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# Moderne Theoretische Physik I

## Grundlagen der Quantenmechanik

Summer Semester 2024

Exercise Sheet 11

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Due date: 12. 07. 2024.

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The problems whose solutions you need to upload are designated with stars.

### ★ Problem 1 ★ Entanglement entropy of the 2-site Quantum Ising model in a transverse field

Consider the Hamiltonian for two spin-1/2 particles:

$$\hat{H} = -J\hat{\sigma}_1^z\hat{\sigma}_2^z - h\hat{\sigma}_1^x - h\hat{\sigma}_2^x \quad (J, h \geq 0) \quad (1)$$

where  $\hat{\sigma}^x$  and  $\hat{\sigma}^z$  are Pauli matrices.

A convenient orthonormal basis of states which spans the full Hilbert space for this model consists of a direct product of eigenstates of  $\hat{\sigma}^z$  denoted, for example,

$$|\phi_1\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2, \quad |\phi_2\rangle = |\downarrow\rangle_1 \otimes |\downarrow\rangle_2, \quad |\phi_3\rangle = |\uparrow\rangle_1 \otimes |\downarrow\rangle_2, \quad |\phi_4\rangle = |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 \quad (2)$$

where  $\hat{\sigma}_{1,2}^z|\uparrow\rangle_{1,2} = |\uparrow\rangle_{1,2}$  and  $\hat{\sigma}_{1,2}^z|\downarrow\rangle_{1,2} = -|\downarrow\rangle_{1,2}$ . **Note:** you may use Wolfram Mathematica for this problem.

1. Find the matrix elements for this Hamiltonian,  $h_{\alpha\beta} = \langle\phi_\alpha|\hat{H}|\phi_\beta\rangle$ , with  $\alpha, \beta = 1, 2, 3, 4$ .
2. Find the eigenstate and eigenvalue of the matrix  $h$  with the lowest eigenvalue. If one denotes this (normalized) eigenstate as  $|\Psi\rangle$ , you should be now able to express it as  $|\Psi\rangle = \sum_{\alpha=1}^4 A_\alpha|\phi_\alpha\rangle$  with known values of the coefficients  $A_\alpha$ .
3. We are interested in the entanglement entropy of the state  $|\Psi\rangle$  for a bipartition that divides sites 1 and 2. First consider a density matrix of the full system simply given by  $|\Psi\rangle$ ,

$$\hat{\rho} = |\Psi\rangle\langle\Psi| \quad (3)$$

To calculate the entanglement entropy between the 2-sites we first need to find the reduced density matrix, which we denote by  $\hat{\rho}_1$ , for this bipartition. Therefore, calculate

$$\hat{\rho}_1 = Tr_2(\hat{\rho}) \quad (4)$$

where  $Tr_2$  denotes a trace over the Hilbert space of site 2, that is over the 2-states  $|\uparrow\rangle_2, |\downarrow\rangle_2$ . This gives the reduced density matrix  $\hat{\rho}_1$  for the subsystem consisting of site 1.

4. Re-express the density-matrix operator,  $\hat{\rho}_1$  as a  $2 \times 2$  matrix in the basis  $|\uparrow\rangle_1, |\downarrow\rangle_1$ , with matrix elements, for example,  $\langle\uparrow_1|\hat{\rho}_1|\uparrow_1\rangle$  and so on.

5. Diagonalize your  $2 \times 2$  matrix representation of  $\hat{\rho}_1$  to obtain its eigenvalues  $\lambda_i$ .
6. The von Neumann (bi-partite entanglement) entropy is defined as,

$$S_1^{vN} = -Tr_1[\hat{\rho}_1 \ln \hat{\rho}_1] = -\sum_i \lambda_i \ln \lambda_i \quad (5)$$

Calculate  $S_1^{vN}$  as a function of  $h/J$  and make a sketch of  $S_1^{vN}$  versus  $h/J$ .

7. What is the value of  $S_1^{vN}$  as  $\frac{h}{J} \rightarrow \infty$ ? As  $\frac{h}{J} \rightarrow 0$ ? Explain the physics behind these two limits.

## Solution 1

1. Using the fact that

$$\hat{\sigma}^x |\uparrow\rangle = |\downarrow\rangle, \quad \hat{\sigma}^x |\downarrow\rangle = |\uparrow\rangle, \quad \hat{\sigma}^z |\uparrow\rangle = |\uparrow\rangle, \quad \hat{\sigma}^z |\downarrow\rangle = -|\downarrow\rangle \quad (6)$$

$$\hat{H}|\phi_1\rangle = -J|\phi_1\rangle - h(|\phi_3\rangle + |\phi_4\rangle), \quad (7)$$

$$\hat{H}|\phi_2\rangle = -J|\phi_2\rangle - h(|\phi_3\rangle + |\phi_4\rangle), \quad (8)$$

$$\hat{H}|\phi_3\rangle = J|\phi_3\rangle - h(|\phi_2\rangle + |\phi_1\rangle), \quad (9)$$

$$\hat{H}|\phi_4\rangle = J|\phi_4\rangle - h(|\phi_2\rangle + |\phi_1\rangle) \quad (10)$$

Therefore in a matrix representation

$$\hat{H} = \begin{pmatrix} -J & 0 & -h & -h \\ 0 & -J & -h & -h \\ -h & -h & J & 0 \\ -h & -h & 0 & J \end{pmatrix} \quad (11)$$

2. The eigenvalues and corresponding eigenstates are as follows:

$$E_1 = -\Delta, \quad |E_1\rangle = \frac{1}{\sqrt{2(\Delta - J)^2 + 8h^2}} \begin{pmatrix} 2h & 2h & \Delta - J & \Delta - J \end{pmatrix}^T, \quad (12)$$

$$E_2 = -J, \quad |E_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 & 0 & 0 \end{pmatrix}^T, \quad (13)$$

$$E_3 = J, \quad |E_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & -1 & 1 \end{pmatrix}^T, \quad (14)$$

$$E_4 = \Delta, \quad |E_4\rangle = \frac{1}{\sqrt{2(\Delta + J)^2 + 8h^2}} \begin{pmatrix} -2h & -2h & J + \Delta & J + \Delta \end{pmatrix}^T \quad (15)$$

where  $\Delta = \sqrt{J^2 + 4h^2}$

The ground state is  $|E_1\rangle$  and

$$|\Psi\rangle = \frac{1}{\sqrt{2(\Delta - J)^2 + 8h^2}} \left( 2h(|\phi_1\rangle + |\phi_2\rangle) + (\Delta - J)(|\phi_3\rangle + |\phi_4\rangle) \right). \quad (16)$$

3. From Eq. (16),

$$\begin{aligned} \rho = |\Psi\rangle\langle\Psi| &= \frac{1}{2} \frac{1}{(\Delta - J)^2 + 4h^2} \left( 4h^2(|\phi_1\rangle + |\phi_2\rangle)(\langle\phi_1| + \langle\phi_2|) + 2h(\Delta - J)(|\phi_1\rangle + |\phi_2\rangle)(\langle\phi_3| + \langle\phi_4|) \right. \\ &\quad \left. + 2h(\Delta - J)(|\phi_3\rangle + |\phi_4\rangle)(\langle\phi_1| + \langle\phi_2|) + (\Delta - J)^2(|\phi_3\rangle + |\phi_4\rangle)(\langle\phi_3| + \langle\phi_4|) \right) \end{aligned} \quad (17)$$

Using

$$\begin{aligned} Tr_2(|\phi_1\rangle\langle\phi_2|) &= Tr_2(|\phi_1\rangle\langle\phi_3|) = Tr_2(|\phi_3\rangle\langle\phi_4|) = Tr_2(|\phi_2\rangle\langle\phi_4|) = 0, \\ Tr_2(|\phi_1\rangle\langle\phi_1|) &= |\uparrow\rangle_1\langle\uparrow|_1, \quad Tr_2(|\phi_1\rangle\langle\phi_4|) = |\uparrow\rangle_1\langle\downarrow|_1, \quad Tr_2(|\phi_3\rangle\langle\phi_3|) = |\uparrow\rangle_1\langle\uparrow|_1, \\ Tr_2(|\phi_2\rangle\langle\phi_2|) &= |\downarrow\rangle_1\langle\downarrow|_1, \quad Tr_2(|\phi_2\rangle\langle\phi_3|) = |\downarrow\rangle_1\langle\uparrow|_1, \quad Tr_2(|\phi_4\rangle\langle\phi_4|) = |\downarrow\rangle_1\langle\downarrow|_1 \end{aligned}$$

and the fact that  $(Tr_2(|\phi_i\rangle\langle\phi_j|))^{\dagger} = Tr_2(|\phi_j\rangle\langle\phi_i|)$ , we can obtain

$$Tr_2(\rho) = \frac{1}{2} \frac{1}{(\Delta - J)^2 + 4h^2} \left[ \left( 4h^2 + (\Delta - J)^2 \right) \left( |\uparrow\rangle_1\langle\uparrow|_1 + |\downarrow\rangle_1\langle\downarrow|_1 \right) + 4h(\Delta - J) \left( |\uparrow\rangle_1\langle\downarrow|_1 + |\downarrow\rangle_1\langle\uparrow|_1 \right) \right] \quad (18)$$

4. In a matrix representation,

$$Tr_2(\rho) = \frac{1}{2} \frac{1}{(\Delta - J)^2 + 4h^2} \begin{pmatrix} 4h^2 + (\Delta - J)^2 & 4h(\Delta - J) \\ 4h(\Delta - J) & 4h^2 + (\Delta - J)^2 \end{pmatrix} \quad (19)$$

5. The eigenvalues and eigenstates of  $Tr_2(\rho)$  are

$$\lambda_1 = \frac{1}{2} \frac{(2h - J + \Delta)^2}{4h^2 + (J - \Delta)^2}, \quad |\lambda_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (20)$$

$$\lambda_2 = \frac{1}{2} \frac{(2h + J - \Delta)^2}{4h^2 + (J - \Delta)^2}, \quad |\lambda_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (21)$$

6. Using the eigenvalues, the von-Neumann entropy is given by

$$\begin{aligned} S_1^{vN} &= - \sum_i \lambda_i \ln \lambda_i = - \frac{1}{2} \frac{(2h - J + \Delta)^2}{4h^2 + (J - \Delta)^2} \ln \left( \frac{1}{2} \frac{(2h - J + \Delta)^2}{4h^2 + (J - \Delta)^2} \right) - \frac{1}{2} \frac{(2h + J - \Delta)^2}{4h^2 + (J - \Delta)^2} \ln \left( \frac{1}{2} \frac{(2h + J - \Delta)^2}{4h^2 + (J - \Delta)^2} \right) \\ &= - \frac{(2x - 1 + \tilde{\Delta})^2}{4x^2 + (1 - \tilde{\Delta})^2} \ln |2x - 1 + \tilde{\Delta}| - \frac{(2x + 1 - \tilde{\Delta})^2}{4x^2 + (1 - \tilde{\Delta})^2} \ln |2x + 1 - \tilde{\Delta}| \\ &\quad + \ln 2 + \ln(4x^2 + (1 - \tilde{\Delta})^2) \end{aligned} \quad (22)$$

where  $x = h/J$  and  $\tilde{\Delta} = \sqrt{1 + 4x^2}$ .

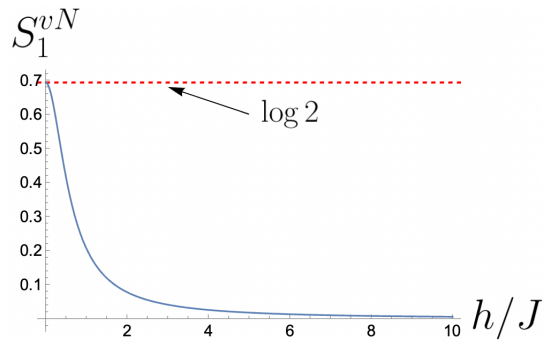


Figure 1:  $S_1^{vN}$  as a function of  $h/J$ .

7. (i)  $\frac{h}{J} \rightarrow 0$  limit

$$\tilde{\Delta}(x) \rightarrow 1 \Rightarrow S_1^{vN} \rightarrow -2 \ln 2x + \ln(2x^2) + \ln 2 = \ln 2 \quad (23)$$

In this limit, the Hamiltonian can be approximated into

$$\hat{H} \approx -J\hat{\sigma}_1^z\hat{\sigma}_2^z \quad (24)$$

and the corresponding ground state is singlet state which is maximally entangled state. Therefore the entanglement entropy is given by  $\ln 2$ .

(ii)  $\frac{h}{J} \rightarrow \infty$  limit

$$\tilde{\Delta}(x) \rightarrow 2x \Rightarrow S_1^{vN} \rightarrow 2 \ln 4x + \ln 8x^2 + \ln 2 = 0 \quad (25)$$

In this limit, the Hamiltonian can be approximated into

$$\hat{H} \approx -h(\hat{\sigma}_1^x + \hat{\sigma}_2^x) \quad (26)$$

and the corresponding ground state is product state ( $|\uparrow\rangle_1 \otimes |\downarrow\rangle_2$ ). As a result, the entanglement entropy is zero.

## ★ Problem 2 ★ Operator in Heisenberg picture

Consider a harmonic oscillator with the Hamiltonian

$$H = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \quad (27)$$

Where  $\hat{a}^\dagger$  and  $\hat{a}$  are the creation and annihilation operators respectively. In the Heisenberg picture, in contrast to the Schrödinger picture, the states are time-independent, but the operators for them are time-dependent.

1. Use the Heisenberg equation of motion to calculate the time evolution of the operators  $\hat{a}(t)$  and  $\hat{a}^\dagger(t)$ .
2. Calculate the time evolution of the operators  $\hat{x}(t)$  and  $\hat{p}(t)$ .
3. Use the results of the previous parts of the task to calculate the commutators  $[\hat{x}(t_1), \hat{x}(t_2)]$  and  $[\hat{x}(t_1), \hat{p}(t_2)]$  of the now time-dependent operators.
4. At time  $t = 0$ , the system is in the ground state  $|\psi(0)\rangle = |0\rangle$ . Calculate the correlation function  $\langle \hat{x}(0)\hat{x}(t) \rangle$ .

## Solution 2

The Heisenberg equation of motion for an operator  $\hat{A}(t)$  is

$$\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}(t)] + \frac{\partial \hat{A}(t)}{\partial t} \quad (28)$$

where the  $\hat{H}$  is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \quad (29)$$

1. The equations of motion for  $a(t)$  and  $a^\dagger(t)$  are given by

$$\frac{da}{dt} = \frac{i}{\hbar}[\hat{a}, \hat{H}] = i\omega[\hat{a}, \hat{a}^\dagger\hat{a}] = -i\omega\hat{a} \Rightarrow \hat{a}(t) = e^{-i\omega t}\hat{a}(0), \quad (30)$$

$$\frac{da^\dagger}{dt} = \frac{i}{\hbar}[\hat{a}^\dagger, \hat{H}] = i\omega[\hat{a}^\dagger, \hat{a}^\dagger\hat{a}] = i\omega\hat{a}^\dagger \Rightarrow \hat{a}^\dagger(t) = e^{i\omega t}\hat{a}^\dagger(0), \quad (31)$$

$$(32)$$

2.  $\hat{x}(t)$  and  $\hat{p}(t)$  are obtained from the above result:

$$\hat{x}(t) = \sqrt{\frac{\hbar}{m\omega}}(\hat{a}^\dagger(t) + \hat{a}(t)) = x(0) \cos \omega t + \frac{p(0)}{m\omega} \sin \omega t, \quad (33)$$

$$\hat{p}(t) = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger(t) - \hat{a}(t)) = p(0) \cos \omega t - m\omega x(0) \sin \omega t. \quad (34)$$

The operators satisfy the classical equations of motion.

The same results can be obtained by solving the system of equations

$$\frac{d\hat{x}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{x}(t)] = \frac{\hat{p}(t)}{m}, \quad (35)$$

$$\frac{d\hat{p}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{p}(t)] = -m\omega^2 \hat{x}(t) \quad (36)$$

3. Using the above results, we can obtain following values of commutators  $[\hat{x}(t_1), \hat{x}(t_2)]$  and  $[\hat{x}(t_1), \hat{p}(t_2)]$ :

$$\begin{aligned} [\hat{x}(t_1), \hat{x}(t_2)] &= \frac{1}{m\omega} \cos \omega t_1 \sin \omega t_2 [\hat{x}(0), \hat{p}(0)] + \frac{1}{m\omega} \sin \omega t_1 \cos \omega t_2 [\hat{p}(0), \hat{x}(0)] \\ &= \frac{i\hbar}{m\omega} \sin \omega(t_2 - t_1), \end{aligned} \quad (37)$$

$$\begin{aligned} [\hat{x}(t_1), \hat{p}(t_2)] &= \cos \omega t_1 \cos \omega t_2 [\hat{x}(0), \hat{p}(0)] - \sin \omega t_1 \sin \omega t_2 [\hat{p}(0), \hat{x}(0)] \\ &= i\hbar \cos \omega(t_2 - t_1) \end{aligned} \quad (38)$$

4. The system is in the ground state  $|\psi(0)\rangle = |0\rangle$  at  $t = 0$ . To calculate the correlation function we switch back to the Heisenberg picture where  $\hat{x}(0) = \hat{x}$ .

$$\begin{aligned} \langle \hat{x}(0)\hat{x}(t) \rangle &= \langle 0|\hat{x}e^{i\hat{H}t/\hbar}\hat{x}e^{-i\hat{H}t/\hbar}|0\rangle = \frac{\hbar}{2m\omega} \langle 0|(\hat{a}^\dagger + \hat{a})e^{i\hat{H}t/\hbar}(\hat{a}^\dagger + \hat{a})|0\rangle e^{-i\omega t/2} \\ &= \frac{\hbar}{2m\omega} \langle 1|e^{i\hbar Ht/\hbar}|1\rangle e^{-i\omega t/2} = \frac{\hbar}{2m\omega} e^{i\omega t} \end{aligned} \quad (39)$$

### Problem 3 Spin in a time-dependent magnetic field

In the lecture, the Larmor precession of the electron spin in a static magnetic field in the  $z$ -direction  $\mathbf{B} = B\hat{z}$  was discussed. In the following, the behavior of the spin- $\frac{1}{2}$  particle will be investigated when a periodic magnetic field is additionally applied in the  $xy$ -plane.

Consider an electron spin in a time-dependent external magnetic field:

$$\mathbf{B}(t) = B_1 \cos \omega t \hat{e}_x + B_1 \sin \omega t \hat{e}_y + B_0 \hat{e}_z \quad (40)$$

1. Write the Hamiltonian of the system explicitly in matrix form.
2. Show that the problem can be transformed into the problem of an electron in a static magnetic field  $\bar{\mathbf{B}} = B_x \hat{e}_x + B_z \hat{e}_z$  by using a suitable transformation:

$$\psi_\uparrow(t) = a(t)\bar{\psi}_\uparrow(t), \quad \psi_\downarrow(t) = b(t)\bar{\psi}_\downarrow(t). \quad (41)$$

3. Use the time evolution operator  $\hat{U}(t, 0)$  to calculate the time evolution of the state  $|\bar{\psi}(t)\rangle$  of the electron spin in the effective static magnetic field  $\bar{\mathbf{B}}$ .
4. At time  $t = 0$  the particle is in the state  $|\psi(0)\rangle = |\uparrow\rangle$ . Calculate the probability  $P_\downarrow(t)$  of finding the spin at time  $t$  in the state  $|\downarrow\rangle$ . For which frequency  $\omega$  of the external field and after which time does the probability become maximum?

### Solution 3

1. The Hamiltonian in the matrix representation is given by

$$\hat{H} = \mu_B \boldsymbol{\sigma} \cdot \mathbf{B} = \mu_B B_1 \left[ \cos \omega t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin \omega t \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right] + \mu_B B_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (42)$$

If we define the frequencies  $\omega = 2\mu_B B$  it can be written compactly as

$$\hat{H} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \quad (43)$$

2. From the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix} \quad (44)$$

we obtain the equations of motion for the components  $\psi_{\uparrow}(t)$  and  $\psi_{\downarrow}(t)$

$$i\frac{\partial \psi_{\uparrow}(t)}{\partial t} = \frac{\omega_0}{2} \psi_{\uparrow} + \frac{\omega_1}{2} e^{-i\omega t} \psi_{\downarrow}, \quad (45)$$

$$i\frac{\partial \psi_{\downarrow}(t)}{\partial t} = \frac{\omega_1}{2} e^{i\omega t} \psi_{\uparrow} - \frac{\omega_0}{2} \psi_{\downarrow} \quad (46)$$

Now let us consider the following transformation:

$$\psi_{\uparrow}(t) = e^{-i\omega t/2} \bar{\psi}_{\uparrow}(t), \quad \psi_{\downarrow}(t) = e^{i\omega t/2} \bar{\psi}_{\downarrow}(t) \quad (47)$$

Then the equations of the motions in terms of the  $\bar{\psi}_{\uparrow, \downarrow}$  are given by

$$i\frac{\partial \bar{\psi}_{\uparrow}}{\partial t} = -\frac{\omega - \omega_0}{2} \bar{\psi}_{\uparrow} + \frac{\omega_1}{2} \bar{\psi}_{\downarrow}, \quad (48)$$

$$i\frac{\partial \bar{\psi}_{\downarrow}}{\partial t} = \frac{\omega_1}{2} \bar{\psi}_{\uparrow} + \frac{\omega - \omega_0}{2} \bar{\psi}_{\downarrow}. \quad (49)$$

We have now transformed the problem to a system with the effective Hamiltonian

$$\hat{\bar{H}} = \frac{\hbar}{2} \begin{pmatrix} -(\omega - \omega_0) & \omega_1 \\ \omega_1 & \omega - \omega_0 \end{pmatrix} \quad (50)$$

This corresponds to an electron spin in the static magnetic field  $\bar{\mathbf{B}} = (B_1, 0, \frac{\Delta\omega}{2\mu_B})$  with  $\Delta\omega = \omega - \omega_0$ .

The transformation (47) can also be written in matrix form as follows:

$$|\psi\rangle = e^{-i\omega t\sigma_z/2} |\bar{\psi}\rangle \quad (51)$$

It is nothing but a time-dependent rotation in spin space around the z-axis. We have switched to a rotating reference system and follow the rotation of the magnetic field  $B_1(t)$ .

3. To determine the time evolution of the state  $|\bar{\psi}(t)\rangle$ , we apply the time evolution operator of  $\hat{\bar{H}}$ .

$$\bar{U}(t, t') = e^{-\frac{i}{\hbar}(t-t')\hat{\bar{H}}}, \quad (52)$$

$$|\bar{\psi}(t)\rangle = e^{-\frac{i}{\hbar}t\hat{\bar{H}}} |\bar{\psi}(0)\rangle = e^{-i(\omega_1\sigma_x/2 - \Delta\omega\sigma_z/2)t} |\bar{\psi}(0)\rangle$$

Using the fact that

$$e^{i\boldsymbol{\sigma} \cdot \hat{n}\theta} = \cos \theta + i\boldsymbol{\sigma} \cdot \hat{n} \sin \theta \quad (53)$$

$$|\bar{\psi}\rangle = \left( \cos \frac{\Omega}{2} - i\frac{1}{\Omega}(\omega_1\sigma_x - \Delta\omega\sigma_z) \sin \frac{\Omega t}{2} \right) |\bar{\psi}(0)\rangle \quad (54)$$

where  $\Omega = \sqrt{\omega_1^2 + \Delta\omega^2}$ .

4. The amplitude for a spin flip from  $|\psi(0)\rangle = |\uparrow\rangle$  to  $|\psi(t)\rangle = |\downarrow\rangle$  is

$$\begin{aligned}\langle\downarrow|\psi(t)\rangle &= \langle\downarrow|e^{-i\omega t\sigma_z/2}|\bar{\psi}(t)\rangle = e^{i\omega t/2}\langle\downarrow|\left(\cos\frac{\Omega t}{2} - i\frac{1}{\Omega}(\omega_1\sigma_x - \Delta\omega\sigma_z)\sin\frac{\Omega t}{2}\right)|\uparrow\rangle \\ &= -ie^{i\omega t/2}\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2},\end{aligned}\tag{55}$$

where we used  $|\bar{\psi}(0)\rangle = |\psi(0)\rangle = |\uparrow\rangle$ . We obtain the probability

$$P_{\downarrow}(t) = |\langle\downarrow|\psi(t)\rangle|^2 = \frac{\omega_1^2}{2\Omega^2}(1 - \cos\Omega t).\tag{56}$$

The probability  $P_{\downarrow}(t)$  reaches the maximum value

$$\frac{\omega_1^2}{\Omega^2} = \frac{\omega_1^2}{(\omega - \omega_0)^2 + \omega_1^2}\tag{57}$$

after a  $\pi$ -pulse,  $t = \frac{\pi}{\Omega}$ .

For a resonant magnetic field  $\omega = \omega_0$ , this has the largest value with  $P_{\downarrow}(\pi/\Omega) = 1$ , and the spin then changes with certainty over time.