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

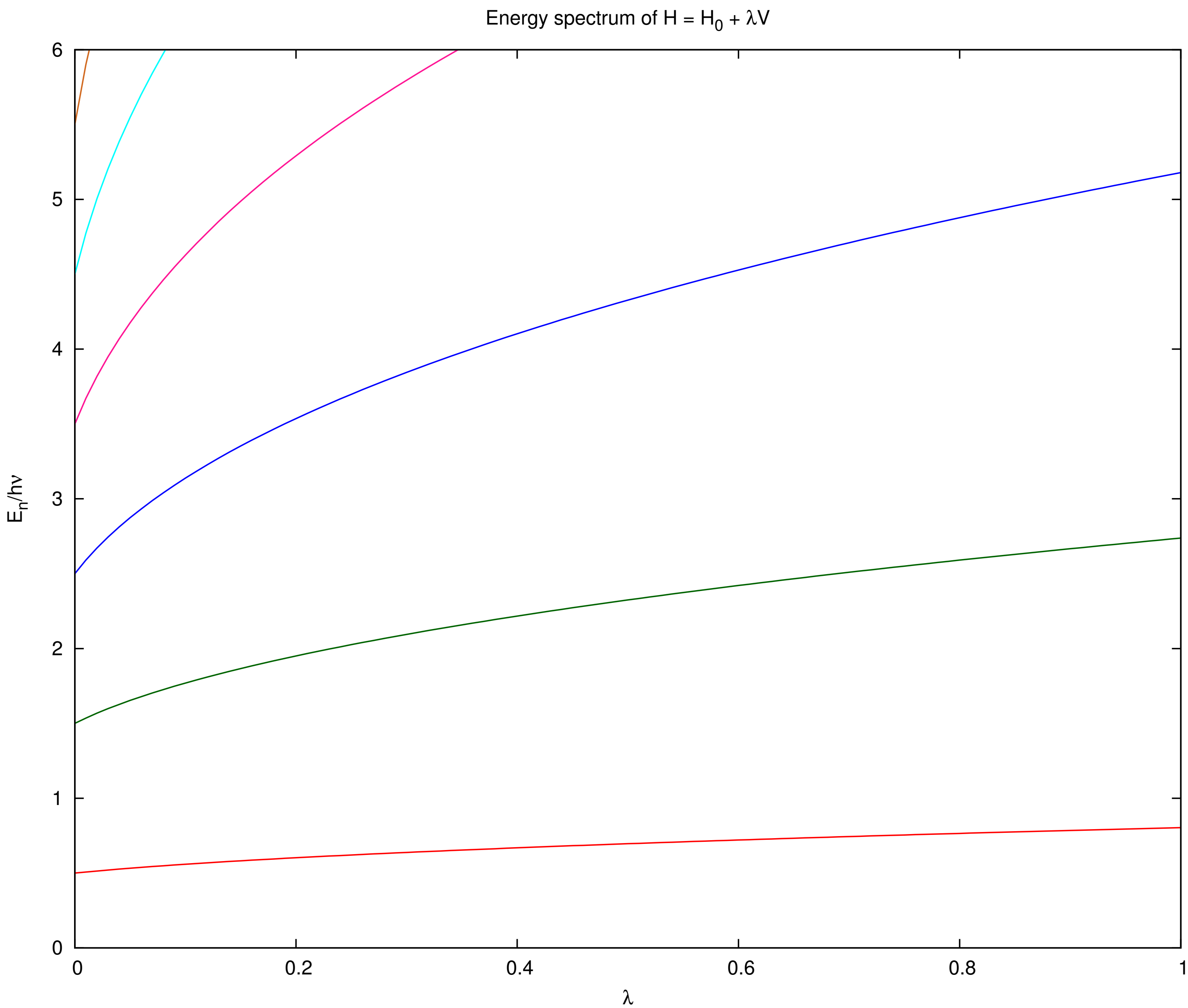
$$\cancel{x} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

and the matrix for V is simply $\hbar\omega\cancel{x}^4$. 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
E_n/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 $H'(t) = \hbar\Omega(a^\dagger + a)\theta(t)$ 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:

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

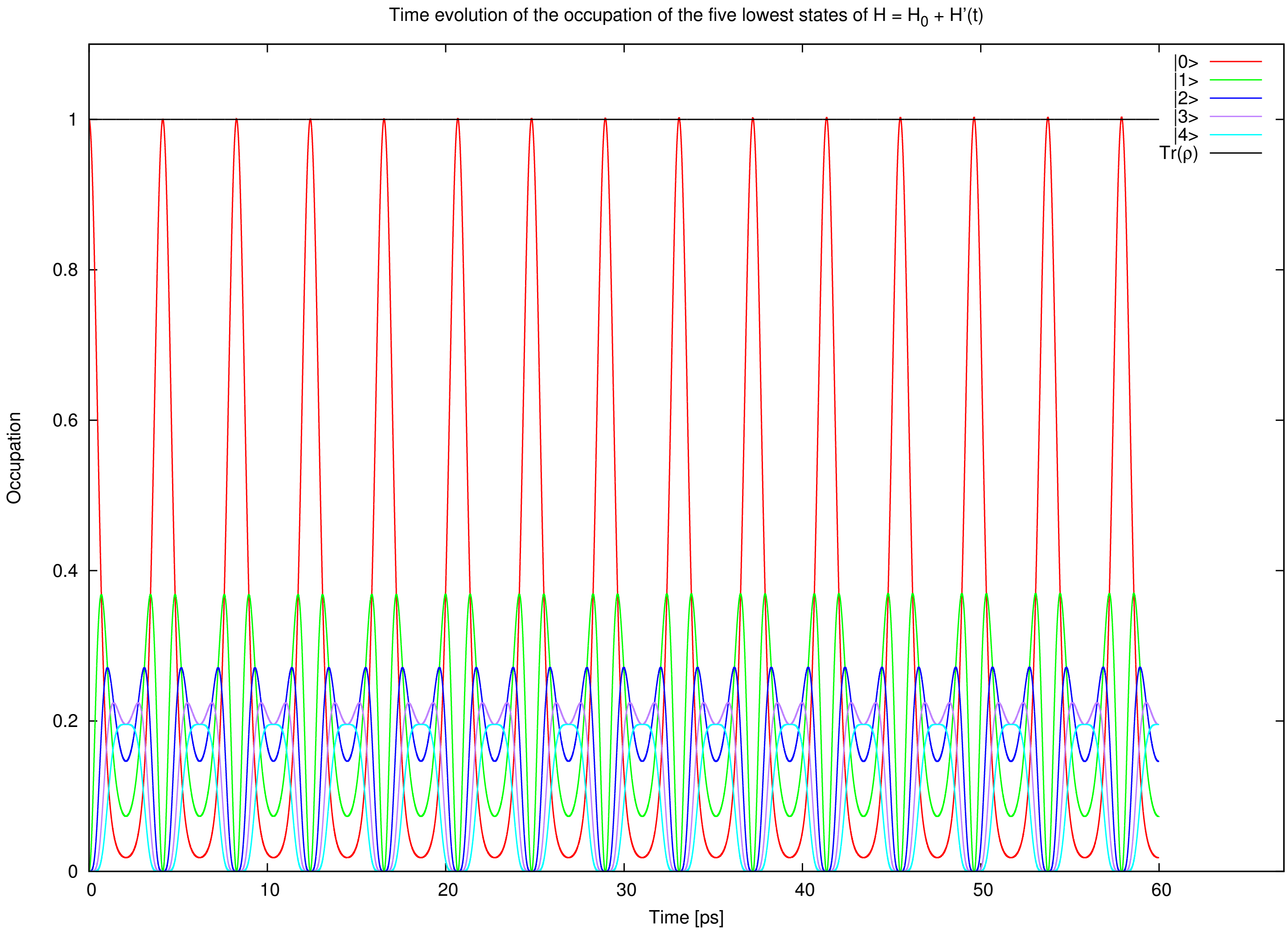
we can add these matrices in a truncated basis and then calculate the time evolution of the system using the Liouville-von Neumann equation:

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

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 $t_{n+1} = t_n + \Delta t$. In the graph below we show the time evolution of the occupation of the five lowest states assuming the initial state is $|0>$, the timestep is $\Delta t = 1fs$ and that $\hbar\omega = \hbar\Omega = 1meV$.


Time evolution of the occupation of the five lowest states of H = H0 + H'(t)
|0>
|1>
|2>
|3>
|4>
Tr(ρ)
Occupation
0
0.2
0.4
0.6
0.8
1
0
10
20
30
40
50
60
Time [ps]

Now we find $< x >$ and $< x^2 >$ (actually weĺl find $< \frac{x}{a} >$ and $< (\frac{x}{a})^2 >$ where a is the same as in project 1) 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 as in project 1) and the trace of $\rho \mathbb{x}^2$. The graph below assumes again that the initial state is $|0>$, the timestep is $\Delta t = 1fs$ and that $\hbar\omega = \hbar\Omega = 1meV$.