Phys 637, I-Semester 2022/23, Assignment 5

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Due-date: 28.10.2022

(1) Let's build us a quantum computer (theorist version): The register of a quantum computer with 2 qubits can be described by the basis $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. Let's call the first qubit A and the second B, i.e. $|00\rangle$ really is $|0_A 0_B\rangle$. It has been shown that it is sufficient if it can perform arbitrary single qubit operation[1] and one of a set of universal two qubit gates. One of the latter is the controlled-Z gate, with the truth-table:

$$|00\rangle \to |00\rangle,$$
$$|01\rangle \to |01\rangle,$$
$$|10\rangle \to |10\rangle,$$
$$|11\rangle \to -|11\rangle. \tag{1}$$

The quantum computer has a Hamiltonian

$$\hat{H} = \sum_{n \in \{A,B\}} \frac{\Omega^{(n)}(t)}{2} \hat{\sigma}_x^{(n)} + \frac{\Delta^{(n)}(t)}{2} \hat{\sigma}_z^{(n)} + U(t)(\hat{\sigma}_z^{(A)} - \mathbb{1})(\hat{\sigma}_z^{(B)} - \mathbb{1}), \tag{2}$$

where we interpret each qubit as a pseudospin $\{|0\rangle \leftrightarrow |\downarrow\rangle, |1\rangle \leftrightarrow |\uparrow\rangle\}$ so that we can use a Pauli matrix notation, and $^{(n)}$ implies that an operator acts on qubit $n \in \{A, B\}$ only. The control parameters $\Omega^{(n)}(t)$, $\Delta^{(n)}(t)$ and $U(t)$ are written explicitly time dependent, so that a sequence of different operations can be performed.

A real quantum computer will also suffer from decoherence due to the external environment. Let that be described by Lindblad operators $\hat{L}_{\mu=1} = \sqrt{\gamma_A}\hat{\sigma}_z^{(A)}$ and $\hat{L}_{\mu=2} = \sqrt{\gamma_B}\hat{\sigma}_z^{(B)}$, where the γ_n are decoherence rates.

(1a) Ignoring decoherence, design a sequence for control parameters that implements the following:

(i) Starting in the initialstate $|\Psi_{ini}\rangle = |00\rangle$, initialise qubit A in the register separately into a non-trivial (exemplary picked) qubit state. Hence the final state for this part should be $|\Psi_1\rangle = (c_{A0}|0\rangle + c_{A1}|1\rangle) \otimes |0\rangle$, with $|c_{A0}|^2 + |c_{A1}|^2 = 1$.

(ii) In the next step, initialise qubit B into another non-trivial qubit state. Hence the final state for this part should be $|\Psi_2\rangle = (c_{A0}|0\rangle + c_{A1}|1\rangle) \otimes (c_{B0}|0\rangle + c_{B1}|1\rangle)$ with $|c_{B0}|^2 + |c_{B1}|^2 = 1$.

(iii) On this register state, subsequently operate with the controlled-Z gate above.

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[1]That means it can map any input state $|\Psi_A\rangle = c_0|0_A\rangle + c_1|1_A\rangle$ with $|c_0|^2 + |c_1|^2 = 1$ into any other state $|\Psi_A'\rangle = c_0'|0_A\rangle + c_1'|1_A\rangle$, similarly for B.

Hints: Global phases do not matter. Revisit Rabi oscillations in two level systems. Maybe read up on the concept of a "Bloch sphere". For finite duration $\tau < T$ pulses of some Rabi frequency such that $\int_0^T dt' \Omega(t') = \pi/2$, π, 2π we call this a ($\pi/2$, π, 2π)-pulse. One knows that starting from e.g. state $|0\rangle$ and $\Delta = 0$, the outcomes of these pulses are $(|0\rangle - i|1\rangle)/\sqrt{2}$, $-i|1\rangle$ and $-|0\rangle$ respectively. Also consider separately which effect the Ω and the Δ terms have on a wavefuction .[5 points].

Solution: The following is just one selected example to generate a non-trivial quantum state

(i) *To initialise qubit A, let us execute a Rabi-$\pi/2$ pulse on it. We (arbitrarily) pick a duration $\tau = 0.25$ (dimensionless units), and then fix $\Omega^{(A)}(0 \leqslant t < 0.25) = (\pi/2)/0.25$ and zero otherwise. All other control parameters ($\Delta^{(A)}$, $\Omega^{(B)}$, $\Delta^{(B)}$, U) remain zero. By construction $\int_0^T dt' \Omega(t') = \pi/2$, and we expect the state at the end of the pulse to be $|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) \otimes |0\rangle$ (see hint, or check code in Q3). This pulse drives Rabi oscillations (see QM-II), based on which we know that we can achieve* any *relative ratio of population in 0 or 1 choosing the appropriate duration of the oscillation (revisit that).*

However, the relative phase between $|0\rangle$ and $|1\rangle$ is fixed by the solution of Rabi oscillations (see QM-II), so we need a separate trick to control that one. For this we can use the energy shift given by $\Delta^{(A)}$, so to demonstrate how this can be also controlled, as a second part of the initialisation sequence, we now set $\Delta^{(A)}(0.5 \leqslant t < 1.0) = 0.25\pi\hbar/0.25$ for a duration $\tau = 0.25$. Since $|0\rangle$ and $|1\rangle$ are eigenstates of $\hat{\sigma}_z^{(A)}$, each will acquire a complex phase $e^{-iE_{0,1}/\hbar\tau}$ which is $e^{i\pi/4} = (1+i)/\sqrt{2}$ for $|0\rangle$ and $e^{-i\pi/4} = (1-i)/\sqrt{2}$ for $|1\rangle$. The final state after completing the initialisation of qubit A is thus: $|\Psi_1\rangle = \frac{1}{\sqrt{2}}(e^{i0.25\pi}|0\rangle - ie^{-i0.25\pi}|1\rangle) \otimes |0\rangle$. It should be hopefully believable, that using these two pulses of variable duration, and the fact that a global phase of the state is not interesting, any arbitrary qubit state can be initialised.

(ii) *Since the single qubit part of the Hamiltonian for qubit (B) does not affect (A) and the reverse, we can now do a similar sequence for qubit B, choosing again $\Omega^{(B)}(1 \leqslant t < 1.25) = (\pi/2)/0.25$ and $\Delta^{(B)}(1.5 \leqslant t < 1.75) = -0.25\pi\hbar/0.25$ with all other parameters remaining zero. We could have done these operations at the same time as those for qubit A, since they are independent from each other, the reason we did them sequentially is just for clarity when comparing with the simulation in Q3. The outcome after $t = 1.75$ will be $|\Psi_2\rangle = \frac{1}{2}(e^{i\pi/4}|0\rangle - ie^{-i\pi/4}|1\rangle) \otimes (e^{-i\pi/4}|0\rangle - ie^{i\pi/4}|1\rangle)$.*

(iii) *Expanding the tensor product, $|\Psi_2\rangle = \frac{1}{2}(|00\rangle + |01\rangle - |10\rangle - |11\rangle)$. For the controlled-Z gate, we need to flip the sign of the $|11\rangle$ coefficient (and nothing else). Inspecting the Hamiltonian, we see that the last (interaction) term, provides an energy shift* only *if the state is $|11\rangle$. We can thus achieve the sign flip by enabling these interactions for the correct duration, say $U(t) = U_0$ during a time interval τ. This gives a complex phase factor $e^{-iU_0\tau/\hbar}$, which we adjust such that $e^{-iU_0\tau/\hbar} = e^{-i\pi}$, hence we need $U_0 = \hbar\pi/\tau$. Doing this for example during the time interval*

$U(2 \leqslant t < 2.25) = (\pi)/\hbar/0.25$, so in the very end we have reached $|\Psi_{final}\rangle = \frac{1}{2}(|00\rangle + |01\rangle - |10\rangle + |11\rangle)$

(1b) Work out the Lindblad Master equation (4.25) for this quantum computer. Describe in words what the terms $\sim \gamma_{A/B}$ are doing and what you expect their physical effect to be. [5 points]

Solution: We can do this in bra-ket notation or explicitly, since we have just four basis states and thus a 4×4 density matrix. Since mathematica can help is in the explicit version, we follow that and write the general time evolving density matrix (basis ordering $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$) as:

$$\rho = \begin{pmatrix} \rho_{00;00} & \rho_{00;01} & \rho_{00;10} & \rho_{00;11} \\ \rho_{01;00} & \rho_{01;01} & \rho_{01;10} & \rho_{01;11} \\ \rho_{10;00} & \rho_{10;01} & \rho_{10;10} & \rho_{10;11} \\ \rho_{11;00} & \rho_{11;01} & \rho_{11;10} & \rho_{11;11} \end{pmatrix}, \tag{3}$$

with all elements functions of t. The complete Hamiltonian can then also be written in matrix form, using the same basis ordering as:

$$H = \begin{pmatrix} \frac{-\Delta_A-\Delta_B}{2} & \frac{\Omega_B}{2} & \frac{\Omega_A}{2} & 0 \\ \frac{\Omega_B}{2} & \frac{-\Delta_A+\Delta_B}{2} & 0 & \frac{\Omega_A}{2} \\ \frac{\Omega_A}{2} & 0 & \frac{\Delta_A-\Delta_B}{2} & \frac{\Omega_B}{2} \\ 0 & \frac{\Omega_A}{2} & \frac{\Omega_B}{2} & \frac{\Delta_A+\Delta_B}{2} + U \end{pmatrix}. \tag{4}$$

The first term of Eq. 4.25 is $-i(H\rho - \rho H)$ and can be calculated just by matrix products of Eq. (3) and Eq. (4). Finally we also write the Lindblad operators in matrix form, using

$$\sigma_{z_A} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad and \quad \sigma_{z_B} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

The second term of Eq. 4.25 is $\frac{\gamma_A}{2}\left(\frac{2\sigma_{Z_A}\rho\sigma_{Z_A} - \sigma_{Z_A}\sigma_{Z_A}\rho - \rho\sigma_{Z_A}\sigma_{Z_A}}{2}\right)$. The third term of Eq. 4.25 is $\frac{\gamma_B}{2}\left(\frac{2\sigma_{Z_B}\rho\sigma_{Z_B} - \sigma_{Z_B}\sigma_{Z_B}\rho - \rho\sigma_{Z_B}\sigma_{Z_B}}{2}\right)$. Adding all these terms we will get the right hand side of the Lindblad Master Eq. 4.25. The final equation system is:

$$\dot{\rho}_{0000} = -i\left(-\frac{\rho_{0010}\Omega_A}{2} + \frac{\rho_{1000}\Omega_A}{2} - \frac{\rho_{0001}\Omega_B}{2} + \frac{\rho_{0100}\Omega_B}{2}\right) \tag{6}$$

$$\dot{\rho}_{1111} = -i\left(-\frac{\rho_{0111}\Omega_A}{2} + \frac{\rho_{1101}\Omega_A}{2} + \frac{\rho_{0001}\Omega_B}{2} - \frac{\rho_{0100}\Omega_B}{2}\right)$$

$$\dot{\rho}_{2222} = -i\left(\frac{\rho_{0010}\Omega_A}{2} - \frac{\rho_{1000}\Omega_A}{2} - \frac{\rho_{1011}\Omega_B}{2} + \frac{\rho_{1110}\Omega_B}{2}\right)$$

$$\dot{\rho}_{3333} = -i\left(\frac{\rho_{0111}\Omega_A}{2} - \frac{\rho_{1101}\Omega_A}{2} + \frac{\rho_{1011}\Omega_B}{2} - \frac{\rho_{1110}\Omega_B}{2}\right)$$

$$\dot{\rho}_{0001} = -\gamma_B\rho_{0001} + \frac{1}{2}i(2\Delta_B\rho_{0001} + \rho_{0011}\Omega_A - \rho_{1001}\Omega_A + \rho_{0000}\Omega_B - \rho_{0101}\Omega_B)$$

$$\dot{\rho}_{0100} = -\gamma_B\rho_{0100} - \frac{1}{2}i(2\Delta_B\rho_{0100} - \rho_{0110}\Omega_A + \rho_{1100}\Omega_A + \rho_{0000}\Omega_B - \rho_{0101}\Omega_B)$$

$$\dot{\rho}_{0010} = -\gamma_A\rho_{0010} + \frac{1}{2}i(2\Delta_A\rho_{0010} + \rho_{0000}\Omega_A - \rho_{1010}\Omega_A + \rho_{0011}\Omega_B - \rho_{0110}\Omega_B)$$

$$\dot{\rho}_{0011} = \frac{1}{2}i(2U\rho_{0011} + 2i\gamma_A\rho_{0011} + 2i\gamma_B\rho_{0011} + 2\Delta_A\rho_{0011} + 2\Delta_B\rho_{0011} + \rho_{0001}\Omega_A$$
$$- \rho_{1011}\Omega_A + \dot{\rho}_{0010}\Omega_B - \rho_{0111}\Omega_B)$$

$$\dot{\rho}_{1100} = -\frac{1}{2}i(2U\rho_{1100} - 2i\gamma_A\rho_{1100} - 2i\gamma_B\rho_{1100} + 2\Delta_A\rho_{1100} + 2\Delta_B\rho_{1100} + \rho_{0100}\Omega_A$$
$$- \rho_{1110}\Omega_A + \dot{\rho}_{1000}\Omega_B - \rho_{1101}\Omega_B)$$

$$\dot{\rho}_{0110} = -\gamma_A\rho_{0110} - \gamma_B\rho_{0110} + \frac{1}{2}i(2\Delta_A\rho_{0110} - 2\Delta_B\rho_{0110} + \rho_{0100}\Omega_A - \rho_{1110}\Omega_A - \rho_{0010}\Omega_B + \dot{\rho}_{0111}\Omega_B)$$

$$\dot{\rho}_{1001} = -\gamma_A\rho_{1001} - \gamma_B\rho_{1001}\frac{1}{2}i(2\Delta_A\rho_{1001} - 2\Delta_B\rho_{1001} + \rho_{0001}\Omega_A - \rho_{1011}\Omega_A - \rho_{1000}\Omega_B + \dot{\rho}_{1101}\Omega_B)$$

$$\dot{\rho}_{0111} = \frac{1}{2}i(2U\rho_{0111} + 2i\gamma_A\rho_{0111} + 2\Delta_A\rho_{0111} + \rho_{0101}\Omega_A - \rho_{1111}\Omega_A - \rho_{0011}\Omega_B + \rho_{0110}\Omega_B)$$

$$\dot{\rho}_{1000} = -\frac{1}{2}i(2U\rho_{1101} - 2i\gamma_A\rho_{1101} + 2\Delta_A\dot{\rho}_{1101} + \rho_{0101}\Omega_A - \rho_{1111}\Omega_A + \rho_{1001}\Omega_B - \rho_{1100}\Omega_B)$$

$$\dot{\rho}_{1011} = \frac{1}{2}i(2U\rho_{1011} + 2i\gamma_B\rho_{1011} + 2\Delta_B\rho_{1011} - \rho_{0011}\Omega_A + \rho_{1001}\Omega_A + \rho_{1010}\Omega_B - \rho_{1111}\Omega_B)$$

$$\tag{7}$$

By comparing this with Eq. (4.28) from the lecture, we see that the coefficients $\gamma_{A/B}$ separately damp the coherence between $|0\rangle$ and $|1\rangle$ for either qubit A or B respectively. They do not cause any direct population change.

(2) Bath correlation functions *Consider an environment of N non-interacting harmonic oscillators and numerically explore their bath-correlation functions.*

(2a) Make a mathematica script that generates masses, frequencies and system-oscillator coupling constants for N oscillators randomly from some specifically chosen distribution. Use that to plot histograms of those distributions and the resultant correlation function $C(\tau)$ for zero temperature and some meaningful nonzero temperature T. [6 pts]

Solution: Some exemplary distribution $P(\kappa) = \frac{1}{\sigma\sqrt{2\pi}}exp[-\frac{1}{2}(\frac{x-\kappa_0}{\sigma})]$ for κ is shown in Fig. 1, for $\sigma = 10$ and $\kappa_0 = 1$. The correlation function calculated for these two distributions is shown in Fig. 2, (left) at $T = 0$ and (right) at $T = 200$. Since only the real part of the correlation function has a temperature dependent prefactor, which tends to increase
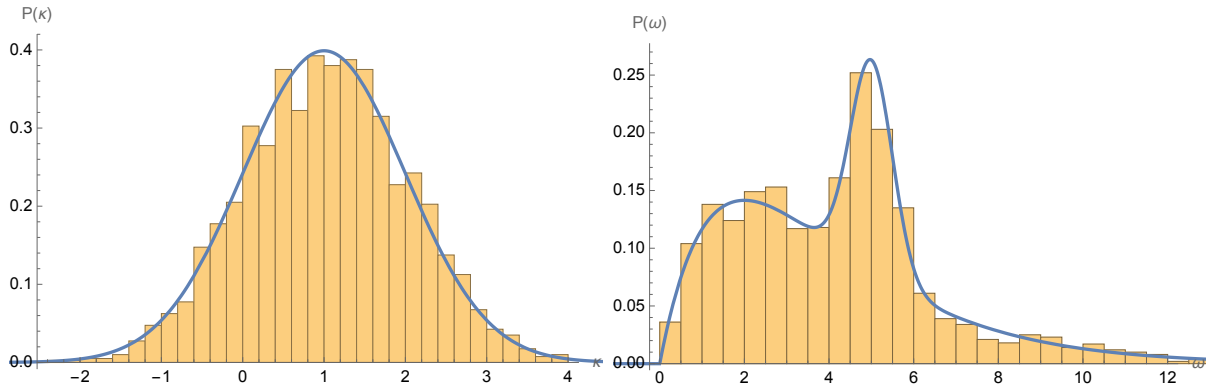
it, the latter appears mainly real.

Figure 1: (left) Probability distribution for coupling (solid blue) $P(\kappa)$ and histogram of the individual generated κ_j (yellow) (right) The same for the distribution $P(\omega)$ of frequencies ω_j.
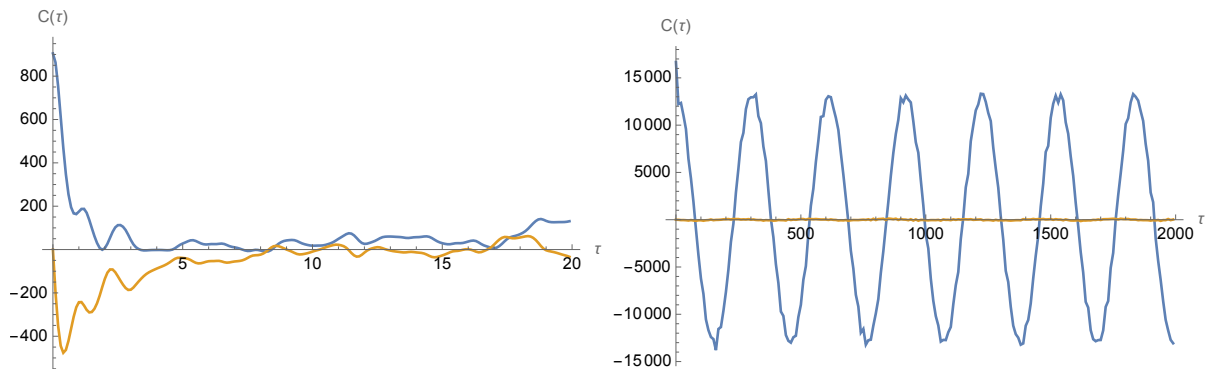

Figure 2: Correlation function $C(\tau)$ build from $N = 200$ oscillators distributed according to the distributions shown in Fig. 1 at $k_B T = 0$ left, and $k_B T = 2$ (right).

(2b) Explore some different distribution shapes, means and widths and varying N. Particular find out how the width (standard deviation) of the frequency distribution $\Delta\omega$, the number of oscillators N and the temperature T affect the correlation function [4 pts].

Hints: Let us assume we have chosen some dimensionless units so that all parameters are of order "one". This still means we can let them vary between e.g. 0.01 and 100 or such. Then, it might be ok to set all masses equal to one (why is that?). Check the documentation of the mathematica commands `Table`, `RandomVariate`, `NormalDistribution`, `MixtureDistribution`, `ChiSquareDistribution`, `Histogram`, `PDF`, `Sum`, `ListPlot`. *Initially start with $N = 20$, but in the end try to crank it up to as high as $N = 2000$.*

Solution: If instead of directly having $N = 2000$ bath oscillators as in Fig. 2(left), we

have much fewer, the correlation function no longer quickly decays and shows much more persistent oscillations. Shis is shown in Fig. 3
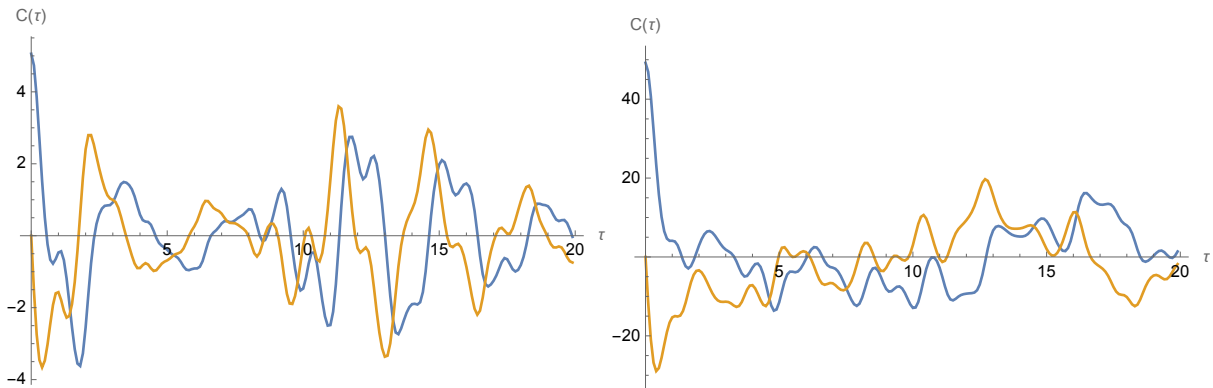

Figure 3: Change of correlations with number of oscillators for the distributions shown in Fig. 1 at zero temperature $T = 0$. Left: $N = 20$, Right: $N = 100$, for $N = 2000$ see Fig. 2

Going back to $N = 2000$ in the following, we see in Fig. 4 when we make the narrow peak in the frequency distribution much more important, we get a more regular envelope decay of oscillations. Then if the frequency distribution is wider, the decay is faster (recall the time-energy uncertainty relation or Fourier theory).
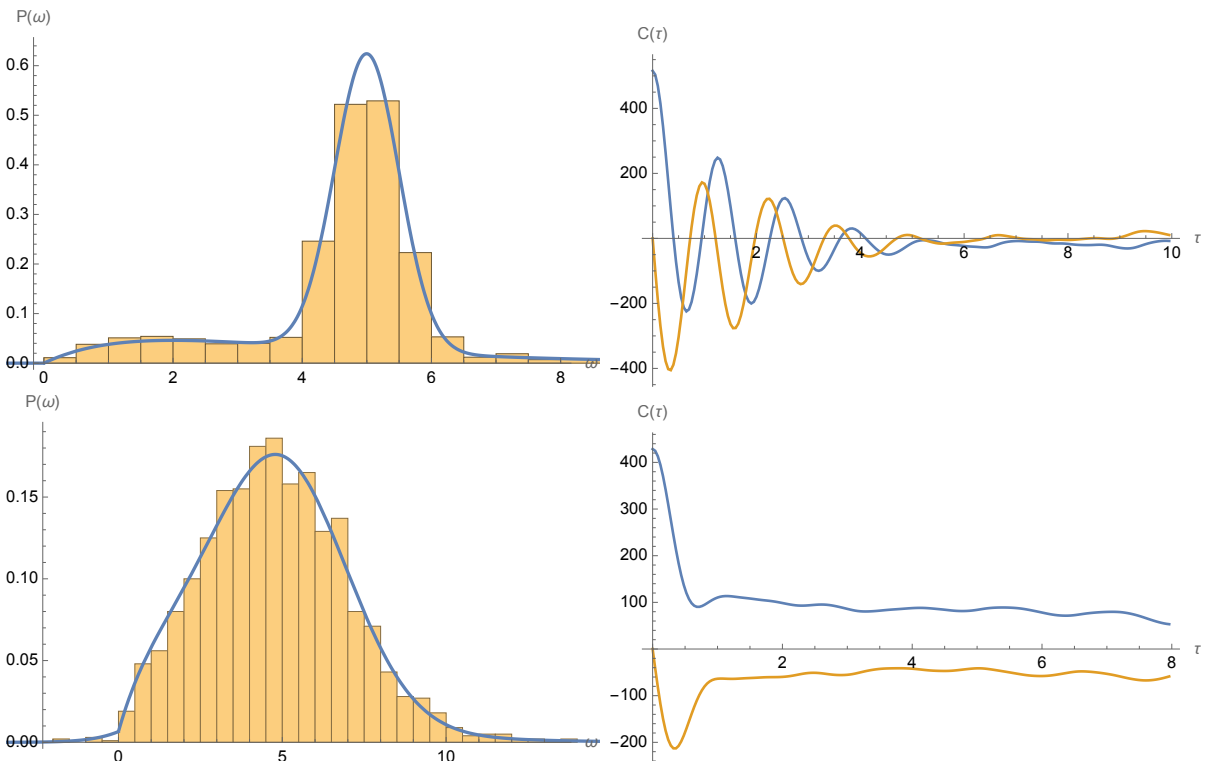

Figure 4: Correlations functions for the same case as in Fig. 2 (left), but changing the frequency distribution to the ones shown on the left.

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Finally, if we play similarly with the coupling distribution, that has much less of an effect on decay times, see Fig. 5
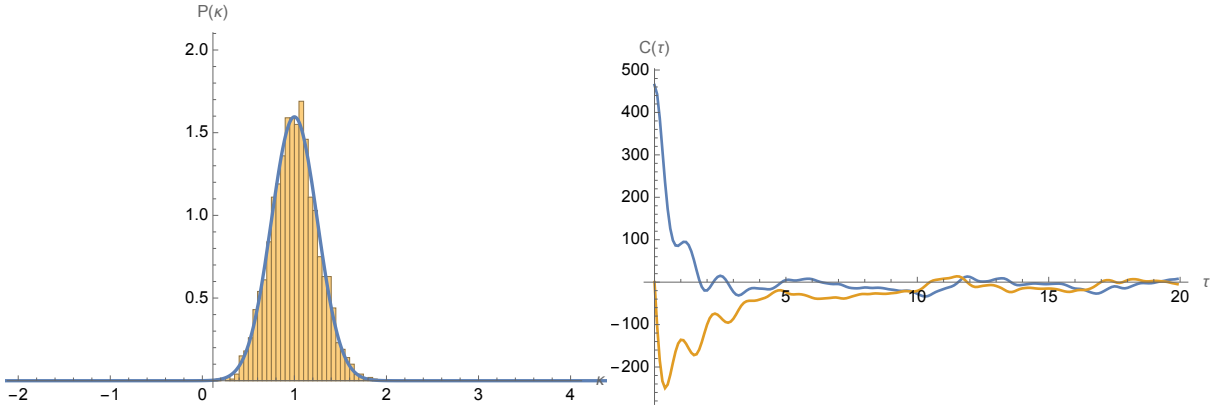

Figure 5: Correlations functions for the same case as in Fig. 2 (left), but changing the coupling distribution to the one shown on the left.

(3) Simulating decoherence in a quantum computer The code `Assignment5_program_draft_v1.xmds` is set up to numerically solve a Lindblad equation, for the density matrix of question 1:

$$\hat{\rho}(t) = \sum_{ab;cd \in \{0,1\}} \rho_{ab;cd}(t) |ab\rangle\langle cd|. \tag{8}$$

(3a) Implement your Lindblad equation from Q1b at XXX and your time sequence for initialisation of the initial state and controlled-Z gate at ZZZ. Some manipulations on A and B could be done in parlallel, best do them sequentially. Also derive the energy as a function of $\hat{\rho}$ and implement that at YYYY. [4 points].

Solution: For implementation see `Assignment5_program_solution_v2b.xmds`. *The energy is given by* $E = \langle\hat{H}\rangle = Tr[\hat{\rho}\hat{H}]$, *which we can again find most easily using the matrix representations above. That gives:*

$$E = 1/2(2U\rho_{1111} + \Delta_B(-\rho_{0000} + \rho_{0101} - \rho_{1010} + \rho_{1111}) + \Delta_A(-\rho_{0000} - \rho_{0101} + \rho_{1010} + \rho_{1111})$$
$$+ \rho_{0010}\Omega_A + \rho_{0111}\Omega_A + \rho_{1000}\Omega_A + \rho_{1101}\Omega_A + \rho_{0001}\Omega_B + \rho_{0100}\Omega_B + \rho_{1011}\Omega_B + \rho_{1110}\Omega_B) \tag{9}$$

(3b) Check that your density matrix remains normalised properly and that energy is conserved <u>for constant parameters and no dephasing only,</u> using `Assignment5_plot_checks_v1.m`*. Discuss what happens to these checks if parameters are varying in time, or you add dephasing, and why. Hint: In the likely case that none of that works on first attempt, use* `Assignment5_plot_populations_v1.m` *to check what your control parameters and populations are doing,* `Assignment5_check_hermiticity_v1.m` *to make sure the density matrix remains Hermitian, in case it doesn't, use*

`Assignment5_check_coherences_v1.m` to find the culprit. [2 points].

Solution: See Fig. 6, the trace of the density matrix has to remain one no matter what, as is shown in the leftmost panel. Energy is only conserved, if the Hamiltonian is time independent and we have a closed system. Setting all control parameters nonzero put constant is thus the only way to check your equations of motion by confirming energy conservation. The (mid) panel in Fig. 6 demonstrates explicitly that system-energy is NOT conserved, if we vary the parameters in the Hamiltonian vary in time. No matter what, the density matrix must be hermitian, and the provided script checks that by calculating the matrix $\hat{\rho} - \hat{\rho}^\dagger$ and then taking the maximum modulus of all the matrix elements as a function of time. Since the matrix itself should be full of zeros, this should remain zero as shown in the right panel.
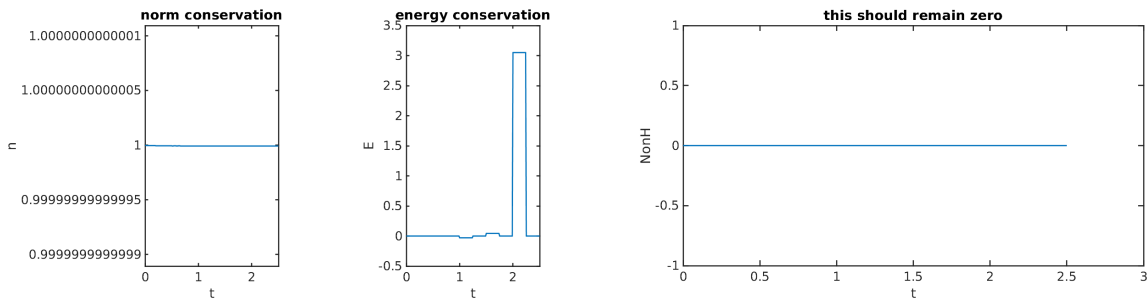

Figure 6: (left) normalisation of density matrix, (mid) energy as per Eq. (9), for a case with non-constant pulse sequence, in this case the one shown in Fig. 7 (mid). (right) For $\hat{\bar{\rho}} = \hat{\rho} - \hat{\rho}^\dagger$ we show $\max_{ij}[\bar{\rho}_{ij}](t)$, where $\bar{\rho}_{ij}$ are the matrix elements of $\hat{\bar{\rho}}$.

If it is not zero, you must find out which matrix element is the culprit, for that `Assignment5_check_coherences_v1.m` *would be useful. It loops through all matrix element (ij) and plots ρ_{ij} and (effectively) ρ_{ji}^*. Since one is the complex conjugate of each other, these solid and dashed lines always should lie on top of each other. See Fig. 7 (left).*
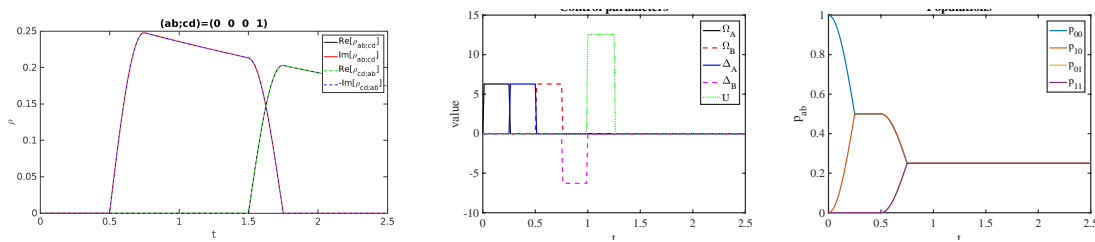

Figure 7: (left) For $\rho_{ab;cd}$ as shown on top, we show the real and imaginary parts of $\rho_{ab;cd}$ and $\rho_{cd;ab}$ as listed in the legend, including dephasing in this case. (mid) Time evolution of control parameters, to check the sequence from Q1(a) is implemented as planned. (right) Probabilities / populations for each of the four basis states.

(3c) Check that your sequence correctly does steps (i) and (iii) from Q1a, using

`Assignment5_check_quantum_computer_v2.m.` , *if there is no decoherence ($\gamma_n = 0$) [2 points].*

Solution: We first can get an idea by plotting the pulse-sequence (Fig. 7 (mid)) and populations (Fig. 7 (right)) noting that they are doing the right thing. Of course this only is a necessary condition for everything to go as planned, since we have not yet looked at the complex phase of the wavefunction. This is done in Fig. 8, where we plot all density matrix elements, which contain the phases in the off diagonal. The provided script compares the real output from the simulation, which the expected output (e.g. your sequence from Q1) for comparison.
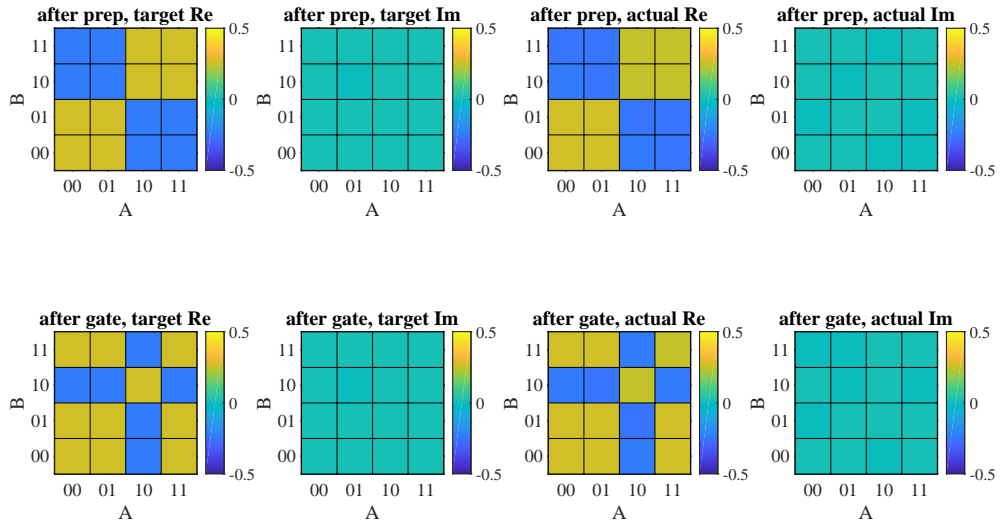

Figure 8: Density matrix elements at the moments listed in subplot titles. We are showing real parts and imaginary parts separately. The left four panels are from the simulation of Eq. (6) without dephasing, the right four panels are the expected states based on your target sequence (here we take the one from Q1(a). We can see that it works as expected, and also that the density matrix elements indeed correspond to the states proposed in Q1.

(3d) Check how this changes when decoherence is added. How large can γ_n be before your quantum computer breaks down. What does that mean for the design principles of quantum computers? [2 points]. Solution: Now when we add dephasing, qubits decohere slightly between steps. This is for example shown in the coherence decay of Fig. 7 (left). We can again compare simulations density matrix elements including decoherence, with expected density matrix elements for the case of no decoherence, in Fig. 9 and see how bad the difference is. The bigger it is, the less well your quantum computer will work.
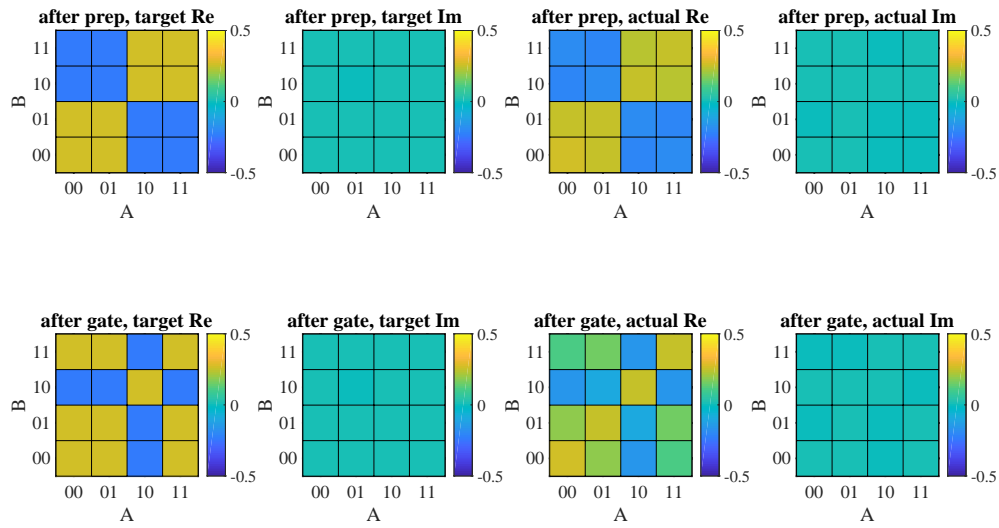
Figure 9: The same as Fig. 8 but <u>with</u> dephasing. $\gamma_A = \gamma_B = 1/5$. Now, when checking out the real parts of density matrix elements in the simulation (bottom row, third from the left), we notice a significant difference to expectation.