Phys 321
Spring 2023

Quantum Theory I: Homework 11

Due: 10 March 2023

1 Generating rotations

The aim of this problem is to construct a specific rotation in two ways and to verify that these give the same result.

a) Recall that a rotation through angle φ about the axis $\hat{\mathbf{n}}$ is represented by the following operator on kets

$$\hat{R}(\varphi \boldsymbol{n}) := e^{-i\varphi/2} \, |+\hat{\boldsymbol{n}}\rangle \langle +\hat{\boldsymbol{n}}| + e^{+i\varphi/2} \, |-\hat{\boldsymbol{n}}\rangle \langle -\hat{\boldsymbol{n}}| \, .$$

Use this to determine the matrix representation of $\hat{R}(\varphi \boldsymbol{x})$.

b) Determine, by exponentiating explicitly, the matrix representing the operator $e^{-i\varphi\hat{\sigma}_x/2}$ where the matrix representing $\hat{\sigma}_x$ in the $\{|+\hat{\boldsymbol{z}}\rangle, |-\hat{\boldsymbol{z}}\rangle\}$ basis is

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Verify that

$$\hat{R}(\varphi \boldsymbol{x}) = e^{-i\varphi\hat{\sigma}_x/2}.$$

2 Evolution under a magnetic field in the y direction

A spin-1/2 particle of mass m, charge q and with g-factor g is subjected to an SG $\hat{\boldsymbol{z}}$ measurement and emerges with $S_z = +\hbar/2$. It is then subjected to a constant magnetic field, $\mathbf{B} = B_0\hat{\mathbf{y}}$ for time t.

a) Determine the state of the particle at time t after the field was first applied.

b) Determine the probability that a SG $\hat{\boldsymbol{z}}$ device will yield $S_z = \hbar/2$ at time t after the field was first applied.

3 Engineering an evolution

A spin-1/2 particle evolves according to

$$|\Psi(t)\rangle = \cos\left(\frac{\omega t}{2}\right)|+\hat{\boldsymbol{z}}\rangle + \sin\left(\frac{\omega t}{2}\right)|-\hat{\boldsymbol{z}}\rangle$$

where $\omega > 0$.

a) Which of the following represents the direction of a constant magnetic field that could produce this time evolution? Explain your answer.

   i) $\mathbf{B} = B_0\hat{\mathbf{x}}$

   ii) $\mathbf{B} = B_0\hat{\mathbf{y}}$

   iii) $\mathbf{B} = B_0\hat{\mathbf{z}}$

   iv) $\mathbf{B} = B_0\left(\frac{1}{\sqrt{2}}\hat{\mathbf{x}} + \frac{1}{\sqrt{2}}\hat{\mathbf{z}}\right)$

A spin-1/2 particle evolves according to

$$|\Psi(t)\rangle = \cos\left(\frac{\omega t}{2}\right)|+\hat{\boldsymbol{z}}\rangle + e^{i\pi/4}\sin\left(\frac{\omega t}{2}\right)|-\hat{\boldsymbol{z}}\rangle$$

where $\omega > 0$.

b) Which of the following represents the direction of a constant magnetic field that could produce this time evolution? Explain your answer.

   i) $\mathbf{B} = B_0\hat{\mathbf{x}}$

   ii) $\mathbf{B} = B_0\hat{\mathbf{y}}$

   iii) $\mathbf{B} = B_0\hat{\mathbf{z}}$

   iv) $\mathbf{B} = B_0\left(\frac{1}{\sqrt{2}}\hat{\mathbf{x}} + \frac{1}{\sqrt{2}}\hat{\mathbf{z}}\right)$

   v) $\mathbf{B} = B_0\left(\frac{1}{\sqrt{2}}\hat{\mathbf{x}} + \frac{1}{\sqrt{2}}\hat{\mathbf{y}}\right)$

   vi) $\mathbf{B} = B_0\left(\frac{1}{\sqrt{2}}\hat{\mathbf{x}} - \frac{1}{\sqrt{2}}\hat{\mathbf{y}}\right)$

4 Evolution under multiple magnetic fields

A spin-1/2 particle of mass m, charge q and with g-factor g undergoes the following.

Stage 1 At time $t = 0$ particle is prepared in the state $|\psi(t=0)\rangle = |+\hat{\boldsymbol{x}}\rangle$.

Stage 2 After the preparation the particle is subjected to a constant magnetic field, $\vec{B} = B_0 \hat{\mathbf{z}}$ for time t. The effects of the field be described in terms of the Hamiltonian

$$\hat{H} = \frac{\hbar\omega_0}{2}\hat{\sigma}_z$$

where $\omega_0 = -gqB_0/2m$ and, in the $\{|+\hat{\boldsymbol{z}}\rangle, |-\hat{\boldsymbol{z}}\rangle\}$ basis,

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Stage 3 The particle is subjected to an SG$\,\hat{\boldsymbol{x}}$ measurement.

a) Find the matrix representation, in the $\{|+\hat{\boldsymbol{z}}\rangle, |-\hat{\boldsymbol{z}}\rangle\}$ basis, of the evolution operator $\hat{U}(t)$, which describes the effects of the constant magnetic field in stage 2.

b) Determine the ket in terms of $\{|+\hat{\boldsymbol{z}}\rangle, |-\hat{\boldsymbol{z}}\rangle\}$ basis, that represents the state of the particle at the end of stage 2.

c) Determine the probability that the outcome of the stage 3 measurement is $S_x = +\hbar/2$.

5 Expectation values of spin observables in NMR

Nuclear magnetic resonance (NMR) is a technique for manipulating nuclear spins within molecules. Certain atomic nuclei, such as H,^{13}C, have spin 1/2, which interacts with magnetic fields in the ways which have been described in class. Modern NMR experiments typically consist of three stages. In the *preparation stage*, the nuclear spins relax to equilibrium in the presence of a strong magnetic field $\mathbf{B_0} = B_0\hat{\mathbf{z}}$ and there is little variation as to how this is accomplished (merely wait for long enough). In the *"pulse sequence" stage* a variety of additional external magnetic fields are applied, interspersed with periods of free evolution under the $\mathbf{B_0}$ field and various internuclear interactions. In the (data) *acquisition stage* the nuclear spins precess freely in the $\mathbf{B_0}$ field (all others are off during this phase) while slowly relaxing toward equilibrium. During the acquisition stage the NMR spectrometer measures both $\langle S_x\rangle$ and $\langle S_y\rangle$ as functions of the time elapsed since the start of the acquisition stage, t. This data can be manipulated mathematically to produce quantities such as $\sqrt{\langle S_x\rangle^2 + \langle S_y\rangle^2}$ or, more commonly, $\langle S_x\rangle + i\langle S_y\rangle$. This question concerns the acquisition stage for an ensemble of spin-1/2 particles.

Consider an ensemble of spin-1/2 particles, such that, **immediately after the end of the "pulse sequence" stage,** each is in the state

$$|+\hat{\boldsymbol{n}}\rangle = \cos\left(\frac{\theta}{2}\right)|+\hat{\boldsymbol{z}}\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\,|-\hat{\boldsymbol{z}}\rangle.$$

As a preparatory step, ignore the precession of the nuclear spins during the acquisition stage. Rather, suppose that every particle undergoes an instantaneous transformation described via

$$\hat{U} = e^{-i\varphi\,\hat{\sigma}_z/2}$$

where φ is an arbitrary angle and this is followed by measurement of $\langle S_x\rangle$ and $\langle S_y\rangle$.

a) Determine $\langle S_x \rangle$ for the ensemble of particles. Does this depend on φ?

b) Determine $\langle S_y \rangle$ for the ensemble of particles. Does this depend on φ?

c) The two expectation values $\langle S_x \rangle$ and $\langle S_y \rangle$ are real and can be incorporated into a real two dimensional vector $\mathbf{S} = \langle S_x \rangle \hat{\mathbf{x}} + \langle S_y \rangle \hat{\mathbf{y}}$. Sketch this vector, indicating φ.

Now consider an ensemble of spin-1/2 particles, each in the state $|+\hat{\boldsymbol{n}}\rangle$ **immediately prior to the acquisition.** The Hamiltonian which determines (but is not equal to) the evolution operator during the acquisition period is

$$\hat{H} = \frac{\hbar\omega_0}{2}\,\hat{\sigma}_z.$$

d) Determine $\langle S_x \rangle (t), \langle S_y \rangle (t)$ for the ensemble of particles where t is the time elapsed since the start of the acquisition stage. Do these depend on ω_0 or t? Could you determine $|+\hat{\boldsymbol{n}}\rangle$ from these measurements (i.e. could you determine θ and ϕ which determine the state)? If so, how? If not, why not?