# Phys 435,I-Semester 2022/23, Assignment 1 solution

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**(1) Quantum mechanical postulates:** For the following quantum systems, in the given state $|\Psi\rangle$, list all possible outcomes of measuring the observables $\hat{O}$, the probability of each outcome, and the state of the system *after* having found a given outcome [3 points].

| System | $\|\Psi\rangle$ | $\hat{O}$ |
|---|---|---|
| two spin-1/2 | $\frac{1}{\sqrt{6}}\|\uparrow\uparrow\rangle + \frac{1}{\sqrt{6}}\|\uparrow\downarrow\rangle + \sqrt{\frac{2}{3}}\|\downarrow\downarrow\rangle$ | $\hat{S}_z^{(1)}$, $\hat{S}_z^{(2)}$ |
| two harmonic oscillators | $(\frac{1}{\sqrt{2}}\|0\rangle + \frac{1}{\sqrt{2}}\|1\rangle) \otimes (\frac{1}{\sqrt{2}}\|1\rangle + \frac{1}{\sqrt{2}}\|2\rangle)$ | $\hat{x}^{(1)}, \hat{p}^{(2)}, \hat{H}^{(1)}$ |

*Solution:*

- *Spins:*
  $\hat{S}_z^{(1)}$*: outcome* $+\hbar/2$*, probability* $p = 1/6 + 1/6 = 1/3$*, collapsing the state to*

$$|\Psi\rangle \rightarrow \frac{1}{\sqrt{2}}|\uparrow\rangle \otimes (|\uparrow\rangle + |\downarrow\rangle). \tag{1}$$

  *To see this formally we have to apply the projection operator* $\hat{P} = (|\uparrow\rangle\langle\uparrow|^{(1)}$ *onto the quantum state, where* $^{(1)}$ *indicates that this is acting on spin 1 only. This gives*

$$\hat{P}|\Psi\rangle = \frac{1}{\sqrt{6}}\underbrace{|\uparrow\rangle\langle\uparrow|^{(1)}|\uparrow\uparrow\rangle}_{|\uparrow\uparrow\rangle} + \frac{1}{\sqrt{6}}\underbrace{|\uparrow\rangle\langle\uparrow|^{(1)}|\uparrow\downarrow\rangle}_{=|\uparrow\downarrow\rangle} + \sqrt{\frac{2}{3}}\underbrace{|\uparrow\rangle\langle\uparrow|^{(1)}|\downarrow\downarrow\rangle}_{=0}$$
$$= \frac{1}{\sqrt{6}}|\uparrow\uparrow\rangle + \frac{1}{\sqrt{6}}|\uparrow\downarrow\rangle \equiv |\Psi_P\rangle \tag{2}$$

  *This state is now wrongly normalised* $\langle\Psi_P|\Psi_P\rangle = 1/3$*, so we divide by the square root of this wrong normalisation* $|\Psi_P\rangle \rightarrow |\Psi_P\rangle/\sqrt{1/3}$ *to fix it, and then reach (1).*
  *For outcome* $-\hbar/2$*,* $p = 2/3$*, collapsing the state to* $|\Psi\rangle \rightarrow |\downarrow\downarrow\rangle$*.*
  $\hat{S}_z^{(2)}$*: outcome* $+\hbar/2$*, probability* $p = 1/6$*, collapsing the state to* $|\Psi\rangle \rightarrow |\uparrow\uparrow\rangle$ *and outcome* $-\hbar/2$*, probability* $p = 1/6 + 2/3 = 5/6$*, collapsing the state to*

$$|\Psi\rangle \rightarrow (\frac{1}{\sqrt{5}}|\uparrow\rangle + \sqrt{\frac{4}{5}}|\downarrow\rangle) \otimes |\downarrow\rangle. \tag{3}$$

- *oscillators: In principle the position* $\hat{x}^{(1)}$ *can take any value, to find the probability of each we write the entire state in the position representation* $\Psi(x_1, x_2) = \phi(x_1)\phi(x_2)$*, which takes a product form here, with* $\phi(x_1) = \frac{1}{\sqrt{2}}(\varphi_0(x_1) + \varphi_1(x_1))$ *and* $\phi(x_2) = \frac{1}{\sqrt{2}}(\varphi_1(x_2) + \varphi_2(x_2))$*, where* $\varphi_k(x)$ *is the position space wavefunction of the kth eigenstate of the harmonic oscillator. The probability to find oscillator one at a specific position* $x_1 = \bar{x}$ *within a small interval* $\Delta x$ *is* $|\phi(\bar{x})|^2\Delta x$*. We* *only have to look at the wavefunction for oscillator 1 since the state as separable. Had that not been the case, the answer here would be* $\int dx_2 |\Psi(\bar{x}, x_2)|^2 \times \Delta x$. *After the position measurement, the state "is"* $\Psi(x_1, x_2) = \delta(x_1 - \bar{x})\phi(x_2)$, *where* $\delta(x_1 - \bar{x})$ *is a delta-function centered on* $\bar{x}$. *Replace the delta function with a very narrow Gaussian, if this hurts you. For momentum we take the Fourier transform* $\tilde{\Psi}(k_1, k_2) = \tilde{\phi}(k_1)\tilde{\phi}(k_2)$, *then we shall measure a result near the specific value* $p_2 = \bar{p} = \hbar\bar{k}$ *within the interval* $\Delta p$ *with probability* $|\tilde{\phi}(k_2)|^2 \Delta p$ *and the state after that measurement will be* $\Psi(x_1, x_2) = \phi(x_1)\frac{e^{i\bar{k}x_2}}{\mathcal{V}}$. *For the energy of oscillator one* $\hat{H}^{(1)}$, *we can find* $E^{(1)} = E_0 = \frac{1}{2}\hbar\omega$ *with probability* 1/2, *and post-measurement state* $|\,0\,\rangle \otimes (\frac{1}{\sqrt{2}}|\,1\,\rangle + \frac{1}{\sqrt{2}}|\,2\,\rangle)$. *The second possibility is* $E^{(1)} = E_1 = \frac{3}{2}\hbar\omega$ *with probability* 1/2, *after which the overall state will be* $|\,1\,\rangle \otimes (\frac{1}{\sqrt{2}}|\,1\,\rangle + \frac{1}{\sqrt{2}}|\,2\,\rangle)$

**(2) Many-body states and operators:** Consider an abstract many-body quantum system, where a single *spin* with $s = 1/2$ is interacting with an environment of many *harmonic oscillators*. The basis of the entire system can thus be written as $\mathcal{B} = \{|\,s_z; n_1, n_2, n_3, \cdots, n_4\,\rangle\}$. Where the first index denotes the z-component of the spin $s_z = -1/2, 1/2$, and ladder operators for the harmonic oscillators act on these states as e.g. $\hat{a}_3|\,s_z; n_1, n_2, n_3, \cdots, n_4\,\rangle = \sqrt{n_3}|\,s_z; n_1, n_2, n_3 - 1, \cdots, n_4\,\rangle$ etc.

(2a) Determine for each of the following states if the spin is entangled with the oscillators [3 points]

*Solution*: For this we can use e.g. the purity of the reduced density matrix of the first spin. If it is $P = 1$, the states were separable, otherwise entangled. Additionally we have a useful exercise in calculating reduced density matrices. The reduced density matrix for the spin will be

$$\hat{\rho}_{red} = \sum_{ss'} \left[ \sum_{n_1,n_2,n_3} \langle\, n_1, n_2, n_3 \,||\, \Psi \,\rangle\langle\, \Psi \,||\, n_1, n_2, n_3 \,\rangle \right] |\,s\,\rangle\langle\, s'\,| \tag{4}$$

(There was a typo in the assignment sheet, which was fixed for this solution (marked in red). Methods in the solution also work for the typoed starting point.

$$\begin{aligned} |\,\Psi_1\,\rangle &= \frac{1}{\sqrt{3}}|\downarrow; 011\,\rangle - \frac{1}{\sqrt{6}}|\uparrow; 011\,\rangle + \frac{1}{3}|\downarrow; 101\,\rangle + \frac{1}{3\sqrt{2}}|\uparrow; 101\,\rangle - \frac{\sqrt{2}}{3}|\downarrow; 110\,\rangle + \frac{1}{3}|\uparrow; 110\,\rangle \\ &\equiv c_{\downarrow;011}|\downarrow; 011\,\rangle + c_{\uparrow;011}|\uparrow; 011\,\rangle + c_{\downarrow;101}|\downarrow; 101\,\rangle + c_{\uparrow;101}|\uparrow; 101\,\rangle + c_{\downarrow;110}|\downarrow; 110\,\rangle + c_{\uparrow;110}|\uparrow; 110\,\rangle \end{aligned} \tag{5}$$

We can see that this state involves only 6 basis states, so we can write the relevant part of the density matrix as 6 by 6 matrix, with basis ordering $\{|\downarrow; 011\,\rangle, |\downarrow; 101\,\rangle, |\downarrow; 110\,\rangle, |\uparrow; 011\,\rangle, |\uparrow; 101\,\rangle, |\uparrow; 110\,\rangle\}$. All other elements are zero. We have chosen the basis ordering such that all states with $\downarrow$ come before those with $\uparrow$, in this way the spin part of the density matrix corresponds to four large blocks. We recognise that formula (4) instructs us to separately take the trace in each block, and write those entries into the reduced density matrix. Hence we do not even have to construct any other elements of the matrix and can leave them blank (even though they are non-zero):

$$\hat{\rho}_{red} = \left[\begin{array}{ccc|ccc} |c_{\downarrow;011}|^2 = \frac{1}{3} & & & c_{\downarrow;011}c^*_{\uparrow;011} = -\frac{1}{\sqrt{18}} & & \\ & |c_{\downarrow;101}|^2 = \frac{1}{9} & & & c_{\downarrow;101}c^*_{\uparrow;101} = \frac{1}{9\sqrt{2}} & \\ & & |c_{\downarrow;110}|^2 = \frac{2}{9} & & & c_{\downarrow;110}c^*_{\uparrow;110} = -\frac{\sqrt{2}}{9} \\ \hline c_{\uparrow;011}c^*_{\downarrow;011} = -\frac{1}{\sqrt{18}} & & & |c_{\uparrow;011}|^2 = \frac{1}{6} & & \\ & c_{\uparrow;101}c^*_{\downarrow;101} = \frac{1}{9\sqrt{2}} & & & |c_{\uparrow;101}|^2 = \frac{1}{18} & \\ & & c_{\uparrow;110}c^*_{\downarrow;110} = -\frac{\sqrt{2}}{9} & & & |c_{\uparrow;110}|^2 = \frac{1}{9} \end{array}\right] \tag{6}$$

Taking the trace separately in each block we find

$$\hat{\rho}_{red} = \begin{pmatrix} \frac{2}{3} & -\frac{2\sqrt{2}}{9} \\ -\frac{2\sqrt{2}}{9} & \frac{1}{3} \end{pmatrix} \tag{7}$$

(basis ordering up, down) with purity $P = \frac{61}{81} < 1$ hence, this is entangled. There are other ways to show this, e.g. you can write that, if the state was separable, we should be able to write it as

$$|\,\Psi_1\,\rangle = (c_1|\uparrow\rangle + c_2|\downarrow\rangle) \otimes (c_3|\,011\,\rangle + c_4|\,101\,\rangle + c_5|\,110\,\rangle). \tag{8}$$

Expanding the product, we get 6 equations for the 5 unknown coefficients, which have no solution here. If you can find a solution to those, can the state have been separable.

$$|\,\Psi_2\,\rangle = -\frac{1}{3\sqrt{2}}|\downarrow;010\,\rangle - \frac{1}{3}|\uparrow;010\,\rangle + \frac{1}{\sqrt{6}}|\downarrow;011\,\rangle + \frac{1}{\sqrt{3}}|\uparrow;011\,\rangle + \frac{1}{3}|\downarrow;120\,\rangle + \frac{\sqrt{2}}{3}|\uparrow;120\rangle,$$

$\hat{\rho}_{red} = \begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & \frac{2}{3} \end{pmatrix}$ with purity $P = 1$ hence not entangled.

$$|\,\Psi_3\,\rangle = \frac{1}{\sqrt{3}}|\downarrow;011\,\rangle - \frac{1}{\sqrt{6}}|\uparrow;011\,\rangle - \frac{1}{3}|\downarrow;101\,\rangle + \frac{1}{3\sqrt{2}}|\uparrow;101\,\rangle - \frac{\sqrt{2}}{3}|\downarrow;110\,\rangle + \frac{1}{3}|\uparrow;110\,\rangle.$$

$\hat{\rho}_{red} = \begin{pmatrix} \frac{2}{3} & -\frac{\sqrt{2}}{3} \\ -\frac{\sqrt{2}}{3} & \frac{1}{3} \end{pmatrix}$ with purity $P = 1$ hence not entangled. (9)

(2b) Determine the following matrix elements [4 points]

*Solution*:

$$\mathcal{M}_1 = \langle \downarrow; 020\,|\hat{S}_x\hat{S}_z|\uparrow; 101\,\rangle = 0 \qquad \mathcal{M}_2 = \langle \downarrow; 020\,|\hat{S}_y|\uparrow; 020\,\rangle = -i\frac{\hbar}{2},$$
$$\mathcal{M}_3 = \langle \downarrow; 113\,|\hat{S}_z\hat{a}_3|\downarrow; 112\,\rangle = 0, \qquad \mathcal{M}_4 = \langle \uparrow; 303\,|\hat{a}_2(\hat{a}_3^\dagger)^2|\uparrow; 301\,\rangle = 0,$$
$$\mathcal{M}_5 = \langle \downarrow; 301\,|\hat{S}_z(\hat{a}_1^\dagger)^3\hat{S}_x\hat{a}_2^2|\uparrow; 021\,\rangle = -\sqrt{12}\left(\frac{\hbar}{2}\right)^2, \qquad \mathcal{M}_6 = \langle \downarrow; 103\,|\hat{S}_y\hat{a}_2|\downarrow; 113\,\rangle = 0. \tag{10}$$

**(3) Dynamics of a spin with environment:** Let us assume the Hamiltonian for a system as above is:

$$\hat{H}_S = \frac{1}{2}\hbar\omega_0\hat{\sigma}_z - \frac{1}{2}\hbar\Delta_0\hat{\sigma}_x, \tag{11}$$
$$\hat{H}_\mathcal{E} = \sum_i \hbar\omega_i\left(\hat{a}_i^\dagger\hat{a}_i + \frac{1}{2}\right) + \hbar\chi_i\hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i, \tag{12}$$
$$\hat{H}_{\text{int}} = \hat{\sigma}_z \otimes \sum_i \bar{\kappa}_i\left(\hat{a}_i + \hat{a}_i^\dagger\right). \tag{13}$$

Study this Hamiltonian in an interaction picture (IP)where $\hat{H}_0 = \hat{H}_S + \hat{H}_\mathcal{E}$, and $\hat{V} = \hat{H}_{\text{int}}$.

(3a) Determine the IP Heisenberg equations for $\hat{a}_k$, $\hat{a}_k^\dagger$, $\sigma_{x,y,z}$. Solve these for $\Delta_0 = \chi_i = 0$ to determine the IP time evolution of $\hat{H}_{\text{int}}$. [4 points]
*Solution*:

$$\frac{d\hat{\sigma}_z}{dt} = \frac{i}{\hbar}\left[\hat{H}_0, \hat{\sigma}_z\right] = i\Delta_0/2\hat{\sigma}_y \tag{14}$$
$$\frac{d\hat{a}_k}{dt} = \frac{i}{\hbar}\left[\hat{H}_0, \hat{a}_k\right] = -i\omega_k\hat{a}_k - 2i\chi_k\hat{a}_k^\dagger\hat{a}_k\hat{a}_k \tag{15}$$
$$\frac{d\hat{a}_k^\dagger}{dt} = \frac{i}{\hbar}\left[\hat{H}_0, \hat{a}_k^\dagger\right] = i\omega_k\hat{a}_k^\dagger + 2i\chi_k\hat{a}_k^\dagger\hat{a}_k^\dagger\hat{a}_k \tag{16}$$

*The simplified versions with* $\Delta_0 = \chi_i = 0$ *have the solutions:*

$$\hat{\sigma}_z(t) = \hat{\sigma}_z(0) \tag{17}$$
$$\hat{a}_k(t) = \hat{a}_k(0)e^{-i\omega_k t} \tag{18}$$
$$\hat{a}_k^\dagger(t) = \hat{a}_k^\dagger(0)e^{i\omega_k t} \tag{19}$$

*Thus* $\hat{H}_{int}(t) = \hat{\sigma}_z(0) \otimes \sum_i \bar{\kappa}_i\left(\hat{a}_i(0)e^{-i\omega_i t} + \hat{a}_i^\dagger(0)e^{i\omega_i t}\right)$.

(3b) Evaluate the IP time-evolution operator $\hat{U}$ for quantum states by integration [2 points] *Hint: It turns out the time-ordering in Eq. (1.34) will only cause an unimportant phase factor, so ignore it now, but keep in mind that it would be crucial in many other calculations. Still* $\Delta_0 = \chi_i = 0$. [3 points]

*With the hint we can just write from Eq. (1.36) in the lecture, for the interaction picture Eq. (1.40)*

$$\hat{U}(t) = e^{-i\int_0^t \hat{H}_{int}(t')dt'} = e^{-i\left(\hat{\sigma}_z(0)\otimes\sum_i \bar{\kappa_i}\left(\hat{a}_i(0)\int_0^t e^{-i\omega_i t'}dt' + \hat{a}_i^\dagger(0)\int_0^t e^{i\omega_i t'}dt'\right)\right)}$$

$$= e^{\frac{1}{2}\hat{\sigma}_z(0)\otimes\sum_i\left(\hat{a}_i^\dagger(0)\lambda_i(t) - \hat{a}_i(0)\lambda_i^*(t)\right)}, \tag{20}$$

$$\tag{21}$$

*with* $\lambda_i(t) \equiv 2\frac{\bar{\kappa_i}}{\omega_i}(1 - e^{i\omega_i t})$.

(3c) Consider an initial spin-environment state $|\,\Psi(0)\,\rangle = (c_1|\downarrow\rangle + c_2|\uparrow\rangle)|\,0,\cdots,0\,\rangle$, where $|\,0,\cdots,0\,\rangle$ denotes all oscillators in the ground-state. How is this state classified? Now apply $\hat{U}$ from (3b) onto the state to find its time-evolution. Discuss the result. Classify the time evolving state. *Hint: Try to recognise the displacement operator* $\hat{D}(\alpha)$ *generating coherent states in the expression for the time-evolution.* [3 points]

*The initial state given is* seperable. *We see that (21) contains one displacement operator as in Eq. (1.25) for each oscillator mode. We have to identify the appropriate* $\alpha$. *For that, first apply the spin part* $\hat{\sigma}_z(0)$ *in (21) to the initial state. We find*

$$\hat{U}(t)|\,\Psi(0)\,\rangle = (c_1 e^{\frac{1}{2}(-1)\otimes\sum_i\left(\hat{a}_i^\dagger(0)\lambda_i(t) - \hat{a}_i(0)\lambda_i^*(t)\right)}|\downarrow\rangle$$

$$+ c_2 e^{\frac{1}{2}(+1)\otimes\sum_i\left(\hat{a}_i^\dagger(0)\lambda_i(t) - \hat{a}_i(0)\lambda_i^*(t)\right)}|\uparrow\rangle) \otimes |\,0,\cdots,0\,\rangle \tag{22}$$

$$= (c_1 \prod_i \hat{D}(-\lambda_i(t)/2)|\downarrow\rangle + c_2 \prod_i \hat{D}(\lambda_i(t)/2)|\uparrow\rangle) \otimes |\,0,\cdots,0\,\rangle$$

$$= c_1|\downarrow\rangle|\,\mathcal{E}_-\,\rangle + c_2|\uparrow\rangle|\,\mathcal{E}_+\,\rangle, \tag{23}$$

*where* $|\,\mathcal{E}_+\,\rangle = |\,\lambda_1(t)/2\,\rangle \otimes |\,\lambda_2(t)/2\,\rangle \otimes \ldots$ *is a state where each oscillator is in a specific coherent state with amplitude* $\lambda_i(t)$.

**(4) Numerical confirmation and extension:** Now implement a numerical solution for the time evolution above, for just a single oscillator, changing to the Schrödinger picture. Write the state as $|\,\Psi(t)\,\rangle = \sum_{s,n} c_{sn}(t)|\,s,n\,\rangle$, where $s \in \{\uparrow,\downarrow\}$ and $n \in \mathbb{N}$. From the Hamiltonian (11)-(13) and Schrödinger's equation, derive the equations of motion for $c_{sn}(t)$. Implement your equations in the file `Assignment1_program_draft_v1.xmds` provided online. Follow the info-sheet `Numerics_assignments_info.pdf` to run your code once implemented.

*The equations are*

$$i\hbar\dot{c}_{\uparrow,n} = \big(\frac{\hbar\omega_0}{2} + \hbar\omega_n n + \hbar\chi_n n(n-1)\big)c_{\uparrow,n} + \frac{\hbar\Delta_0}{2}c_{\downarrow,n} + \bar{\kappa}_n(\sqrt{n}c_{\uparrow,n-1} + \sqrt{n+1}c_{\uparrow,n+1}), \tag{24}$$

$$i\hbar\dot{c}_{\downarrow,n} = \big(\frac{-\hbar\omega_0}{2} + \hbar\omega_n n + \hbar\chi_n n(n-1)\big)c_{\downarrow,n} + \frac{\hbar\Delta_0}{2}c_{\uparrow,n} + \bar{\kappa}_n(\sqrt{n}c_{\downarrow,n-1} + \sqrt{n+1}c_{\downarrow,n+1}). \tag{25}$$

*(where for the last term each we understand that e.g.* $_{\downarrow,-1} = 0$*/ does not exist). See webpage for solution codes.* (4a) The file assumes parameters $\Delta_0 = \chi_i = 0$ as in Q3. For this case, check that normalisation and energy are conserved, using `Assignment1_plot_checks_v1.m`. Then inspect dynamics in the oscillator basis `Assignment1_plot_coefficients_v1.m`. Then view a slideshow of the position-basis dynamics `Assignment1_density_slideshow_v1.m`. Formally here, here the "if up"density is defined as $n(x) = |\sum_n c_{\uparrow,n}\varphi_n(x)|^2$ with oscillator states $\varphi_n(x)$, etc. Compare with Q3 and discuss [7 points]

*See webpage for solution plots. If the equations are correct, we find that norm and energy are conserved up to numerical precision. For the dynamics, all oscillators are moving to more and more excited states, but then return for a complete revival in the initial ground-state. When viewing the slideshow we see that the position space wavefunction remains in Gaussian shape at all times, as is characteristic for a coherent state. We also see that the part of the wavefunction for spin up is moving to the left, while the part for spin down is moving to the right. All this agrees well with out analytical solution in Eq. 3(c).*

(4b) The numerics allow us to also study $\Delta_0 = \chi_i \neq 0$, which makes the analytical solution as in Q3 impossible. Now copy paste your equations also into `Assignment1_program_draft_partb_v1.xmds`, but initially set there $\bar{\kappa}_i = 0$. Plot the total spin populations in $\uparrow$ and $\downarrow$ using `Assignment1_plot_spin_oscillations_v1.m`. Also plot now for $\bar{\kappa}_i = (2\pi) \times 0.15$. Compare and discuss. [3 points]

*Solution plots online. For* $\bar{\kappa}_i = 0$ *but* $\Delta_0 = \chi_i \neq 0$ *we see coherent oscillations between both spin-states. In the presence of an oscillator* $\bar{\kappa}_i = (2\pi) \times 0.15$*, these become quite irregular. In the presence of* many *oscillators, these turn into damped oscillations, as we see later.*