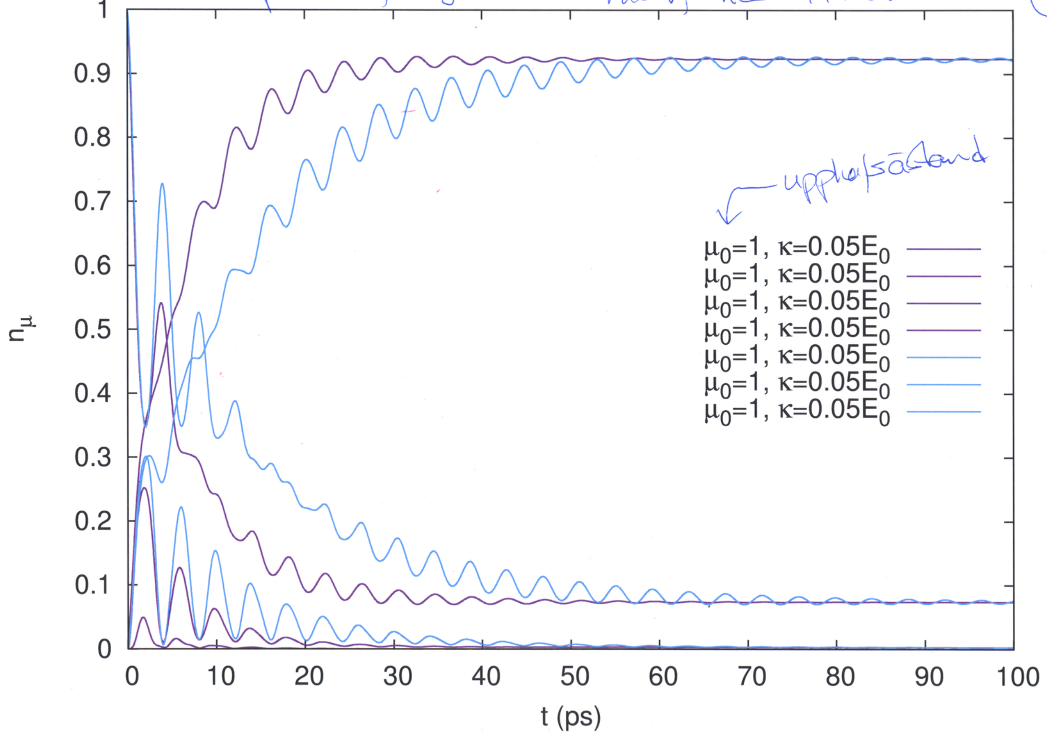
and try to figure out what messages it conways

Occupation, $E_0 = \hbar\omega_0 = 1$ meV, $\hbar\Omega = 0,4$ meV

9



Occupation, $E_0 = \hbar\omega_0 = 1\,\mathrm{meV}$, $\hbar\Omega = 0.4\,\mathrm{meV}$ 10



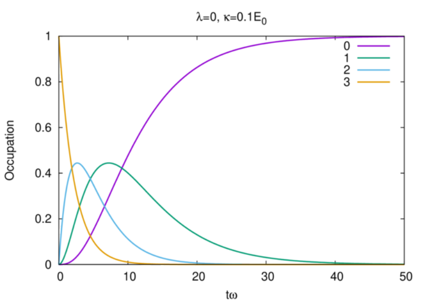
It is also interesting to use the model to see how an excited HO decays into its ground state, see next two figures.

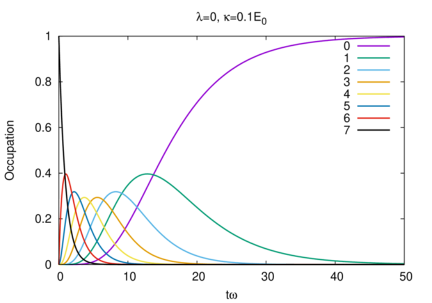
The derivation of the dissipation is complex and care has to be taken when the system is not only a HO, see

C.W. Gardiner and M.J. Collett, PRA 31, 3761 (1985)

For example one might want to do the calculation for the anharmonic oscillator, in its own eigenbasis

We can discuss this issue in class. . . .


λ=0, κ=0.1E$_0$
Occupation
tω
0
1
2
3
0
0.2
0.4
0.6
0.8
1
0
10
20
30
40
50



λ=0, κ=0.1E0
Occupation
tω
0
1
2
3
4
5
6
7
0
0.2
0.4
0.6
0.8
1
10
20
30
40
50