Phys 435, I-Semester 2022/23, Assignment 2

Instructor: Sebastian Wüster
Due-date: Fri 2.9.2022

(1) Coupled harmonic oscillators: Consider two quantum mechanical harmonic oscillators of mass $m = 1$, described with the Hamiltonian

$$\hat{H} = \hbar\omega\big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\big) + \hbar\omega\big(\hat{b}^\dagger\hat{b} + \frac{1}{2}\big) + \hbar\kappa\big(\hat{a}^\dagger + \hat{a}\big)\big(\hat{b}^\dagger + \hat{b}\big). \tag{1}$$

where $\hat{a}^\dagger$, $\hat{a}$ are ladder operators for oscillator 1, and $\hat{b}^\dagger$, $\hat{b}$ for oscillator 2.

This corresponds to the classical Hamiltonian

$$H = \frac{1}{2}\Big(p_1^2 + \omega^2 x_1^2\Big) + \frac{1}{2}\Big(p_2^2 + \omega^2 x_2^2\Big) + 2\kappa\omega x_1 x_2. \tag{2}$$

(1a) Writing a quantum state $|\,\Psi(t)\,\rangle = \sum_{nm} c_{nm}(t)|\,n,m\,\rangle$, where $|\,n,m\,\rangle$ are two-oscillator number states as defined at the end of section 2.1. in the lecture, find the time evolution equation for all $c_{nm}(t)$. [3 points]

(1b) Suppose you have solved these, find the reduced density matrix for the first oscillator only, in the state $|\,\Psi(t)\,\rangle$ (i.e. in terms of some general $c_{nm}(t)$). [2 points]

(1c) Nextly, find the general expression for the Purity of that reduced density matrix. [5 points]

(2) Numerical solution: Now implement a numerical solution for the time evolution you found in (1a). Implement your equations in the file `Assignment2_program_draft_v1.xmds` provided online. Follow the info-sheet `Numerics_assignments_info.pdf` to run your code once implemented. The code is set up to begin in a product of coherent states initially, with $|\,\Psi(0)\,\rangle = |\,\alpha\,\rangle \otimes |\,\beta\,\rangle$.

(2a) First, check that normalisation and energy are conserved, using `Assignment2_plot_checks_v1.m`. Then inspect dynamics of the mean phase space coordinates in `Assignment2_plot_oscillations_v1.m` to check they make sense. Also run `Assignment2_classical_osc_v1.xmds` into which you still have to insert the classical Newton's equations following from (2). Finally plot a comparison of quantum expectation values and classical results using `Assignment2_compare_oscillations_v1.m`, and discuss all your results. [5 points]

(2b) Implement your result for the purity from (1c) in the code as instructed at the end of the .xmds file, and plot this for the same dynamics as in (2a). Then for testing, run it with no coupling $\kappa = 0$ and plot again. What did you expect, what did you find? Discuss. Finally change the initial state for the second oscillator to $(|\,2\,\rangle + |\,5\,\rangle)/\sqrt{2}$ by uncommenting the corresponding lines. Plot the purity also now and discuss [5 points].

(3) Diagonal system and thermal environment: Let us consider a multi-state (indexed by k) system with an environment of M harmonic oscillators [1], with Hamiltonian $\hat{H} = \hat{H}_S + \hat{H}_{int} + \hat{H}_E$ using

$$\begin{aligned} \hat{H}_S &= \sum_k \epsilon_k | \, k \, \rangle \langle \, k \, |, \\ \hat{H}_{int} &= \sum_k \kappa_k | \, k \, \rangle \langle \, k \, | \otimes \hat{E}_k, \\ \hat{H}_E &= \sum_{n=1}^{M} \hbar \omega_n \hat{b}_n^\dagger \hat{b}_n. \end{aligned} \tag{3}$$

where $\hat{E}_k$ can be expressed as some function of the $\hat{b}_n$ and $\hat{b}_n^\dagger$.

(3a) Show that the Hamiltonian is block-diagonal in terms of $| \, k \, \rangle$. [1 point]

(3b) Write the thermal state density matrix $\hat{\rho}_{E,T}$ for the environment at temperature T, in terms of many-body oscillator states $| \, \mathbf{n} \, \rangle \equiv | \, n_1, n_2, \cdots, n_M \, \rangle$. [1 point]

(3c) Let $| \, \Psi_{k,\mathbf{n}}(t) \, \rangle$ be the many body state of system and environment that arises through time evolution (using Schrödinger's equation) from the initial state $| \, \phi_{k;\mathbf{n}}(0) \, \rangle = | \, k \, \rangle \otimes | \, \mathbf{n} \, \rangle$. Then show that a density matrix of the form

$$\hat{\rho}(t) = \sum_{k,k'} \sum_{\mathbf{n}} p_{\mathbf{n}} \left[c_k c_{k'}^* | \, \Psi_{k,\mathbf{n}}(t) \, \rangle \langle \, \Psi_{k',\mathbf{n}}(t) \, | \right], \tag{4}$$

fulfills the von-Neumann equation (3.2)[2] from the separable initial state $\hat{\rho}(0) = | \, \psi_S(0) \, \rangle \langle \, \psi_S(0) \, | \otimes \hat{\rho}_{E,T}$, where the initial system state is $| \, \psi_S(0) \, \rangle = \sum_k c_k | \, k \, \rangle$. Determine $p_{\mathbf{n}}$. [4 points]

(3d) Derive the reduced density matrix $\hat{\rho}_S$ for the system only, similar to the discussion in section 3.1.4. Suppose there initially was a coherence between two system basis-states, say $k = 0$ and $k' = 1$. Inspect the coherence matrix element $\langle \, k \, | \hat{\rho}_S | \, k' \, \rangle$ and discuss under which conditions this coherence might disappear? Does it always? Which part of the Hamiltonian decides if it does? How can you interpret the $\sum_{\mathbf{n}} p_{\mathbf{n}}$ part? [4 points]

[1] Just to be definite, the discussion works for any environment.

[2] Maybe start by showing that one.