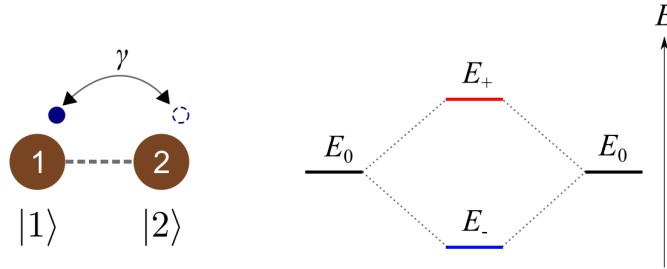


**— Soluções —****Problema 1 | Molécula diatômica numa aproximação de 2 níveis**

Consideremos a molécula diatômica esquematizada abaixo, cujos átomos 1 e 2 são do *mesmo* elemento. Em cada átomo, é apenas relevante considerar a sua orbital de valência, que pode ser ocupada por um eletrão. Quando os átomos estão isolados, a energia do eletrão nessa orbital de valência é  $E_0$ .



Ao aproximarmos os 2 átomos, passa a existir uma probabilidade finita de um eletrão inicialmente na orbital de valência do átomo 1 “saltar” (efeito túnel) para a orbital correspondente do átomo 2, e vice-versa. Este processo é quantificado por uma taxa de transição  $\gamma > 0$ , sendo que o Hamiltoniano deste sistema tem a representação

$$\hat{H} \mapsto H = \begin{bmatrix} E_0 & -\gamma \\ -\gamma & E_0 \end{bmatrix}, \quad \text{na base } \{|1\rangle, |2\rangle\}, \quad (1.1)$$

em que  $|1\rangle$  e  $|2\rangle$  representam as orbitais de valência no átomo 1 e 2, respetivamente.

1. Determine o espectro de energia,  $E_{\pm}$ , que o eletrão terá nesta molécula. Mostre que a menor destas energias é sempre inferior à energia do eletrão no átomo isolado:  $E_- \leq E_0$ .
2. Determine o auto-estado associado à menor energia obtida acima.
3. No estado de menor energia, qual é a probabilidade de encontrar o eletrão em cada um dos átomos 1 e 2?
4. Mostre que a matriz  $H$  que representa o Hamiltoniano em (1.1) pode ser escrita como

$$H = \alpha \mathbf{1} + \beta (\sigma_x n_x + \sigma_y n_y + \sigma_z n_z), \quad (1.2)$$

onde  $\mathbf{1}$  é a matriz identidade,  $\beta > 0$ ,  $\sigma_{x,y,z}$  são as matrizes de Pauli, e  $n_x^2 + n_y^2 + n_z^2 = 1$ . Expresse as constantes  $\alpha$ ,  $\beta$  e as componentes  $n_{x,y,z}$  em termos dos parâmetros  $E_0$  e  $\gamma$  deste problema.

5. Verifique que os auto-estados de (1.1) coincidem com os autoestados da matriz  $\sigma \cdot \mathbf{n}$ , onde  $\mathbf{n}$  é o vetor unitário que obteve na questão anterior, e  $\sigma$  é o “vetor de matrizes de Pauli”.
6. Escreva a matriz que representa o operador de evolução temporal,  $\hat{U}(t, 0)$ , na base  $\{|1\rangle, |2\rangle\}$ .
7. Suponha que se prepara o eletrão de forma a que, para  $t = 0$ , o seu vetor de estado é

$$|\psi(0)\rangle = |1\rangle. \quad (1.3)$$

- a) Determine a probabilidade  $\mathcal{P}_2(t)$  de o encontrar no átomo 2 em função do tempo.
- b) Esquematize graficamente a função  $\mathcal{P}_2(t)$ . Interprete este gráfico em termos da localização do eletrão em função do tempo. Explique porque é razoável apelidar o parâmetro  $\gamma$  de “taxa de transição”.
- c) Em que instantes poderemos encontrar o eletrão no átomo 2? Em quais desses instantes estará o eletrão, com certeza, no átomo 2?

### Solution

1. The Hamiltonian matrix is

$$H = \begin{bmatrix} E_0 & -\gamma \\ -\gamma & E_0 \end{bmatrix}.$$

Solving for the eigenvalues:

$$\begin{vmatrix} E_0 - \lambda & \gamma \\ \gamma & E_0 - \lambda \end{vmatrix} = 0 \Leftrightarrow (E_0 - \lambda)^2 = \gamma^2 \Leftrightarrow \lambda = E_0 \pm \gamma$$

Therefore the energy spectrum consists of the two values

$$E_+ = E_0 + \gamma \quad \text{and} \quad E_- = E_0 - \gamma.$$

The lowest energy state for the electron is

$$E_- = E_0 - \gamma \leq E_0 \quad (\text{because } \gamma > 0).$$

So, when the electron is in this eigenstate, the total energy of the system is clearly smaller than it is if the coupling  $\gamma$  is zero (which corresponds to the atoms being far apart).

2. Solving for the eigenvectors of  $H$  we obtain:

$$\begin{bmatrix} E_0 - \lambda & -\gamma \\ -\gamma & E_0 - \lambda \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = 0 \Leftrightarrow \frac{v}{u} = \frac{E_0 - \lambda}{\gamma} \Leftrightarrow \frac{v}{u} = \begin{cases} -1, & \lambda = E_+ \\ 1, & \lambda = E_- \end{cases}$$

and the normalized eigenstates are thus

$$E_{\pm} \longrightarrow |\varepsilon_{\pm}\rangle = \frac{1}{\sqrt{2}}(|1\rangle \mp |2\rangle).$$

Since the lowest energy eigenvalue is  $E_-$ , the corresponding eigenstate is

$$|\varepsilon_-\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle.$$

(This linear combination with positive sign is called a *bonding* state in quantum chemistry.)

3. In the eigenstate  $|\varepsilon_-\rangle$ , the probability of finding the electron in either atom is the same, because

$$\mathcal{P}_1 = |\langle 1|\varepsilon_-\rangle|^2 = \frac{1}{2} \quad \text{and} \quad \mathcal{P}_2 = |\langle 2|\varepsilon_-\rangle|^2 = \frac{1}{2}.$$

4. The Hamiltonian matrix can split into a diagonal and an off-diagonal term as

$$H = \begin{bmatrix} E_0 & -\gamma \\ -\gamma & E_0 \end{bmatrix} = E_0 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \gamma \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = E_0 \mathbf{1} - \gamma \sigma_x.$$

This is a particular form of the given matrix

$$\alpha \mathbf{1} + \beta (\sigma_x n_x + \sigma_y n_y + \sigma_z n_z),$$

with the parameters

$$\alpha = E_0, \quad \beta = \gamma, \quad n_x = -1, \quad n_{y,z} = 0.$$

5. From the previous result we see that the term proportional to  $\alpha$  is just the identity matrix. If we call  $\lambda_H$  to the eigenvalues of  $H$  and  $\lambda_\sigma$  to the eigenvalues of  $\sigma_x$ , we can write

$$\begin{aligned} \text{Eigenvalue of } H &= E_0 - \gamma \times \text{Eigenvalue of } \sigma_x \\ &\downarrow \\ \lambda_H &= E_0 - \gamma \lambda_\sigma. \end{aligned}$$

We also know that the eigenvalues of  $\sigma_x$  are  $\lambda_\sigma = \pm 1$ . Therefore, the lowest ( $E_-$ ) and highest ( $E_+$ ) energy eigenvalues are

$$E_- = E_0 - \gamma \quad (\text{corresponds to } \lambda_\sigma = +1),$$

$$E_+ = E_0 + \gamma \quad (\text{corresponds to } \lambda_\sigma = -1).$$

As a result, the eigenstates associated with these energies will be

$$|\varepsilon_\pm\rangle = |\mp\rangle_x = \frac{1}{\sqrt{2}}|1\rangle \mp \frac{1}{\sqrt{2}}|2\rangle.$$

In this last step we used the result we know from previous problems/lectures for the eigenstates  $|\pm\rangle_x$  of  $\sigma_x$ .

This is indeed what we had obtained earlier in question 2. The advantage is that we showed that the Hamiltonian for this two-level system can be expressed in terms

of a linear combination of the different Pauli matrices (just  $\sigma_x$  in this particular case). This is an example of the general discussion in the lectures, where we showed that we need only to know the eigenstates and eigenvalues of  $\boldsymbol{\sigma} \cdot \mathbf{n}$  to know the complete solution of any two-level system. In the end, we have only to identify what  $\alpha$ ,  $\beta$  and  $\mathbf{n}$  are in terms of the original parameters of the problem. But the spectrum and eigenstates can be written immediately.

6. Since the Hamiltonian is not explicitly dependent on time, we know that the evolution operator will be given by

$$\hat{U}(t, 0) = e^{-i\hat{H}t/\hbar}.$$

Therefore we need to calculate the exponential of the  $H$  matrix. As was shown in the previous question, we can write it as

$$H = \alpha \mathbf{1} + \beta \boldsymbol{\sigma} \cdot \mathbf{n},$$

and hence

$$U(t, 0) = e^{-i\alpha \mathbf{1}t/\hbar - i\beta \boldsymbol{\sigma} \cdot \mathbf{n}t/\hbar}.$$

At this point you should recall one of the results from “Folha de Problemas 1”, which states that, if  $A$  and  $B$  are two commuting matrices, then we can write

$$e^{A+B} = e^A e^B = e^B e^A.$$

The two matrices in the evolution operator are  $\mathbf{1}$  and  $\boldsymbol{\sigma} \cdot \mathbf{n}$ , which obviously commute. We can therefore write

$$U(t, 0) = e^{-i\alpha \mathbf{1}t/\hbar} e^{-i\beta \boldsymbol{\sigma} \cdot \mathbf{n}t/\hbar}.$$

In “Folha de Problemas 1” it was also shown that

$$e^{i\nu \boldsymbol{\sigma} \cdot \mathbf{n}} = \mathbf{1} \cos \nu + i \boldsymbol{\sigma} \cdot \mathbf{n} \sin \nu.$$

We can use this result to write the evolution operator as

$$U(t, 0) = e^{-i\alpha t/\hbar} \left[ \mathbf{1} \cos \frac{\beta t}{\hbar} - i \boldsymbol{\sigma} \cdot \mathbf{n} \sin \frac{\beta t}{\hbar} \right].$$

For our case,  $\alpha = E_0$ ,  $\beta = \gamma$ , and  $\mathbf{n} = -\mathbf{u}_x$ , so that the above becomes

$$U(t, 0) = e^{-iE_0 t/\hbar} \left[ \mathbf{1} \cos \frac{\gamma t}{\hbar} + i \sigma_x \sin \frac{\gamma t}{\hbar} \right].$$

If, for convenience, we define  $\omega \equiv 2\gamma/\hbar$ , and  $\omega_0 \equiv E_0/\hbar$ , the explicit matrix form of  $U(t, 0)$  is

$$U(t, 0) = e^{-i\omega_0 t} \begin{bmatrix} \cos \frac{\omega t}{2} & i \sin \frac{\omega t}{2} \\ i \sin \frac{\omega t}{2} & \cos \frac{\omega t}{2} \end{bmatrix}.$$

7. The given initial state is

$$|\psi(0)\rangle = |1\rangle.$$

a) The desired probability is given by

$$\mathcal{P}_2(t) = |\langle 2 | \psi(t) \rangle|^2.$$

Therefore, we need to know the time-evolved state  $|\psi(t)\rangle$ . Since we calculated explicitly the evolution operator above, we can immediately obtain this state from the relation

$$|\psi(t)\rangle = U(t, 0)|\psi(0)\rangle.$$

In the basis  $\{|1\rangle, |2\rangle\}$  the right-hand side of this equation reads

$$U(t, 0)|\psi(0)\rangle \longrightarrow e^{-i\omega_0 t} \begin{bmatrix} \cos \frac{\omega t}{2} & i \sin \frac{\omega t}{2} \\ i \sin \frac{\omega t}{2} & \cos \frac{\omega t}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = e^{-i\omega_0 t} \begin{bmatrix} \cos \frac{\omega t}{2} \\ i \sin \frac{\omega t}{2} \end{bmatrix},$$

or, back to Dirac notation,

$$|\psi(t)\rangle = \cos \frac{\omega t}{2} |1\rangle + i \sin \frac{\omega t}{2} |2\rangle.$$

(We discarded the global phase factor  $e^{-i\omega_0 t}$  which is irrelevant to define the state.)

Plugging this into the definition of  $\mathcal{P}_2(t)$  we obtain:

$$\mathcal{P}_2(t) = \sin^2 \frac{\omega t}{2} = \frac{1 - \cos \omega t}{2}.$$

b) The function  $\mathcal{P}_2(t)$  oscillates periodically between 0 and 1, with period

$$T = \frac{2\pi}{\omega} = \frac{\pi\hbar}{\gamma}.$$

Physically, this oscillation tells us that the probability of finding the electron in a given atom oscillates in time; this is equivalent to saying that the expectation value of its position oscillates back and forth between the two atoms.

Moreover, because the initial state is  $|\psi(0)\rangle = |1\rangle$ , then half a period of oscillation ( $T/2$ ) corresponds to the time it takes for the electron to transition (i.e., to “jump”) from one atom to the other. Schematically,

$$|\psi(0)\rangle = |1\rangle \xrightarrow{t=T/2} |\psi(T/2)\rangle = |2\rangle \xrightarrow{t=T} |\psi(T)\rangle = |1\rangle \xrightarrow{t=3T/2} |\psi(3T/2)\rangle = |2\rangle \dots$$

The number of such transitions per unit time is proportional to  $1/T \propto \gamma$ . Consequently, the parameter  $\gamma$  controls the *rate* of such transitions, which justifies its designation.

c) At times that are integer multiples of  $T$ , the probability of finding the electron at atom 2 is zero, because

$$\mathcal{P}_2(nT) = \frac{1 - \cos(2n\pi)}{2} = 0, \quad (n = 1, 2, 3, \dots).$$

Hence, if a measurement of its position is made, we will find it on atom 1 with certainty. At any other time, we have  $\mathcal{P}_2(t) \neq 0$ , which means that there is some

finite probability that the electron is at atom 2.

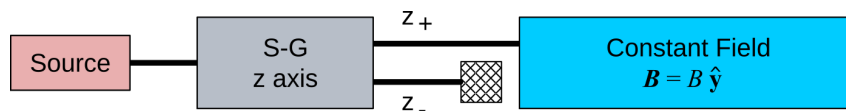
For the electron to be found in atom 2 with *certainty*, we need to have  $\mathcal{P}_2(t) = 1$ , which occurs whenever

$$\cos \omega t = -1 \quad \Rightarrow \quad t = \frac{T}{2} + nT,$$

where  $T = 2\pi/\omega = \pi\hbar/\gamma$  is the period of oscillation defined in the previous question. Therefore, at these times the electron will be found at atom 2 with probability 1 (with certainty).

## Problema 2 | Precessão de spin num campo externo

Considere uma coleção de partículas neutras com spin  $S = 1/2$  que são filtradas por um seletor de Stern-Gerlach (S-G) orientado segundo a direção  $\hat{z}$ , como esquematizado abaixo.



Imediatamente após o seletor, essas partículas entram numa região onde existe um campo magnético constante  $\mathbf{B} = B \hat{y}$ . O Hamiltoniano que descreve a energia de interação entre o spin destas partículas e o campo magnético é dado, genericamente, por

$$\hat{H} = -\hat{\boldsymbol{\mu}} \cdot \mathbf{B} = \omega \hat{\mathbf{S}} \cdot \mathbf{u}_B, \quad \omega \equiv \frac{eB}{m},$$

onde  $\mathbf{u}_B$  é um vetor unitário na direção do campo magnético.

1. Qual é o ket  $|\psi\rangle$  que descreve o estado de spin das partículas à saída do seletor?
2. Invocando o teorema de Ehrenfest, determine quais de entre as projeções  $\hat{S}_x$ ,  $\hat{S}_y$ ,  $\hat{S}_z$  são constantes na região de campo magnético constante.
3. Considere uma das partículas que entra na região de campo constante no instante  $t = 0$ :
  - a) Determine o seu vetor de estado num instante subsequente,  $|\psi(t)\rangle$ , expressando-o na base dos auto-estados de  $\hat{S}_z$ .
  - b) De acordo com o  $|\psi(t)\rangle$  que obteve, em que instantes  $t = T$  estará o spin desta partícula a apontar precisamente segundo a direção positiva de  $\hat{x}$ ?
  - c) Descreva qualitativamente o movimento do spin nesta região de campo constante e interprete o resultado anterior nesse contexto.
4. Se acrescentarmos, à saída da região onde existe o campo  $\mathbf{B}$  constante, um medidor de S-G orientado segundo  $\hat{y}$ , que fração de partículas serão defletidas em cada uma das direções?

## Solution

1. Since they have been selected with spin pointing along the positive  $\hat{z}$  direction, the spin state will be that associated with the positive eigenvalue of  $\hat{S}_z$ :

$$|\psi(0)\rangle = |+\rangle_z.$$

2. We can answer this question without calculating the time evolution explicitly, because we know that an observable will be a constant of the motion if it commutes with the Hamiltonian, and if it is not explicitly time dependent. Therefore, since in this problem

$$\hat{H} = \omega \hat{S}_y,$$

it follows that

$$[\hat{S}_i, \hat{H}] = \omega [\hat{S}_i, \hat{S}_y] = \begin{cases} i\hbar\omega\hat{S}_z, & i = x \\ 0, & i = y \\ -i\hbar\omega\hat{S}_x, & i = z \end{cases}.$$

Hence, only  $\hat{S}$  is a constant of the motion. This is what we expect from the qualitative nature of the motion that the spin undergoes in the region with constant external field: the magnetic moment will be precessing around the field direction, which is  $\hat{y}$  in this case, and hence the projection along  $\hat{y}$  should remain constant.

3. The initial state is  $|\psi(0)\rangle = |+\rangle_z$ .

### a) **Solution strategy I (the general approach):**

To find the state vector at a later time it is convenient to express this initial state in the eigenbasis of the Hamiltonian/energy:

$$|\psi(0)\rangle = \alpha|\varepsilon_+\rangle + \beta|\varepsilon_-\rangle,$$

after which we can directly write the time-evolved state as

$$|\psi(t)\rangle = \alpha e^{-iE_+t/\hbar}|\varepsilon_+\rangle + \beta e^{-iE_-t/\hbar}|\varepsilon_-\rangle.$$

Since

$$\hat{H} = \omega \hat{S}_y \quad \left( \omega = \frac{eB}{m} \right),$$

the eigenvalues of the Hamiltonian are simply

$$E_{\pm} = \pm \frac{\hbar\omega}{2}$$

and its eigenstates are the eigenstates of  $\hat{S}_y$  (or  $\sigma_y$ ) which read, in the basis  $\{|\pm\rangle_z\}$ :

$$|\varepsilon_{\pm}\rangle = |\pm\rangle_y = \frac{1}{\sqrt{2}}|+\rangle_z \pm \frac{i}{\sqrt{2}}|-\rangle_z.$$

The coefficients  $\alpha, \beta$  of  $|\psi(0)\rangle$  introduced above are

$$\alpha = \langle \varepsilon_+ | \psi(0) \rangle = {}_y\langle + | + \rangle_z = \frac{1}{\sqrt{2}}, \quad \beta = \langle \varepsilon_- | \psi(0) \rangle = {}_y\langle - | + \rangle_z = \frac{1}{\sqrt{2}},$$

and the initial state can therefore be written as

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|\varepsilon_+\rangle + \frac{1}{\sqrt{2}}|\varepsilon_-\rangle.$$

From here, the time-evolved state follows directly as

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}e^{-i\omega t/2}|\varepsilon_+\rangle + \frac{1}{\sqrt{2}}e^{i\omega t/2}|\varepsilon_-\rangle = \frac{1}{\sqrt{2}}e^{-i\omega t/2}|+\rangle_y + \frac{1}{\sqrt{2}}e^{i\omega t/2}|-\rangle_y.$$

The last step is to write it back in the  $\{|\pm\rangle_z\}$  basis:

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{2}}e^{-i\omega t/2}|+\rangle_y + \frac{1}{\sqrt{2}}e^{i\omega t/2}|-\rangle_y \\ &= \frac{1}{\sqrt{2}}e^{-i\omega t/2} \left( \frac{1}{\sqrt{2}}|+\rangle_z + \frac{i}{\sqrt{2}}|-\rangle_z \right) + \frac{1}{\sqrt{2}}e^{i\omega t/2} \left( \frac{1}{\sqrt{2}}|+\rangle_z - \frac{i}{\sqrt{2}}|-\rangle_z \right) \\ &= \frac{1}{2}e^{-i\omega t/2} (|+\rangle_z + i|-\rangle_z) + \frac{1}{2}e^{i\omega t/2} (|+\rangle_z - i|-\rangle_z) \\ &= \frac{1}{2} \left( e^{-i\omega t/2} + e^{i\omega t/2} \right) |+\rangle_z + \frac{i}{2} \left( e^{-i\omega t/2} - e^{i\omega t/2} \right) |-\rangle_z \\ &= \cos \frac{\omega t}{2} |+\rangle_z + \sin \frac{\omega t}{2} |-\rangle_z \end{aligned}$$

The final answer is therefore

$$|\psi(t)\rangle = \cos \frac{\omega t}{2} |+\rangle_z + \sin \frac{\omega t}{2} |-\rangle_z. \quad (2.1)$$

### **Solution Strategy II (explicit computation via the evolution operator):**

We know that the time-evolved state ket is related to the initial ket by means of the linear transformation effected by the evolution operator:

$$|\psi(t)\rangle = \hat{U}(t, 0)|\psi(0)\rangle.$$

Since the Hamiltonian of this problem is not parametrically dependent on time, the evolution operator has the following form:

$$\hat{U}(t, 0) = e^{-i\hat{H}t/\hbar}.$$

Replacing the particular Hamiltonian for this problem identified in the previous question, the evolution operator reads

$$\hat{U}(t, 0) = e^{-i\omega t \hat{S}_y/\hbar}.$$

Since the target basis is the eigenbasis of  $\hat{S}_z$ , let us write the state  $|\psi(t)\rangle$  as

$$|\psi(t)\rangle = \alpha(t) |+\rangle_z + \beta(t) |-\rangle_z,$$



where the coefficients  $\alpha(t)$  and  $\beta(t)$  are what we need to determine. Writing the relation between the time-evolved and initial states in the matrix representation, we have

$$\begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} = e^{-i\omega t S_y / \hbar} \begin{bmatrix} \alpha(0) \\ \alpha(0) \end{bmatrix} = e^{-i\omega t S_y / \hbar} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

In this basis the spin projection  $\hat{S}_y$  has the matrix representation

$$S_y = \frac{\hbar}{2} \sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \longrightarrow e^{-i\omega t S_y / \hbar} = e^{-i\frac{\omega t}{2} \sigma_y}.$$

We need now to calculate the  $2 \times 2$  matrix corresponding to  $e^{-i\frac{\omega t}{2} \sigma_y}$ . You will recall from Problem set 1 (or from the lecture notes) that the following identity holds for the exponential function of any linear combination of Pauli matrices:

$$e^{i\gamma \boldsymbol{\sigma} \cdot \mathbf{n}} = \cos \gamma \mathbf{1} + i \sin \gamma \boldsymbol{\sigma} \cdot \mathbf{n} \quad (|\mathbf{n}| = 1). \quad (2.2)$$

Applied to the case at hand, this allows us to write

$$e^{-i\frac{\omega t}{2} \sigma_y} = \cos \frac{\omega t}{2} \mathbf{1} - i \sin \frac{\omega t}{2} \sigma_y = \begin{bmatrix} \cos \frac{\omega t}{2} & -\sin \frac{\omega t}{2} \\ \sin \frac{\omega t}{2} & \cos \frac{\omega t}{2} \end{bmatrix},$$

and therefore

$$\begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix} = \begin{bmatrix} \cos \frac{\omega t}{2} & -\sin \frac{\omega t}{2} \\ \sin \frac{\omega t}{2} & \cos \frac{\omega t}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos \frac{\omega t}{2} \\ \sin \frac{\omega t}{2} \end{bmatrix}.$$

This means that,

$$|\psi(t)\rangle = \cos \frac{\omega t}{2} |+\rangle_z + \sin \frac{\omega t}{2} |-\rangle_z,$$

which, of course, is precisely the result obtained above in eq. (2.1)

**Note:** In this second approach we were able to write the matrix representation of the evolution operator without needing to change to the energy eigenbasis. This was possible because of the identity (2.2), which allows us to convert exponentials of Pauli matrices to linear combinations of Pauli matrices. In general (i.e. for systems other than a 2-level system) the task of directly obtaining the matrix representation for  $\hat{U}(t, t_0)$  without going to the energy eigenbasis is not so easy, and the general approach is preferred.

- b) In quantum-mechanical terms, “pointing along the positive  $\hat{x}$  direction” means that if we measure  $\hat{S}_x$  the outcome will be  $+\hbar/2$  with absolute certainty (probability 1). So, to answer the question we need to find  $t = T$  such that

$$|_x \langle + | \psi(T) \rangle|^2 = 1.$$

Taking the solution obtained in (2.1) above for the time-evolved state, and recalling that

$$|+\rangle_x = \frac{1}{\sqrt{2}} |+\rangle_z + \frac{1}{\sqrt{2}} |-\rangle_z,$$

we have:

$$|_x \langle + | \psi(T) \rangle|^2 = 1 \quad \Leftrightarrow \quad \left| \cos \frac{\omega T}{2} + \sin \frac{\omega T}{2} \right|^2 = 2 \quad \Leftrightarrow \quad \sin \omega T = 1.$$

Therefore, when

$$t = T = \frac{\pi}{2\omega} + \frac{2\pi}{\omega}n \quad (n = 0, 1, 2, 3, \dots)$$

the spin will be in the positive eigenstate of  $\hat{S}_x$ , which corresponds to pointing along the positive  $\hat{x}$  direction.

- c) The motion described by a magnetic moment in the presence of a constant magnetic field consists a precession around the field direction with constant angular velocity  $\omega$ , and keeping the projection with the field direction constant. In the current problem the precessing spins rotate in the  $Oxz$  plane. If we make a sketch of this precession we can easily see that, if the spin starts pointing along  $u_z$  at  $t = 0$ , we expect it to point along  $\hat{x}$  after  $\frac{1}{4}$  of a precession period. This means that we would expect it to be directed along  $\hat{x}$  at the times

$$T = \frac{1}{4} \times \frac{2\pi}{\omega} + \frac{2\pi}{\omega}n = \frac{\pi}{2\omega} + \frac{2\pi}{\omega}n$$

which is what we obtained above.

4. In the region containing the constant magnetic field, the spin state is given by the result (2.1) above. The S-G device along  $\hat{y}$  will measure  $S_y$ . The probability of each outcome is given by

$$\begin{aligned} \mathcal{P}(S_y \rightarrow \frac{\hbar}{2}) &= |\langle + | \psi(t) \rangle|^2 \\ &= \left| \left[ \frac{1}{\sqrt{2}} \langle + | - \frac{i}{\sqrt{2}} \langle + | \right] \left[ \cos \frac{\omega t}{2} | + \rangle_z + \sin \frac{\omega t}{2} | - \rangle_z \right] \right|^2 \\ &= \frac{1}{2} \left| \cos \frac{\omega t}{2} - i \sin \frac{\omega t}{2} \right|^2 = \frac{1}{2}, \end{aligned}$$

and, of course,

$$\mathcal{P}(S_y \rightarrow -\frac{\hbar}{2}) = \frac{1}{2}.$$

Note that these probabilities are independent of time (because the time dependence cancels out). Consequently, there's an equal probability for these particles to have either positive or negative spin projection along  $\hat{y}$ . This means that, when sent through a S-G device oriented along  $\hat{y}$ , half will be deflected in each direction.

(Note: since the result above is independent of time, it doesn't matter how much time the particles spend in the region with the constant  $B$  field, or how big that region is.)