

# Introduction to Quantum Mechanics I

Midterm exam, November 22, 2024

2 hours

*Please write as neatly as possible. Any unreadable text will be ignored.*

*This exam is composed of two independent problems.*

*Use separate sets of paper to deal with the two problems.*

*You can write in English or French.*

## Problem 1 : A proton and an electron

In this problem one considers a proton (particle 1) and an electron (particle 2) which form a bound state, as in the hydrogen atom. We concentrate on the spins of the proton and of the electron, and totally disregard their spatial (orbital) properties.

1) Briefly recall what is the appropriate Hilbert space to describe the spin of the electron and what is the appropriate Hilbert space to describe the spin of the proton. What is the appropriate Hilbert space  $\mathcal{H}$  for the combined system ? What is the dimension of  $\mathcal{H}$  ? Give one orthonormal basis for  $\mathcal{H}$ .

2) Assume there is a uniform magnetic field  $\vec{B} = B\vec{e}_z$ . Neglecting any interactions between the electron and the proton, what is the corresponding Hamiltonian  $H_{(1)}$  for the proton, what is the Hamiltonian  $H_{(2)}$  for the electron and what is Hamiltonian  $H$  for the combined system ? What are the eigenstates of  $H$  and what are the corresponding (total) energies? Which state has the minimal energy? (Recall that  $\gamma_p = g_p \frac{e}{2m_p} > 0$  and  $\gamma_e = g_e \frac{(-e)}{2m_e} < 0$  and  $\gamma_p < |\gamma_e|$ .)

3) Suppose a measurement at  $t = 0$  of the total energy has given the lowest energy value. What is the state of the system right after the measurement? One then turns off (at  $t = 0+$ ) the uniform magnetic field. (We assume that turning off the magnetic field does not change the quantum state.) Now one takes into account the interaction between the magnetic moments of the proton and electron as described by the hyperfine Hamiltonian (as appropriate for an orbital wave function 1s):

$$H_{\text{hf}} = \frac{\epsilon}{\hbar^2} \vec{S}^{(1)} \cdot \vec{S}^{(2)}, \quad (1.1)$$

with some positive constant  $\epsilon$ . What is the unit of  $\epsilon$  ? What are the eigenstates and eigenvalues of  $H_{\text{hf}}$  ? Determine the state of the system at any later time  $t > 0$ .

4) Suppose at  $t = t_1 > 0$  one measures the  $z$ -component of the spin of the proton. What is the probability to find  $+\frac{\hbar}{2}$  ? Suppose one has found  $+\frac{\hbar}{2}$ . Immediately afterwards one measures the  $z$ -component of the spin of the electron. What does one find?

5) If instead of measuring the  $z$ -component of the spin of the proton, at  $t = t_1 > 0$ , one measures its  $x$ -component, what is the probability to find  $+\frac{\hbar}{2}$  ? Suppose one has found  $+\frac{\hbar}{2}$ . Immediately afterwards one measures the  $z$ -component of the spin of the electron. What are the probabilities to find  $+\frac{\hbar}{2}$  and  $-\frac{\hbar}{2}$  ?

## Problem 2 : Transverse field Ising model

The so-called one-dimensional transverse field Ising model (also referred to as quantum Ising model or spin chain) consists of  $N$  spins (or  $N$  q-bits), with corresponding spin-operators  $\vec{S}^{(a)} = (S_x^{(a)}, S_y^{(a)}, S_z^{(a)})$ ,  $a = 1, \dots, N$ , and a Hamiltonian given by

$$H = \sum_{a=1}^N \left( \frac{2J}{\hbar^2} S_z^{(a)} S_z^{(a+1)} + \frac{2b}{\hbar} S_x^{(a)} \right), \quad (1.2)$$

where one assumes “periodic boundary conditions”, by identifying  $\vec{S}^{(N+1)} \equiv \vec{S}^{(1)}$ . In this problem, we will restrict ourselves to the simplest case,  $N = 2$ .

1) What is the dimension of the Hilbert space  $\mathcal{H}$ ? Give the “standard” tensor product basis in this Hilbert space, made from the individual  $|\pm\rangle_z$ . Write out explicitly  $H$  for the present case  $N = 2$ . (You should find a sum of 3 terms.)

2) Recall how  $S_x^{(1)}$  acts on  $|1 : \pm\rangle_z$  and similarly  $S_x^{(2)}$  on  $|2 : \pm\rangle_z$ . Compute the action of  $H$  on the states of the tensor product basis, and give the corresponding matrix  $\hat{H}$ . Explain why it is non-trivial to compute the partition function  $Z$  given by the trace of  $e^{-\beta H}$ , i.e.  $Z = \text{tr} e^{-\beta H}$ . Show that for  $b = 0$  the computation can be easily done and give the result (which is the partition function of the corresponding classical Ising chain for  $N = 2$ ).

3) Compute  $[S_j^{(1)}, H]$  for  $j = x, y, z$ .

4) Consider now a general normalised state  $|\psi(t)\rangle$  satisfying the Schrödinger equation with an arbitrary (self-adjoint) Hamiltonian  $H$ . For any observable  $A$ , express  $i\hbar \frac{d}{dt} \langle A \rangle_\psi$  in terms of  $\langle [H, A] \rangle_\psi$ , where  $\langle (\dots) \rangle_\psi$  means the expectation value in the state  $|\psi(t)\rangle$ .

5) Coming back to our transverse field Ising model, we assume that at  $t = 0$  one has  $\langle S_z^{(1)} \rangle = +\frac{\hbar}{2}$ . Show that this implies that the state necessarily is a factorised state. Then apply the previous general result to obtain  $\frac{d}{dt} \langle S_j^{(1)} \rangle$  ( $j = x, y, z$ ) at arbitrary times and then specialise your result for  $t = 0$ . Show that, for small times,  $\langle S_z^{(1)} \rangle$  will decrease quadratically as  $\langle S_z^{(1)} \rangle = \frac{\hbar}{2} - Ct^2$  with a constant  $C$  to be determined.

6) In order to try to find the eigenvalues and eigenvectors of the Hamiltonian, compute its action on the Bell basis, as given in eq. (5.68) of the lecture notes, namely

$$\begin{aligned} |\Phi^+\rangle &= \frac{1}{\sqrt{2}}(|++\rangle + |--\rangle) & , & & |\Phi^-\rangle &= \frac{1}{\sqrt{2}}(|++\rangle - |--\rangle) & , \\ |\Psi^+\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) & , & & |\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) & . \end{aligned} \quad (1.3)$$

Using your result, determine all the eigenvalues and eigenvectors of  $H$ . Also compute the partition function  $Z$ .

# Solutions

## Problem 1 : A proton and an electron

1) Each particle has a spin  $\frac{1}{2}$  which means that the corresponding Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  are each 2-dimensional, with basis  $\{|1 : +\rangle, |1 : -\rangle\}$  for the first particle (proton) and basis  $\{|2 : +\rangle, |2 : -\rangle\}$  for the second particle (electron). The combined system has as Hilbert space  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$  of dimension 4, with 4 basis states

$$\begin{aligned} |1 : +\rangle \otimes |2 : +\rangle &\equiv |++\rangle, & |1 : +\rangle \otimes |2 : -\rangle &\equiv |+-\rangle, \\ |1 : -\rangle \otimes |2 : +\rangle &\equiv |-+\rangle, & |1 : -\rangle \otimes |2 : -\rangle &\equiv |--\rangle. \end{aligned} \quad (1.4)$$

This is an orthonormal basis.

2) We have

$$\begin{aligned} H_{(1)} &= -\vec{m}_p \cdot \vec{B} = -\gamma_p \vec{S}^{(p)} \cdot \vec{B} = -\gamma_p B S_z^{(p)} \equiv -\gamma_p B S_z^{(1)}, \\ H_{(2)} &= -\vec{m}_e \cdot \vec{B} = -\gamma_e \vec{S}^{(e)} \cdot \vec{B} = -\gamma_e B S_z^{(e)} = |\gamma_e| B S_z^{(e)} \equiv |\gamma_e| B S_z^{(2)}. \end{aligned} \quad (1.5)$$

Then  $H = H_{(1)} \otimes \mathbf{1} + \mathbf{1} \otimes H_{(2)}$ . Now the basis states (1.4) are all eigenstates of this  $H$  :

$$\begin{aligned} H |++\rangle &= (|\gamma_e| - \gamma_p) B \frac{\hbar}{2} |++\rangle, & H |+-\rangle &= -(\gamma_p + |\gamma_e|) B \frac{\hbar}{2} |+-\rangle, \\ H |-+\rangle &= (|\gamma_e| + \gamma_p) B \frac{\hbar}{2} |-+\rangle, & H |--\rangle &= -(|\gamma_e| - \gamma_p) B \frac{\hbar}{2} |--\rangle, \end{aligned} \quad (1.6)$$

The lowest eigenvalue clearly is  $-(\gamma_p + |\gamma_e|)B$  with corresponding eigenvector  $|+-\rangle$ .

3) At  $t = 0+$  the state gets projected to  $|+-\rangle$ . In terms of the triplet state  $|1, 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$  and the singlet state  $|0, 0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$ , this is  $|\psi(0+)\rangle = |+-\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 0\rangle)$ .

We know from the lecture that  $\vec{S}^{(1)} \cdot \vec{S}^{(2)} = \frac{1}{2} \vec{S}_{\text{tot}}^2 - \frac{3\hbar^2}{4}$  and that

$$\vec{S}^{(1)} \cdot \vec{S}^{(2)} |1, 0\rangle = \frac{\hbar^2}{4} |1, 0\rangle, \quad \vec{S}^{(1)} \cdot \vec{S}^{(2)} |0, 0\rangle = -\frac{3\hbar^2}{4} |0, 0\rangle, \quad (1.7)$$

so that

$$H_{\text{hf}} |1, 0\rangle = \frac{\epsilon}{4} |1, 0\rangle, \quad H_{\text{hf}} |0, 0\rangle = -\frac{3\epsilon}{4} |1, 0\rangle. \quad (1.8)$$

Then at time  $t$  the state is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{-i\frac{\epsilon t}{4\hbar}} |1, 0\rangle + e^{+i\frac{3\epsilon t}{4\hbar}} |0, 0\rangle \right). \quad (1.9)$$

This can be rewritten as

$$\begin{aligned} |\psi(t)\rangle &= \frac{e^{i\frac{\epsilon t}{4\hbar}}}{\sqrt{2}} \left( e^{-i\frac{\epsilon t}{2\hbar}} |1, 0\rangle + e^{+i\frac{\epsilon t}{2\hbar}} |0, 0\rangle \right) \\ &= \frac{e^{i\frac{\epsilon t}{4\hbar}}}{2} \left( e^{-i\frac{\epsilon t}{2\hbar}} (|+-\rangle + |-+\rangle) + e^{+i\frac{\epsilon t}{2\hbar}} (|+-\rangle - |-+\rangle) \right) \\ &= e^{i\frac{\epsilon t}{4\hbar}} \left( \cos \frac{\epsilon t}{2\hbar} |+-\rangle - i \sin \frac{\epsilon t}{2\hbar} |-+\rangle \right). \end{aligned} \quad (1.10)$$

4) The probability that a measurement of  $S_z^{(1)}$  gives  $+\frac{\hbar}{2}$  is

$$\langle \psi(t) | \left( |+\rangle \langle +| \otimes \mathbf{1} \right) | \psi(t) \rangle = \cos^2 \frac{\epsilon t}{2\hbar} , \quad (1.11)$$

and the state after this measurement (with result  $+\frac{\hbar}{2}$ ) is, up to normalisation,

$$\left( |+\rangle \langle +| \otimes \mathbf{1} \right) | \psi(t) \rangle = e^{i\frac{\epsilon t}{4\hbar}} \cos \frac{\epsilon t}{2\hbar} |+-\rangle , \quad (1.12)$$

or after normalising simply  $|+-\rangle$ . A measurement of  $S_z^{(2)}$  then yields  $-\frac{\hbar}{2}$  with probability 1.

5) If we measure instead the  $x$ -component of the spin of the proton, the probability to find  $+\frac{\hbar}{2}$  is

$$\langle \psi(t) | \left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) | \psi(t) \rangle . \quad (1.13)$$

Now

$$\left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) |+-\rangle = \left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) |+\rangle_z \otimes |-\rangle_z = \left( \langle +|_x |+\rangle_z \right) |+\rangle_x \otimes |-\rangle_z = \frac{1}{\sqrt{2}} |+\rangle_x \otimes |-\rangle_z , \quad (1.14)$$

and similarly

$$\left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) |-+\rangle = \left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) |-\rangle_z \otimes |+\rangle_z = \left( \langle +|_x |-\rangle_z \right) |+\rangle_x \otimes |+\rangle_z = \frac{1}{\sqrt{2}} |+\rangle_x \otimes |+\rangle_z , \quad (1.15)$$

so that

$$\left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) | \psi(t) \rangle = \frac{e^{i\frac{\epsilon t}{4\hbar}}}{\sqrt{2}} |+\rangle_x \otimes \left( \cos \frac{\epsilon t}{2\hbar} |-\rangle_z - i \sin \frac{\epsilon t}{2\hbar} |+\rangle_z \right) . \quad (1.16)$$

Then the probability (1.13) is

$$\langle \psi(t) | \left( |+\rangle_x \langle +|_x \otimes \mathbf{1} \right) | \psi(t) \rangle = \frac{1}{2} \left( \cos \frac{\epsilon t}{2\hbar} \langle -|_z + i \sin \frac{\epsilon t}{2\hbar} \langle +|_z \right) \left( \cos \frac{\epsilon t}{2\hbar} |-\rangle_z - i \sin \frac{\epsilon t}{2\hbar} |+\rangle_z \right) = \frac{1}{2} . \quad (1.17)$$

Right after the measurement, the state is given, up to normalisation, by (1.16). Normalising it yields

$$|+\rangle_x \otimes \left( \cos \frac{\epsilon t}{2\hbar} |-\rangle_z - i \sin \frac{\epsilon t}{2\hbar} |+\rangle_z \right) \quad (1.18)$$

Then the probabilities that a measurement of  $S_z^{(2)}$  yields  $+\frac{\hbar}{2}$  is  $\sin^2 \frac{\epsilon t}{2\hbar}$  and that it yields  $-\frac{\hbar}{2}$  is  $\cos^2 \frac{\epsilon t}{2\hbar}$ .

## Problem 2 : Transverse field Ising model

1) The Hilbert space  $\mathcal{H}$  is the  $N$ -fold tensor product of the two-dimensional single spin Hilbert spaces, and the dimension is  $2^N$ . The standard basis is composed of the  $|\pm\rangle \otimes |\pm\rangle \otimes \dots |\pm\rangle = |\pm \pm \dots \pm\rangle$ .

2) For  $N = 2$  we have

$$H = \frac{4J}{\hbar^2} S_z^{(1)} S_z^{(2)} + \frac{2b}{\hbar} (S_x^{(1)} + S_x^{(2)}) . \quad (1.19)$$

We take the basis elements in the following order :  $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$ . We have  $S_x^{(1)} |+\pm\rangle = \frac{\hbar}{2} |-\pm\rangle$  and  $S_x^{(1)} |-\pm\rangle = \frac{\hbar}{2} |+\pm\rangle$  and similarly for  $S_x^{(2)}$ . It follows that

$$\begin{aligned} H |++\rangle &= J |++\rangle + b |+-\rangle + b |+-\rangle , \\ H |+-\rangle &= -J |+-\rangle + b |--\rangle + b |++\rangle , \\ H |-+\rangle &= -J |-+\rangle + b |++\rangle + b |--\rangle , \\ H |--\rangle &= J |--\rangle + b |+-\rangle + b |-+\rangle . \end{aligned} \quad (1.20)$$

Then the matrix is

$$\hat{H} = \begin{pmatrix} \langle ++ | H | ++ \rangle & \langle ++ | H | +- \rangle & \langle ++ | H | -+ \rangle & \langle ++ | H | -- \rangle \\ \langle +- | H | ++ \rangle & \langle +- | H | +- \rangle & \langle +- | H | -+ \rangle & \langle +- | H | -- \rangle \\ \langle -+ | H | ++ \rangle & \langle -+ | H | +- \rangle & \langle -+ | H | -+ \rangle & \langle -+ | H | -- \rangle \\ \langle -- | H | ++ \rangle & \langle -- | H | +- \rangle & \langle -- | H | -+ \rangle & \langle -- | H | -- \rangle \end{pmatrix} = \begin{pmatrix} J & b & b & 0 \\ b & -J & 0 & b \\ b & 0 & -J & b \\ 0 & b & b & J \end{pmatrix} . \quad (1.21)$$

For  $b \neq 0$  this matrix is not diagonal and to compute  $\text{tr} e^{-\beta H}$  one needs to diagonalise it. Said differently, if  $E_1, \dots, E_4$  are the eigenvalues of this Hamiltonian, then  $Z = \sum_{i=1}^4 e^{-\beta E_i}$ . However, determining the eigenvalues of this  $4 \times 4$ -matrix is non-trivial. On the other hand, for  $b = 0$ , it is already diagonal and the eigenvalues are  $J, -J, -J, J$ , so that  $Z = 4 \cosh(\beta J)$ , which is indeed the result of the classical (periodic) Ising chain for  $N = 2$ .

3) We have

$$\begin{aligned} [S_x^{(1)}, H] &= -i \frac{4J}{\hbar} S_y^{(1)} S_z^{(2)} , \\ [S_y^{(1)}, H] &= i \frac{4J}{\hbar} S_x^{(1)} S_z^{(2)} - i 2b S_z^{(1)} , \\ [S_z^{(1)}, H] &= i 2b S_y^{(1)} . \end{aligned} \quad (1.22)$$

4) This is Ehrenfest's theorem. We assume that  $A$  has no time-dependence. Then

$$\begin{aligned} i\hbar \frac{d}{dt} \langle A \rangle_\psi &= i\hbar \frac{d}{dt} \langle \psi(t) | A | \psi(t) \rangle = ( - \langle \psi(t) | H \rangle A | \psi(t) \rangle + \langle \psi(t) | A (H | \psi(t) \rangle ) \\ &= \langle \psi(t) | [A, H] | \psi(t) \rangle = \langle [A, H] \rangle_\psi . \end{aligned} \quad (1.23)$$

5) Now apply this to  $A = S_a^{(1)}$  and use (1.22) to get (we drop the subscript  $\psi$  on the expectation value)

$$\begin{aligned} i\hbar \frac{d}{dt} \langle S_x^{(1)} \rangle &= -i \frac{4J}{\hbar} \langle S_y^{(1)} S_z^{(2)} \rangle , \\ i\hbar \frac{d}{dt} \langle S_y^{(1)} \rangle &= i \frac{4J}{\hbar} \langle S_x^{(1)} S_z^{(2)} \rangle - i 2b \langle S_z^{(1)} \rangle , \\ i\hbar \frac{d}{dt} \langle S_z^{(1)} \rangle &= i 2b \langle S_y^{(1)} \rangle . \end{aligned} \quad (1.24)$$

If initially at  $t = 0$  one has  $\langle S_z^{(1)} \rangle = +\frac{\hbar}{2}$  then the initial state must be eigenstate of  $S_z^{(1)}$ , which means that the state in the full Hilbert space must be factorised as  $|1 : +\rangle \otimes |2 : \chi\rangle$ . Then, at  $t = 0$ , one has  $\langle S_y^{(1)} S_z^{(2)} \rangle = \langle S_y^{(1)} \rangle_{|1:+\rangle} \langle S_z^{(2)} \rangle_{|2:\chi\rangle} = 0$  since  $\langle S_y^{(1)} \rangle_{|1:+\rangle} = 0$ . Similarly,  $\langle S_x^{(1)} S_z^{(2)} \rangle = \langle S_x^{(1)} \rangle_{|1:+\rangle} \langle S_z^{(2)} \rangle_{|2:\chi\rangle} = 0$ . Thus

$$\begin{aligned} \text{at } t = 0 : \quad i\hbar \frac{d}{dt} \langle S_x^{(1)} \rangle &= 0 , \\ i\hbar \frac{d}{dt} \langle S_y^{(1)} \rangle &= -ib\hbar , \\ i\hbar \frac{d}{dt} \langle S_z^{(1)} \rangle &= 0 . \end{aligned} \quad (1.25)$$

Thus, at small times,  $S_y^{(1)}$  will start to get a non-vanishing expectation value  $\langle S_y^{(1)} \rangle \simeq -bt$ . Then, by (1.24),  $\frac{d}{dt} \langle S_z^{(1)} \rangle \simeq -\frac{2b^2}{\hbar}t$  and, hence,  $\langle S_z^{(1)} \rangle \simeq \frac{\hbar}{2} - \frac{b^2}{\hbar}t^2$  which shows that the expectation value will decrease quadratically in  $t$  at small times. In any case, we also do not expect the state to remain factorised.

6) It follows immediately from (1.20) and the definition of the Bell basis that

$$\begin{aligned} H |\Phi^-\rangle &= J |\Phi^-\rangle , & H |\Psi^-\rangle &= -J |\Psi^-\rangle , \\ H |\Phi^+\rangle &= J |\Phi^+\rangle + 2b |\Psi^+\rangle , & H |\Psi^+\rangle &= 2b |\Phi^+\rangle - J |\Psi^+\rangle . \end{aligned} \quad (1.26)$$

This shows that  $|\Phi^-\rangle$  is eigenvector with eigenvalue  $J$  and  $|\Psi^-\rangle$  is eigenvector with eigenvalue  $-J$ . In the orthogonal subspace with orthonormal basis vectors  $|\Phi^+\rangle$  and  $|\Psi^+\rangle$ ,  $H$  acts as  $\hat{H}_{\text{ortho}} = J\sigma_z + 2b\sigma_x$ . Hence the eigenvalues are  $\pm\sqrt{J^2 + 4b^2}$  and the eigenvectors are

$$|v_+\rangle = \cos \frac{\theta}{2} |\Phi^+\rangle + \sin \frac{\theta}{2} |\Psi^+\rangle , \quad |v_-\rangle = -\sin \frac{\theta}{2} |\Phi^+\rangle + \cos \frac{\theta}{2} |\Psi^+\rangle , \quad \tan \theta = \frac{2b}{J} . \quad (1.27)$$

In particular, the partition function is

$$Z = 2 \cosh(\beta J) + 2 \cosh(\beta \sqrt{J^2 + 4b^2}) . \quad (1.28)$$