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

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

in the book of Griffiths

$a^+ = a_+$
$a = a_-$

We use the more 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

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

Heaviside Step function

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 $T(t)$

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

substitution into L-v N-equation then gives

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

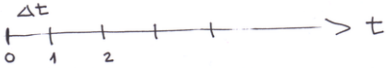
$$-i\hbar\,\dot{T}^{+}(t) = T^{+}(t)\,H(t)$$

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

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

Λ or felli of $\varrho(t)$ is a functional

by introducing a time grid



and use the Cranck-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 each <u>each time step</u>

a) Find the time-evolution of the occupation of few lowest state. Check accuracy with respect to $\hbar\Omega/\hbar\omega$

b) Find $\langle x\rangle(t)$.

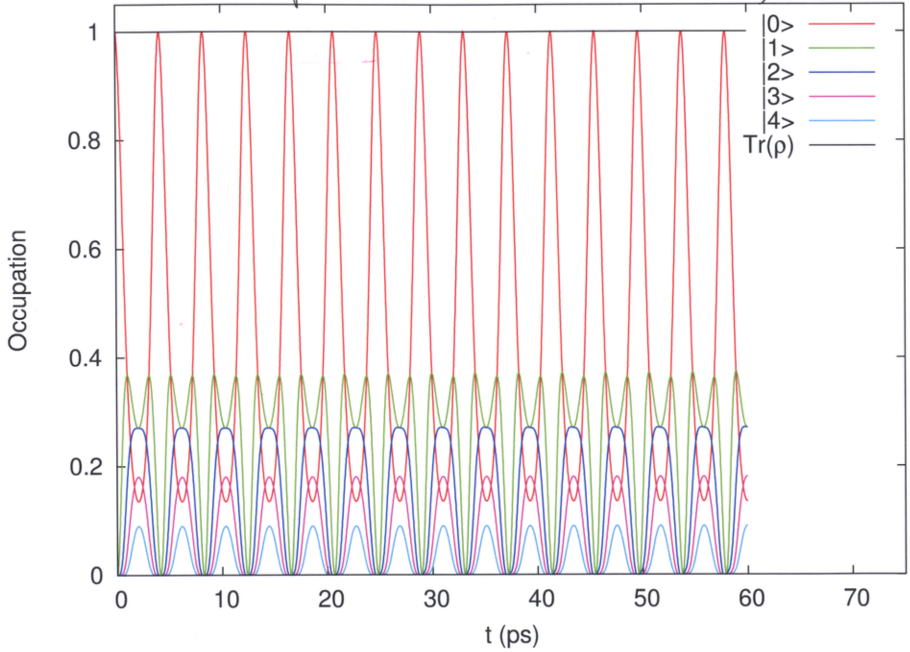
I add here a graph for a). It still has to be confirmed.

Becaus we are working with the L-v N-equation it is possible to add dissipation to our model. let's do it like Björn Birnir i PRL 76, 3309 (1996)

$$i\hbar\dot{\varrho} = [H,\varrho] - \frac{i}{2}\{RS\varrho + S\varrho R\}$$

this is a type of a master equation for a open system that we do not derive here

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



$\delta\rho = \rho(t) - \rho_0$, where ρ_0 is the density matrix for only the ground state occupied.

$$\rho_0 = \begin{pmatrix} 1 & & 0 \\ & 0 & \\ 0 & & 0 \end{pmatrix}$$

and we set

$$R = \begin{pmatrix} \Gamma_1 & & & 0 \\ & \Gamma_1 & & \\ & & \ddots & \\ 0 & & & \Gamma_1 \end{pmatrix}$$

Γ_1 on the diagonal

I select for testing $\Gamma_1 = 0.10\ \hbar\omega$

The dissipation sends the system to the ground state, but $H'(t)$ has and is perturbing it's levels

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

d) Find again $\langle x \rangle (t)$.

The dissipation only changes $\Lambda[\rho(t)]$ in the equation above

With dissipation $\hbar\omega = \hbar\Omega = 1$ meV, $N_f = 16$