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

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(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]

The equations are

$$\begin{aligned} i\hbar\dot{c}_{nm}(t) &= \hbar\omega(n+m+1)c_{nm}(t) + \hbar\kappa\big(\sqrt{n(m+1)}c_{n-1,m+1} + \sqrt{(n+1)m}c_{n+1,m-1} \\ &\quad + \sqrt{nm}c_{n-1,m-1} + \sqrt{(n+1)(m+1)}c_{n+1,m+1}\big), \end{aligned} \tag{3}$$

(where for the last term each we understand that e.g. $c_{n,m} = 0$ *or does not exist, whenever* $n < 0$ *or* $m < 0$*).*

(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]

First we write the density matrix for a pure two-body state $|\,\Psi(t)\,\rangle$ *as above, which is*

$$\rho(t) = \sum_{nm;n'm'} \rho_{nm;n'm'}(t)|\,n,m\,\rangle\langle\,n'm'\,| \equiv \sum_{nm;n'm'} c_{nm}c^*_{n'm'}(t)|\,n,m\,\rangle\langle\,n'm'\,| \tag{4}$$

The we use the definition of the reduced DM for oscillator A as $\hat{\rho}_A = \sum_k \big(\langle\,k\,|_B\big)\hat{\rho}|\,k\,\rangle_B$*, where* $|\,k\,\rangle_B$ *is the oscillator basis for only the second oscillator. With this we obtain*

$$\rho(t)_A = \sum_{nn'k} \rho_{nk,n'k}|\,n\,\rangle_A\langle\,n'\,|_A. \tag{5}$$

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

From the definition the purity is $P(t) = Tr_A[\rho(t)_A^2]$*. Explicit insertion of (5) gives*

$$P(t) = \sum_l \langle\,l\,|\Bigg(\sum_{nn'k}\rho_{nk,n'k}|\,n\,\rangle\langle\,n'\,|\Bigg)\Bigg(\sum_{mm'k'}\rho_{mk',m'k'}|\,m\,\rangle\langle\,m'\,|\Bigg)|\,l\,\rangle \tag{6}$$

(i) We have omitted subscripts $_A$, $_B$, since all states in (6) pertain to oscillator A. (ii) It is very important to use DIFFERENT summation indices in the second copy of $\rho(t)_A$ than in the first. We now use $\langle l \,|\, n \rangle = \delta_{ln}$, $\langle n' \,|\, m \rangle = \delta_{n'm}$ and $\langle m' \,|\, l \rangle = \delta_{m'l}$, which removes three of the seven sums and all of the basis vectors. Thus

$$P(t) = \sum_{lk;mk'} \rho_{lk,mk}\rho_{mk',lk'}. \tag{7}$$

We can now insert coefficients c, but the expression (7) also suffices.

(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]

See solution codes and plots online. Discussion: You should find perfect agreement between the quantum expectation values $\langle x_1 \rangle$, $\langle x_2 \rangle$, $\langle p_1 \rangle$, $\langle p_2 \rangle$ and the corresponding classical results. This is a consequence of the Ehrenfest theorem in quantum mechanics (see e.g. Griffith problem 1.12). This perfect agreement is somewhat special for a harmonic oscillator.

(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].

When $\kappa = 0$, we have to of course find that $P(t) \equiv 1$, since oscillator A must remain in a pure (reduced) state. For nonzero coupling, we find deviations from 1, meaning the oscillator A entangles with oscillator B. How much it does strongly depends on the initial state of oscillator B, see plots.

(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

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

$\hat{H} = \hat{H}_S + \hat{H}_{int} + \hat{H}_E$ using

$$\hat{H}_S = \sum_k \epsilon_k | \, k \, \rangle \langle \, k \, |,$$

$$\hat{H}_{int} = \sum_k \kappa_k | \, k \, \rangle \langle \, k \, | \otimes \hat{E}_k,$$

$$\hat{H}_E = \sum_{n=1}^{M} \hbar \omega_n \hat{b}_n^\dagger \hat{b}_n. \tag{8}$$

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

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

Solution: Let's arrange our basis in the order

$$\mathcal{B} = \{B_0, B_1, B_2, \cdots\} \tag{9}$$

where $B_k = \{| \, k \, \rangle \otimes | \, \mathbf{n} \, \rangle\}$*, for fixed state* $| \, k \, \rangle$ *of the system and* $\mathbf{n}$ *running through* *<u>all</u>* *possible indices of the environment.*

Taking an arbitrary vector $| \, \phi_k \, \rangle$ *from* B_k *and another one* $| \, \phi_{k'} \, \rangle$ *from* $B_{k'}$ *with* $k \neq k'$*, we see that*

$$\langle \, \phi_k \, | \hat{H} | \, \phi_{k'} \, \rangle = 0, \tag{10}$$

since all terms in the Hamiltonian are $\sim | \, k \, \rangle \langle \, k \, |$*. Thus each part of the Hamiltonian with different* $| \, k \, \rangle \langle \, k \, |$ *forms a block, let us call that* $\hat{H}_k$*, even though each block is still infinite dimensional. Then* $\hat{H} = \sum_k \hat{H}_k$*.*

(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] *Solution: Since*

the environment is just a sum of harmonic oscillators, we can read off the Hamiltonian, that $| \, \mathbf{n} \, \rangle$ *is an eigenstate, with energy* $E_{\mathbf{n}} = \sum_\ell \hbar \omega_\ell n_\ell$*. Thus the explicit thermal density matrix is*

$$\hat{\rho}_{E,T} = \frac{1}{Z} \sum_{\mathbf{n}} e^{-\frac{\sum_\ell \hbar \omega_\ell n_\ell}{k_B T}} | \, \mathbf{n} \, \rangle \langle \, \mathbf{n} \, |, \tag{11}$$

with $Z = \sum_{\mathbf{n}} e^{-\frac{\sum_\ell \hbar \omega_\ell n_\ell}{k_B T}}$.

(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

$$\hat{\rho}(t) = \sum_{k,k'} \sum_{\mathbf{n}} p_{\mathbf{n}} \left[c_k c_{k'}^* | \, \Psi_{k,\mathbf{n}}(t) \, \rangle \langle \, \Psi_{k',\mathbf{n}}(t) \, | \right], \tag{12}$$

fulfills the von-Neumann equation from the separable initial state

$$\hat{\rho}(0) = |\,\psi_S(0)\,\rangle\langle\,\psi_S(0)\,| \otimes \hat{\rho}_{E,T}, \tag{13}$$

where the initial system state is $|\,\psi_S(0)\,\rangle = \sum_k c_k|\,k\,\rangle$. Determine $p_{\mathbf{n}}$. [4 points] *Solution:*

Let us first formalise the statement that $|\,\Psi_{k,\mathbf{n}}(t)\,\rangle$ *arises through time evolution using Schrödinger's equation from the given initial state. This implies:*

$$|\,\Psi_{k,\mathbf{n}}(t)\,\rangle = \hat{U}(t)|\,k\,\rangle \otimes |\,\mathbf{n}\,\rangle = e^{-i\hat{H}t/\hbar}|\,k\,\rangle \otimes |\,\mathbf{n}\,\rangle, \tag{14}$$

where $\hat{U}$ *is the time evolution operator. Due to the block structure found earlier, we can write*

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \prod_k e^{-i\hat{H}_k t/\hbar}, \tag{15}$$

where in the second equality we used that $\left[\hat{H}_k, \hat{H}_{k'}\right] = 0$. *Thus we see that*

$$|\,\Psi_{k,\mathbf{n}}(t)\,\rangle = e^{-i\hat{H}_k t/\hbar}|\,k\,\rangle \otimes |\,\mathbf{n}\,\rangle, \tag{16}$$

i.e. only the "correct block in the Hamiltonian" is going to contribute to the time-evolution of an initial state starting in $|\,k\,\rangle$ *only.*

We know in general, that $\hat{\rho}(t) = e^{-i\hat{H}t/\hbar}\hat{\rho}(0)e^{i\hat{H}t/\hbar}$ *solves the von-Neumann equation from the initial state (initial density matrix)* $\hat{\rho}(0)$. *To see this:*

$$\begin{aligned} i\hbar\dot{\hat{\rho}}(t) &\overset{\textit{product rule}}{=} i\hbar\left[(-\frac{i}{\hbar}\hat{H})e^{-i\hat{H}t/\hbar}\rho(0)e^{i\hat{H}t/\hbar} + e^{-i\hat{H}t/\hbar}\rho(0)e^{i\hat{H}t/\hbar}(\frac{i}{\hbar}\hat{H})\right] \\ &= \hat{H}\hat{\rho}(t) - \hat{\rho}(t)\hat{H} = \left[\hat{H}, \hat{\rho}(t)\right]. \end{aligned} \tag{17}$$

Starting from the initial density matrix given in (13), we thus have to find

$$\hat{\rho}(t) = e^{-i\hat{H}t/\hbar}|\,\psi_S(0)\,\rangle\langle\,\psi_S(0)\,| \otimes \sum_{\mathbf{n}} p_{\mathbf{n}}|\,\mathbf{n}\,\rangle\langle\,\mathbf{n}\,|e^{i\hat{H}t/\hbar}, \tag{18}$$

with coefficients $p_{\mathbf{n}}$ *defined in Eq. (11). We can rewrite this step by step as follows*

$$\begin{aligned} &= \sum_{k,k'} e^{-i\hat{H}t/\hbar}c_k c_{k'}^*|\,k\,\rangle\langle\,k'\,| \otimes \sum_{\mathbf{n}} p_{\mathbf{n}}|\,\mathbf{n}\,\rangle\langle\,\mathbf{n}\,|e^{i\hat{H}t/\hbar}. \\ &= \sum_{k,k'}\sum_{\mathbf{n}} p_{\mathbf{n}}c_k c_{k'}^* e^{-i\hat{H}t/\hbar}|\,k;\mathbf{n}\,\rangle\langle\,k';\mathbf{n}\,|e^{i\hat{H}t/\hbar}. \\ &\overset{\textit{Eq. (15)}}{=} \sum_{k,k'}\sum_{\mathbf{n}} p_{\mathbf{n}}c_k c_{k'}^* e^{-i\hat{H}_k t/\hbar}|\,k;\mathbf{n}\,\rangle\langle\,k';\mathbf{n}\,|e^{i\hat{H}_{k'}t/\hbar}. \\ &\overset{\textit{Eq. (16)}}{=} \sum_{k,k'}\sum_{\mathbf{n}} p_{\mathbf{n}}c_k c_{k'}^*|\,\Psi_{k,\mathbf{n}}(t)\,\rangle\langle\,\Psi_{k',\mathbf{n}}(t)\,|, \end{aligned} \tag{19}$$

which has the form we wanted to reach.

(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]
Solution: Similarly to the discussion in section 3.1.4. we will have to use the basis $|\,\mathbf{n}\,\rangle$ *to perform the trace over the environment explicitly. In preparation for that, we should write*

$$|\,\Psi_{k,\mathbf{n}}(t)\,\rangle = \sum_{\mathbf{m}} d_{\mathbf{m}}^{(k,\mathbf{n})}(t)|\,k,\mathbf{m}\,\rangle. \tag{20}$$

This is always possible since the $|\,\mathbf{m}\,\rangle$ *are a basis of the environmental Hilbertspace. The superscripts* $^{(k,\mathbf{n})}$ *of the complex coefficients* d *mean "these are the coefficients for the state which has evolved from* $|\,k;\mathbf{n}\,\rangle$ *initially". Insertion into (19), and being careful not to name two different summation indices (or summation index vectors) with the same letter, we have*

$$\hat{\rho}(t) = \sum_{k,k'} \sum_{\mathbf{n},\mathbf{m},\mathbf{m}'} p_{\mathbf{n}} c_k c_{k'}^* d_{\mathbf{m}}^{(k,\mathbf{n})}(t) d_{\mathbf{m}'}^{*(k',\mathbf{n})}(t)|\,k,\mathbf{m}\,\rangle\langle\, k',\mathbf{m}'\,|, \tag{21}$$

Now we perform the trace over the environment to obtain the reduced density matrix for the system:

$$\begin{aligned}\hat{\rho}_S(t) = Tr_E[\hat{\rho}(t)] &= \sum_{\mathbf{s}} \langle\,\mathbf{s}\,|\sum_{k,k'} \sum_{\mathbf{n},\mathbf{m},\mathbf{m}'} p_{\mathbf{n}} c_k c_{k'}^* d_{\mathbf{m}}^{(k,\mathbf{n})}(t) d_{\mathbf{m}'}^{*(k',\mathbf{n})}(t)|\,k,\mathbf{m}\,\rangle \underbrace{\langle\, k',\mathbf{m}'\,|\,\mathbf{s}\,\rangle}_{=\langle\, k'\,|\delta_{\mathbf{m}',\mathbf{s}}} \\ &= \sum_{\mathbf{s}} \sum_{k,k'} \sum_{\mathbf{n},\mathbf{m},\mathbf{m}'} p_{\mathbf{n}} c_k c_{k'}^* d_{\mathbf{m}}^{(k,\mathbf{n})}(t) d_{\mathbf{s}}^{*(k',\mathbf{n})}(t) \underbrace{\langle\,\mathbf{s}\,|\,k,\mathbf{m}\,\rangle}_{=|\,k\,\rangle\delta_{\mathbf{m},\mathbf{s}}}\langle\, k'\,|,\end{aligned} \tag{22}$$

where we used the notation $\delta_{\mathbf{v},\mathbf{w}} = \delta_{v_1,w1}\delta_{v_2,w_2}\cdots\delta_{v_M,w_M}$. *Then*

$$\begin{aligned}\hat{\rho}_S(t) &= \sum_{k,k'} \sum_{\mathbf{n}} p_{\mathbf{n}} c_k c_{k'}^* \sum_{\mathbf{s}} d_{\mathbf{s}}^{(k,\mathbf{n})}(t) d_{\mathbf{s}}^{*(k',\mathbf{n})}(t)|\,k\,\rangle\langle\, k'\,| \\ &\overset{Eq.\ (20)}{=} \sum_{k,k'} c_k c_{k'}^* \sum_{\mathbf{n}} p_{\mathbf{n}} \langle\,\Psi_{k',\mathbf{n}}(t)\,|\,\Psi_{k,\mathbf{n}}(t)\,\rangle|\,k\,\rangle\langle\, k'\,|\end{aligned} \tag{23}$$

and the matrix element $\langle\, k\,|\hat{\rho}_S|\, k'\,\rangle$ *is governed by* $\sum_{\mathbf{n}} p_{\mathbf{n}}\langle\,\Psi_{k',\mathbf{n}}(t)\,|\,\Psi_{k,\mathbf{n}}(t)\,\rangle$ *(except the part* $c_k c_{k'}^*$ *coming form the initial state only).*

This contains a thermal average over the environment through the $\sum_{\mathbf{n}} p_{\mathbf{n}}\cdots$, *as well as the feature as seen in section 3.1.4, that the coherence disappears once the states of the environment that* $|\,k\,\rangle$ *and* $|\,k'\,\rangle$ *are entangled with, have become orthogonal.*

Here the coherence can in principle also disappear through the thermal average even for cases where all $\langle\,\Psi_{k',\mathbf{n}}(t)\,|\,\Psi_{k,\mathbf{n}}(t)\,\rangle$ *are non-zero, since these are complex numbers.*