Problem Set 2
(M1 Math Methods 2023-2024)

This problem set is due on Friday, September 29th, 2023, at 23:59. The solutions should be sent as a single PDF (scan of handwritten document or LaTeX) to alexandru.petrescu@minesparis.psl.eu by the deadline. If you collaborate with a colleague, please write clearly their names at the top of your solution sheets. If you submit late without a satisfactory reason, the set will be accepted with a 10% penalty in the score.

I. CONTROLLING A QUBIT (20 POINTS)

Consider a qubit under a monochromatic control tone

$$\frac{\hat{H}}{\hbar} = \frac{1}{2}\omega_q \hat{\sigma}_z + \varepsilon_d \cos(\omega_d t)\hat{\sigma}_x. \tag{1}$$

Assume that we choose our frequencies such that $\omega_d, \omega_q \gg \epsilon_d$.

a) *Time-dependent change of frame.* Show that, given the time-dependent Schrödinger equation for an eigenstate of the Hamiltonian $|\psi(t)\rangle$,

$$\left[\frac{\hat{H}(t)}{\hbar} - i\partial_t\right]|\psi(t)\rangle = 0, \tag{2}$$

and an arbitrary time-dependent unitary transformation $\hat{U}(t)$, then the transformed states $\hat{U}^\dagger(t)|\psi(t)\rangle$ obey the transformed time-dependent Schrödinger equation

$$\begin{aligned} \left[\frac{\hat{H}'(t)}{\hbar} - i\partial_t\right]\hat{U}^\dagger(t)|\psi(t)\rangle = 0, \\ \frac{\hat{H}'}{\hbar}(t) \equiv \hat{U}^\dagger(t)\left[\frac{\hat{H}}{\hbar} - i\partial_t\right]\hat{U}(t). \end{aligned} \tag{3}$$

b) Go to a 'rotating' frame by applying the unitary transformation $\hat{U}(t) = \exp\left(-i\omega_d\hat{\sigma}_z t/2\right)$ and show that in this new rotating frame, up to neglecting terms that contain phase factors that oscillate at large frequencies $\pm(\omega_d + \omega_q)$, the Hamiltonian governing the dynamics is

(introducing $\Delta \equiv \omega_q - \omega_d$)

$$\frac{1}{\hbar}\hat{H}' \approx \frac{1}{2}\Delta\hat{\sigma}_z + \frac{1}{2}\varepsilon_d\hat{\sigma}_x. \tag{4}$$

c) Solve the time-dependent Schrödinger equation in this frame, then report the result in the original laboratory frame, assuming the system is prepared in the initial state $|\psi(t=0)\rangle = |0\rangle$.

d) Now fix $\omega_d = \omega_q$ and find the amount of time it will take the system to go to the excited state $|1\rangle$ (this is a π pulse or NOT gate). What about the time to evolve from $|0\rangle$ into the linear combination $|-\rangle = (|0\rangle - i\,|1\rangle)/\sqrt{2}$ (this would amount to a $\pi/2$ pulse)?

e) Numerically integrate the Schrödinger equation corresponding to Hamiltonian Eq. (1) with initial condition $|\psi(t=0)\rangle = |0\rangle$ for the following parameters $\omega_q/(2\pi) = \omega_d/(2\pi) =$ 5GHz, $\epsilon_d/(2\pi) = 0.25$GHz, and plot the three components of the Bloch vector $\vec{r}$ corresponding to the density matrix, i.e. $\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)| \equiv \frac{1+\vec{r}(t)\cdot\vec{\sigma}}{2}$. Graphically compare the numerical solution to your result in b). Find a sufficiently small control drive amplitude ϵ_d for which the π-pulse infidelity, defined as the minimum of $1 - \mathrm{Tr}\{\hat{\rho}(t)\hat{\rho}_{\mathrm{target}}\}$ as time t is varied with $\hat{\rho}_{\mathrm{target}} = |1\rangle\langle 1|$, is smaller than 5%.

f) Suppose the system is in state $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Now assume that you measure $\hat{\sigma}_z$, for which the two projectors are $\hat{P}_1 = |1\rangle\langle 1|$ and $\hat{P}_0 = |0\rangle\langle 0|$. What is the probability of measuring 0 (or 1) and what is the state of the system right after the measurement in each case? Now, assume that you performed the same measurement, but *without looking at the outcome*. What is the state of the system? *Hint:* This is represented by a density matrix corresponding to a pure state ensemble defined by the states and probabilities that you determined in the previous question.

g) Suppose that someone prepared the system in either the pure state $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ or the mixed state $\rho = \frac{\hat{P}_0 + \hat{P}_1}{2}$. Can you, by performing a combination of π or $\pi/2$ pulses, and $\hat{\sigma}_z$ measurements, figure out whether the system was prepared in one or the other?

SOLUTION

a)[**2 points**] Take an arbitrary unitary $\hat{U}(t)$ and define a new ket $|\psi'(t)\rangle = \hat{U}^\dagger(t)\,|\psi(t)\rangle$. Now make the following trivial insertions into the time-dependent Schrödinger Eq. (2)

$$\hat{U}^\dagger(t)\left[\frac{\hat{H}(t)}{\hbar} - i\partial_t\right]\hat{U}(t)\hat{U}^\dagger(t)\,|\psi(t)\rangle = 0, \tag{5}$$

so we have

$$\hat{U}^\dagger(t)\left[\frac{\hat{H}(t)}{\hbar} - i\partial_t\right]\hat{U}(t)\,|\psi'(t)\rangle = 0. \tag{6}$$

Now the result is obtained by carefully handling the time derivative. It acts on everything to its right, including the unitary $\hat{U}(t)$, so $-i\partial_t\left[\hat{U}(t)\,|\psi'(t)\rangle\right] = -i\left[\partial_t\hat{U}(t)\right]|\psi'(t)\rangle + -i\hat{U}(t)\left[\partial_t\,|\psi'(t)\rangle\right]$. So in the new frame we have the following time-dependent Schrödinger equation

$$\left[\frac{\hat{H}'(t)}{\hbar} - i\partial_t\right]|\psi'(t)\rangle = 0, \tag{7}$$

where

$$\begin{aligned}\hat{H}'(t)/\hbar &= \hat{U}^\dagger(t)\left[\hat{H}(t)/\hbar - i\partial_t\right]\hat{U}(t)\\ &= \hat{U}^\dagger(t)\hat{H}(t)\hat{U}(t)/\hbar - i\hat{U}^\dagger(t)\left[\partial_t\hat{U}(t)\right].\end{aligned} \tag{8}$$

b)[**3 points**] $\hat{\sigma}_x = \hat{\sigma}_+ + \hat{\sigma}_-$, where $\hat{\sigma}_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, and $\hat{\sigma}_- = \hat{\sigma}_+^\dagger$, and therefore $\hat{U}^\dagger(t)\hat{\sigma}_x\hat{U}(t) = \sigma_+ e^{i\omega_d t} + \sigma_- e^{-i\omega_d t}$, which allows us to write the transformed Hamiltonian

$$\frac{\hat{H}'(t)}{\hbar} = \frac{1}{2}\Delta\hat{\sigma}_z + \frac{1}{2}\epsilon_d(e^{i\omega_d t} + e^{-i\omega_d t})(\sigma_+ e^{i\omega_d t} + \sigma_- e^{-i\omega_d t}). \tag{9}$$

In the above, assuming $2\omega_d \gg \epsilon_d$, drop the terms oscillating at frequency $\pm 2\omega_d$ to arrive at the approximate rotating-wave-approximation form

$$\frac{\hat{H}'}{\hbar} \approx \frac{1}{2}\Delta\hat{\sigma}_z + \frac{1}{2}\epsilon_d\hat{\sigma}_x. \tag{10}$$

c)[**3 points**] In this frame, there are two eigenstates, with eigenenergies and eigenprojectors (i.e. projectors onto the two eigenstates) given by

$$\frac{E_\pm}{\hbar} = \pm|\vec{n}| = \pm\sqrt{\left(\frac{\Delta}{2}\right)^2 + \left(\frac{\epsilon_d}{2}\right)^2},\ \hat{P}_\pm = \frac{\hat{I} \pm \hat{n}\cdot\vec{\sigma}}{2}, \tag{11}$$

where $\vec{n} = \left(\frac{\epsilon_d}{2}, 0, \frac{\Delta}{2}\right)$ and $\hat{n} = \vec{n}/|\vec{n}|$, $\hat{I}$ is the 2×2 identity matrix, and $\hat{n}\cdot\vec{\sigma} \equiv \hat{n}_x\hat{\sigma}_x + \hat{n}_y\hat{\sigma}_y + \hat{n}_z\hat{\sigma}_z$.

In the $\hat{H}'$ frame, $|\psi'(t=0)\rangle = |0\rangle = |\psi(t=0)\rangle$ (the ket is the same at the initial time in both frames, since the unitary that connects the frames is the identity at time $t=0$). The subsequent evolution in the $\hat{H}'$ frame is

$$\begin{aligned}
|\psi'(t)\rangle = e^{-i\hat{H}'t/\hbar}|0\rangle &= (e^{-iE_+t/\hbar}\hat{P}_+ + e^{-iE_-t/\hbar}\hat{P}_-)|0\rangle \\
&= \left(e^{-iE_+t/\hbar}\frac{\hat{I}+\hat{n}_x\hat{\sigma}_x+\hat{n}_z\hat{\sigma}_z}{2} + e^{-iE_-t/\hbar}\frac{\hat{I}-\hat{n}_x\hat{\sigma}_x-\hat{n}_z\hat{\sigma}_z}{2}\right)|0\rangle \\
&= \left(e^{-iE_+t/\hbar}\frac{|0\rangle+\hat{n}_x|1\rangle-\hat{n}_z|0\rangle}{2} + e^{-iE_-t/\hbar}\frac{|0\rangle-\hat{n}_x|1\rangle+\hat{n}_z|0\rangle}{2}\right),
\end{aligned} \tag{12}$$

which gives, in the frame of $\hat{H}(t)$,

$$\begin{aligned}
|\psi(t)\rangle = \hat{U}(t)|\psi'(t)\rangle = &\frac{1}{2}e^{i\frac{\omega_d}{2}t}\left[e^{-iE_+t/\hbar}(1-\hat{n}_z) + e^{-iE_-t/\hbar}(1+\hat{n}_z)\right]|0\rangle \\
&+\frac{1}{2}e^{-i\frac{\omega_d}{2}t}\left[e^{-iE_+t/\hbar}\hat{n}_x - e^{-iE_-t/\hbar}\hat{n}_x\right]|1\rangle .
\end{aligned} \tag{13}$$

d)[**4 points**] At $\Delta = 0$, $E_\pm = \pm|\epsilon_d|/2$, $\hat{n}_x = 1$ and $\hat{n}_{y,z} = 0$, so

$$|\psi(t)\rangle = e^{i\frac{\omega_d}{2}t}\cos\left(\frac{\epsilon_d}{2}t\right)|0\rangle - ie^{-i\frac{\omega_d}{2}t}\sin\left(\frac{\epsilon_d}{2}t\right)|1\rangle . \tag{14}$$

A π pulse occurs at time t_π satisfying the condition $t_\pi = \pi/|\epsilon_d|$. At exactly this instant, the state of the system is $|\psi(t_\pi)\rangle = |1\rangle$, up to an irrelevant phase factor. At $t_\pi/2$, the state of the system is, assuming $\epsilon_d > 0$,

$$|\psi(t_\pi/2)\rangle = \frac{1}{\sqrt{2}}\left(e^{i\frac{\omega_d}{4}t_\pi}|0\rangle - ie^{-i\frac{\omega_d}{4}t_\pi}|1\rangle\right), \tag{15}$$

while the expression in the $\hat{H}'$ frame is free of the change-of-frame phase factors

$$|\psi'(t)\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle). \tag{16}$$

e)[**4 points**] Let's write $|\psi(t)\rangle$ as a two-dimensional complex vector $\begin{pmatrix} c_1(t) \\ c_0(t)\end{pmatrix}$. Then Eq. (1) can be recast immediately as a system of linear ordinary differential equations

$$\begin{aligned}
-i\dot{c}_0(t) &= -\frac{1}{2}\omega_q c_0(t) + \epsilon_d\cos(\omega_d t)c_1(t) \\
-i\dot{c}_1(t) &= \frac{1}{2}\omega_q c_1(t) + \epsilon_d\cos(\omega_d t)c_0(t),
\end{aligned} \tag{17}$$

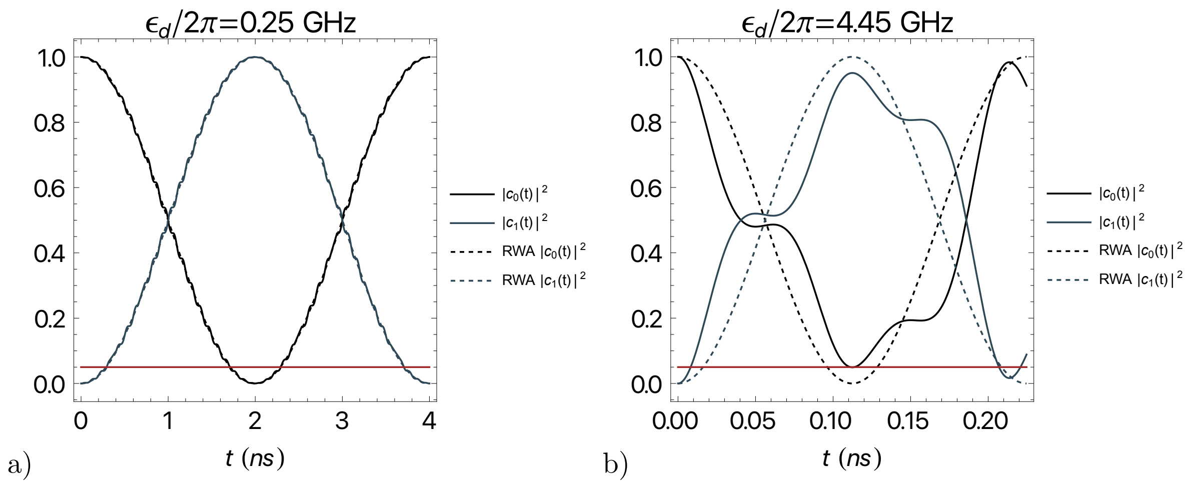

FIG. 1. Result of numerical simulation for $\epsilon_d = 0.25 * 2\pi$GHz, as given in the problem [panel a)], and for $\epsilon_d = 4.45 * 2\pi$GHz [panel b)], a value for which the minimum infidelity is 5% (see text). Rotating-wave approximation according to Eq. (4) is shown in dashed line, full numerical solution of Eq. (1) in solid lines. In panel b), the red line denotes the 5% threshold for infidelity.

to be solved with initial conditions $c_0(t = 0) = 1$ and $c_1(t = 0) = 1$. The numerical solution is shown in Fig. 1, and compared with the RWA of Eq. (4). As the drive amplitude is increased, all else kept equal, there are large deviations from the RWA solution. The $\pi-$pulse infidelity you were asked to compute equals $|c_0(t)|^2$. We find that one needs a very large $\epsilon_d \approx 4.45 \times 2\pi$ GHz to reach a regime where the minimum infidelity is 5%.

f)[**2 points**] If the state of the system is $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ then upon measuring $\hat{\sigma}_z$ one would get $+1$ or -1 with probability 1/2, and the state right after will be $|1\rangle$ or $|0\rangle$, respectively. If you did not look at your measurement outcome, but performed the measurement, the state of the system would be given by the pure state ensemble $\{(1/2, |0\rangle), (1/2, |1\rangle)\}$, i.e. by $\hat{\rho} = \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} = \frac{\hat{P}_0 + \hat{P}_1}{2}$.

g)[**2 points**] $\hat{\rho} = \frac{\hat{P}_0 + \hat{P}_1}{2} = \frac{1}{2}\hat{I}$ where $\hat{I}$ is the identity operator. Therefore $\hat{\rho}$ commutes with any unitary operator, so $\hat{U}\hat{\rho}\hat{U}^\dagger = \hat{\rho}$. On the other hand, let us find a unitary transformation $\hat{U}$ that takes $|\psi\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$ to the ket $|1\rangle$. This can be chosen as $\hat{U} = |1\rangle\langle\psi| + |0\rangle\langle\psi_\perp|$, where $|\psi_\perp\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$ is chosen such that it is orthonormal to $|\psi\rangle$, i.e. $\langle\psi_\perp|\psi\rangle = 0$. $\hat{U}$ as written above is unitary since $\hat{U}\hat{U}^\dagger = |1\rangle\langle 1| + |0\rangle\langle 0| = \hat{I}$ and $\hat{U}^\dagger\hat{U} = |\psi\rangle\langle\psi| + |\psi_\perp\rangle\langle\psi_\perp| = \hat{I}$. Applying this unitary, then measuring $\hat{\sigma}_z$, would immediately allow one to distinguish between the two scenarios. In the first scenario, that of the system being in state $\hat{\rho}$, one would measure

+1 half of the time, and −1 half of the time, whereas in the second scenario, one would always measure $|1\rangle$.

II. COHERENT INTERACTION BETWEEN TWO QUBITS (20 POINTS)

Consider the Hamiltonian

$$\frac{\hat{H}}{\hbar} = \frac{\omega_q}{2}\left(\hat{\sigma}_{z1} + \hat{\sigma}_{z2}\right) + g\left(\hat{\sigma}_{+,1}\hat{\sigma}_{-,2} + \hat{\sigma}_{+,2}\hat{\sigma}_{-,1}\right), \tag{18}$$

where $\hat{\sigma}_{z1}$ is shorthand for $\hat{\sigma}_{z1} \otimes I_2$, and $\hat{\sigma}_{z2}$ for $I_1 \otimes \hat{\sigma}_{z2}$, and $\hat{\sigma}_{+,1}\hat{\sigma}_{-,2} \equiv \hat{\sigma}_{+,1} \otimes \hat{\sigma}_{-,2}$ etc. Note that $\sigma_{\pm,i} \equiv \frac{\sigma_{xi} \pm \sigma_{yi}}{2}$, I_i is the 2×2 identity matrix, and $\sigma_{xi}, \sigma_{yi}, \sigma_{zi}$ are the three Pauli matrices acting on the qubit $i = 1, 2$.

a) Find the eigenstates and eigenvalues of this Hamiltonian, noting that the observable corresponding to the total number of excitations, $\hat{\sigma}_{z1} + \hat{\sigma}_{z2}$, commutes with the Hamiltonian.

b) Suppose the system is initialized in the one-excitation state $|\psi(t=0)\rangle = |10\rangle$, corresponding to qubit 1 being in the excited state and qubit 2 in the ground state. What is the time evolution of this ket under the Hamiltonian above? How much time will it take for the excitation to get transfered from the first qubit to the second, i.e. find the smallest $t_{swap} > 0$ for which $|\psi(t_{swap})\rangle = |01\rangle$. Similarly, what is $t_{entangle} < t_{swap}$ for which $|\psi(t_{entangle})\rangle = \frac{|10\rangle - i|01\rangle}{\sqrt{2}}$? Find the reduced density matrix corresponding to the first qubit, $\rho_1(t) = \mathrm{Tr}_2\left\{|\psi(t)\rangle\langle\psi(t)|\right\}$, and express its purity, defined as $\mathrm{Tr}\left\{\hat{\rho}_1^2(t)\right\}$, as a function of time.

c) Suppose you measured σ_{z1} exactly at $t_{entangle}$ above, and found outcome '1'. What is the probability of this outcome, and what is state of the system right after this measurement?

SOLUTION

a)[**8 points**] With tensor-product notation, the Hamiltonian reads

$$\frac{\hat{H}}{\hbar} = \frac{\omega_q}{2}\left(\hat{\sigma}_{z1} \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{\sigma}_{z2}\right) + g\left(\hat{\sigma}_{+,1} \otimes \hat{\sigma}_{-,2} + \hat{\sigma}_{-,1} \otimes \hat{\sigma}_{+,2}\right). \tag{19}$$

The following commutators are needed $[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$, and their cyclic permutations, $[\hat{\sigma}_y, \hat{\sigma}_z] = 2i\hat{\sigma}_x$, and $[\hat{\sigma}_z, \hat{\sigma}_x] = 2i\hat{\sigma}_y$. Since $\hat{\sigma}_\pm = \frac{\hat{\sigma}_x \pm i\hat{\sigma}_y}{2}$, you can easily show that $[\hat{\sigma}_z, \hat{\sigma}_\pm] = \pm 2\sigma_\pm$. Finally, recalling the rule $\left(\hat{A} \otimes \hat{B}\right) \cdot \left(\hat{C} \otimes \hat{D}\right) = (\hat{A} \cdot \hat{C}) \otimes (\hat{B} \cdot \hat{D})$, we are ready to show that the relevant commutator vanishes

$$\begin{aligned}
&[\hat{\sigma}_{z1} \otimes \hat{I}_2 + \hat{I}_1 \otimes \sigma_{z2}, \sigma_{+,1} \otimes \sigma_{-,2} + \sigma_{-,1} \otimes \sigma_{+,2}] \\
=&[\hat{\sigma}_{z,1}, \hat{\sigma}_{+,1}] \otimes \hat{\sigma}_{-,2} + \hat{\sigma}_{-,1} \otimes [\hat{\sigma}_{z,2}, \hat{\sigma}_{+,2}] + [\hat{\sigma}_{z,1}, \hat{\sigma}_{-,1}] \otimes \hat{\sigma}_{+,2} + \hat{\sigma}_{+,1} \otimes [\hat{\sigma}_{z,2}, \hat{\sigma}_{-,2}] \\
=&2\hat{\sigma}_{+,1} \otimes \hat{\sigma}_{-,2} + 2\hat{\sigma}_{-,1} \otimes \hat{\sigma}_{+,2} - 2\hat{\sigma}_{-,1} \otimes \hat{\sigma}_{+,2} - 2\hat{\sigma}_{+,1} \otimes \hat{\sigma}_{-,2} \\
=&0.
\end{aligned} \tag{20}$$

The above is an exercise in Pauli algebra, but a more intuitive solution is to write down matrices in the basis of the tensor product Hilbert space $\{|11\rangle, |10\rangle, |01\rangle, |00\rangle\}$, where by $|ij\rangle$ we mean $|i\rangle \otimes |j\rangle$ for any i, j taking values $0, 1$. The matrices are

$$\frac{\hat{H}}{\hbar} = \begin{pmatrix} \omega_q & 0 & 0 & 0 \\ 0 & 0 & g & 0 \\ 0 & g & 0 & 0 \\ 0 & 0 & 0 & -\omega_q \end{pmatrix}, \hat{\sigma}_{z1} + \hat{\sigma}_{z2} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}. \tag{21}$$

The two matrices clearly commute. The eigenvectors and eigenvalues of the Hamiltonian can be easily read off, they are $|11\rangle$ of eigenvalue ω_q, $\frac{|10\rangle \pm |01\rangle}{\sqrt{2}}$ of eigenvalues $\pm g$, and finally $|00\rangle$ of eigenvalue $-\omega_q$. Note that these correspond to the following eigenvalues of total σ_z: 2, 0 (twofold degenerate), and -2, respectively.

b)[**8 points**] In the zero total $\hat{\sigma}_z$ subspace, the dynamics is governed by the two-by-two Hamiltonian

$$\frac{\hat{H}}{\hbar} = \begin{pmatrix} 0 & g \\ g & 0 \end{pmatrix} \equiv g\hat{\tau}_x, \tag{22}$$

where we introduced a new Pauli matrix $\hat{\tau}_x$ that acts on this subspace spanned by the basis vectors $\{|10\rangle, |01\rangle\}$.

Then if one starts in the state $|10\rangle$, the time evolution is given by $|\psi(t)\rangle = e^{-igt\hat{\tau}_x}|10\rangle = \Big(\hat{I}\cos(-gt) + i\hat{\tau}_x \sin(-gt)\Big)|10\rangle = \cos(gt)|10\rangle - i\sin(gt)|01\rangle$. A full transfer of the excitation will occur at time $t = t_{swap} = \pi/(2g)$. The two qubits will be entangled in a Bell-like state at $t_{entangle} = t_{swap}/2 = \pi/(4g)$.

The density matrix corresponding to $|\psi(t)\rangle$ above is $\hat{\rho} = \cos^2(gt)|10\rangle\langle 10| + \sin^2(gt)|01\rangle\langle 01| - i\sin(gt)\cos(gt)|01\rangle\langle 10| + i\sin(gt)\cos(gt)|10\rangle\langle 01|$, whence the reduced density matrix for qubit 1 is $\hat{\rho}_1(t) = \cos^2(gt)|1\rangle\langle 1| + \sin^2(gt)|0\rangle\langle 0|$, and the purity is $\mathrm{Tr}(\rho_1^2(t)) = \cos^4(gt) + \sin^4(gt)$. The purity is then maximal at integer multiples of the swap time, i.e. when the excitation is one of the two qubits.

c)[**4 points**] The probability is 1/2, and the state right after this is $|10\rangle$.