Homework problems, set 1:

Operators, qubits and simple operations

Hand in before 4/4-2018.
Maximum number of points: 62.

1 Qubit time-evolution

The Pauli matrices

$$\hat{\sigma}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \hat{\sigma}_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \hat{\sigma}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1}$$

together with the unit matrix $\hat{\sigma}_0 = \mathbb{1}$ span the set of 2×2 matrices. Thus, we can write

$$\hat{H} = \vec{\mathbf{c}} \cdot \vec{\sigma} = c_0\hat{\sigma}_0 + c_1\hat{\sigma}_1 + c_2\hat{\sigma}_2 + c_3\hat{\sigma}_3 \tag{2}$$

for any 2×2 matrix $\hat{H}$.

a) What are the constrains on the vector $\vec{\mathbf{c}} = (c_0, c_1, c_2, c_3)$ making the matrix $\hat{H}$ hermitian, symmetric or unitary? (3p)

b) Assume $\hat{H}$ is the Hamiltonian generating the time-evolution for a qubit. The time-evolution operator is then (we put $\hbar = 1$)

$$\hat{U}(t) = e^{-i\hat{H}t}. \tag{3}$$

Write down $\hat{U}(t)$ as a 2×2 matrix by using the properties of the Pauli matrices. (4p)

c) If the initial qubit state is

$$|\psi(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{4}$$

give the time-evolved state $|\psi(t)\rangle$ for the cases: *i)* $\vec{\mathbf{c}} = (\omega_0, g, 0, 0)$, *ii)* $\vec{\mathbf{c}} = (\omega_0, 0, g, 0)$ and *iii)* $\vec{\mathbf{c}} = (\omega_0, 0, 0, g)$. Explain with words how the qubit state evolves on the Bloch sphere. (3p)

d) The same as the previous problem but for the initial state (2p)

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left[\begin{array}{c} 1 \\ 1 \end{array}\right]. \tag{5}$$

2 Single qubit gates

In atomic physics one is often talking about π- or $\pi/2$-pulses. The name comes from the fact that one shines a laser pulse on an atom such that two electronic states in the atoms are (dipole) coupled by the laser, and the 'area' of the pulse, $\int dt\,\Omega(t) = A$, equals either π or $\pi/2$. The corresponding unitary operator is given by

$$\hat{U}_A = e^{-i\hat{\sigma}_x A/2}. \tag{6}$$

a) Write down the closed form expressions for $\hat{U}_A$ for the π- ($A = \pi$) and $\pi/2$-pulse ($A = \pi/2$). (2p)

b) For a general qubit state

$$|\psi\rangle = \cos(\theta/2)\,|0\rangle + \sin(\theta/2)\,e^{i\varphi}|1\rangle = \left[\begin{array}{c} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{array}\right], \tag{7}$$

explain what the two pulses (transformations) are doing to these states on the Bloch sphere. (2p)

c) Two other common single qubit gate operations are the *Hadamard* and the *phase* gates defined by the unitaries

$$\hat{U}_H = \frac{1}{\sqrt{2}}\left[\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array}\right], \qquad \hat{U}_\phi = \left[\begin{array}{cc} 1 & 0 \\ 0 & e^{i\phi} \end{array}\right] \tag{8}$$

respectively. Going back to the first problem and Eqs. (2) and (3), find the vectors $\vec{\mathbf{c}}$ which generates these gates, given some time t. (2p)

3 Rotations

If we rescale the Pauli-matrices accordingly,

$$\hat{S}_x = \frac{\hat{\sigma}_1}{2}, \qquad \hat{S}_y = \frac{\hat{\sigma}_2}{2}, \qquad \hat{S}_z = \frac{\hat{\sigma}_3}{2}, \tag{9}$$

the new operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ obey the standard angular momentum commutation relations. Now, having worked out problem 1 and 2, it should be clear that any operation

$$\hat{U}_{\hat{e}_{\vec{\mathbf{n}}}}(\varphi) = e^{i\varphi\hat{e}_{\vec{\mathbf{n}}}\cdot\vec{S}}, \tag{10}$$

with $\hat{e}_{\vec{\mathbf{n}}}$ a unit vector in the direction $\vec{\mathbf{n}}$ and $\vec{S} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$, acts as a rotation of the state $|\psi\rangle$. In particular, you will demonstrate in this problem that the transformation realises a φ-rotation about the $\hat{e}_{\vec{\mathbf{n}}}$-axis.

a) Give a closed expression for $\hat{U}_{\hat{e}_{\vec{\mathbf{n}}}}(2\pi) = \exp(i2\pi\hat{e}_{\vec{\mathbf{n}}}\cdot\vec{S})$. Comment on this result. (2p)

b) Can you, without explicit calculations, explain which qubit states that will be the eigenstates of $\hat{U}_{\hat{e}_{\vec{\mathbf{n}}}}(\varphi) = \exp(i\varphi\hat{e}_{\vec{\mathbf{n}}}\cdot\vec{S})$? (2p)

c) As for any rotations, *e.g.* in euclidian space, we can either consider rotating the vectors (states) or the coordinate system. Thus, $\hat{U}_{\vec{\mathbf{n}}}(\varphi)$ is either acting on the state $|\psi\rangle$ or on the Pauli matrices. Calculate the following rotations (3p)

$$\begin{aligned}
\hat{\sigma}'_\alpha &= \hat{U}_{\hat{e}_x}(\varphi)\hat{\sigma}_z\hat{U}^\dagger_{\hat{e}_x}(\varphi), \\
\hat{\sigma}'_z &= \hat{U}_{\hat{e}_x}(\varphi)\frac{1}{\sqrt{2}}\left(\hat{\sigma}_y - \hat{\sigma}_z\right)\hat{U}^\dagger_{\hat{e}_x}(\varphi), \\
\hat{\sigma}'_{\vec{\mathbf{n}}} &= \hat{U}_{\hat{e}_{\vec{\mathbf{n}}}}(\varphi)\left(\hat{e}_{\vec{\mathbf{n}}}\cdot\vec{\sigma}\right)\hat{U}^\dagger_{\hat{e}_{\vec{\mathbf{n}}}}(\varphi).
\end{aligned} \tag{11}$$

d) Imagine an experimental situation: Our qubit is an atom where the logic states $|0\rangle$ and $|1\rangle$ are represented by two electronic Zeeman levels corresponding to different principle quantum numbers n. One can measure the population in the two states via *state-selected florescence*, *i.e.* it is possible to measure $\hat{\sigma}_z$. In this scenario, the basis $\{|0\rangle, |1\rangle\}$ makes the natural one and one refers to it as the *computational basis*. However, we may want to measure say $\hat{\sigma}_x$ or $\hat{\sigma}_y$ instead. Assume we can perform any qubit rotation, $\hat{U}_{\hat{e}_{\vec{\mathbf{n}}}}(\varphi)$, and we can directly measure $\hat{\sigma}_z$, how should we do to measure $\hat{\sigma}_x$ or $\hat{\sigma}_y$? (3p)

4 Group properties

Group theory and symmetries play an important role in the understanding of quantum physics. In this problem we explore some of the very basic concepts of group theory.

a) Show which of the following that form groups

(i) The set Z of integers under addition. (1p)

(ii) The set Z of integers under multiplication. (1p)

(iii) The set R of real numbers under multiplication. (1p)

(iv) The set S_n of permutations of n objects. (1p)

(v) The set Z_n of integers modulo n under addition. (1p)

(vi) The set C_n of in-plane rotations by an angle $2\pi k/n$ for $k \in Z$. (1p)

b) For any two elements g_1 and g_2 of a group $\mathcal{G}$, the group is said to be *Abelian* if $g_1 g_2 = g_2 g_1$, and *non-Abelian* otherwise. Furthermore, the *order* of the group is the number of elements of the group. For the groups of the a) problem, determine the order of them and whether they are Abelian or not. (3p)

c) The idea of group *isomorphism* is central for the theory of groups. If two groups $\mathcal{G}_1$ and $\mathcal{G}_2$ are *isomorphic* they have the same order and "structure", *i.e.* there exist a one-to-one function f between the two groups that preserves the multiplication; for $a \in \mathcal{G}_1$ then $f(a) \in \mathcal{G}_2$, and if a, $b \in \mathcal{G}_1$ such that $ab = c \in \mathcal{G}_1$ then we have $f(a)f(b) = f(c) \in \mathcal{G}_2$. Are any of the groups in problem a) isomorphic? (3p)

d) Assume that $\mathcal{G}$ is a group and its elements $g \in \mathcal{G}$. If there is a subset of elements $\{h \in \mathcal{G}\}$ which also forms a group, then this is called a sub-group. Futhermore, the center $\mathcal{Z}$ of a group $\mathcal{G}$ is defined as $=\{z \in \mathcal{G}|\, zg = gz \;\; \forall\; g \in \mathcal{G}\}$. Prove that $\mathcal{Z}$ is a subgroup of $\mathcal{G}$. (3p)

5 The $SU(2)$ and $SU(3)$ groups

The Pauli matrices together with the commutation relation

$$[\hat{\sigma}_i, \hat{\sigma}_j] = i2\varepsilon_{ijk}\hat{\sigma}_k \tag{12}$$

defines a *Lie algebra*. The operators $\hat{\sigma}_i$ ($i = 1, 2, 3$) are called *generators* of the $SU(2)$ group[1], meaning that all 2×2 unitary matrix $\hat{U}$ with determinant equal to unity can be written as exponentials of the matrices $\hat{\sigma}_i$, *i.e.* $\hat{U}_{\vec{\mathbf{c}}} = \exp\left(i\vec{\mathbf{c}} \cdot \vec{\sigma}\right)$ with $\vec{\mathbf{c}} = (c_1, c_2, c_3)$. Furthermore, a *Casimir operator* $\hat{C}$ is a matrix that commutes with all the generators.

a) Prove that $\det\left[\hat{U}_{\vec{\mathbf{c}}}\right] = 1$. (2p)

b) Prove that the set of matrices $\left\{\hat{U}_{\vec{\mathbf{c}}}\right\}$ forms a group. (2p)

c) The Lie algebra spanned by the Pauli matrices has one Casimir operator, find it! (2p)

The group $SU(3)$ of unitary 3×3 matrices with unit determinant can be generated from the *Gell-Mann matrices*

$$\hat{\lambda}_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \hat{\lambda}_2 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \hat{\lambda}_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\hat{\lambda}_4 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \hat{\lambda}_5 = \begin{bmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix}, \quad \hat{\lambda}_6 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \tag{13}$$

$$\hat{\lambda}_7 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad \hat{\lambda}_8 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}.$$

The mutual commutation relations of the Gell-Mann matrices obey the $SU(3)$ Lie algebra.

d) Consider all $n \times n$ unitary matrices, show that they form a group, and show also that all $n \times n$ unitary matrices with unit determinant forms a sub-group. (3p)

e) The Gell-Mann matrices (13) are the generators for the $SU(3)$ group, *i.e.* any 3×3 unitary matrix with unit determinant can be written as $\hat{U}_{\vec{\mathbf{d}}} = \exp\left(i\vec{\mathbf{d}} \cdot \vec{\lambda}\right)$ with the same notation as above. By looking at the expressions for the $\hat{\lambda}_i$ matrices, can you show that there are three $SU(2)$ sub-groups of $SU(3)$? (3p)

[1]The S in $SU(2)$ stands for *special* marking that the determinant is equal to 1.

6 "Split-operator" and Trotter decomposition

A useful operator identity is the *Baker-Hausdorff formula* (or its generalisation)

$$e^{(\hat{A}+\hat{B})t} = e^{t\hat{A}}e^{t\hat{B}}e^{-\frac{t^2}{2}[\hat{A},\hat{B}]}e^{\frac{t^3}{6}\left(2[\hat{B},[\hat{A},\hat{B}]]+[\hat{A},[\hat{A},\hat{B}]]\right)}\dots. \tag{14}$$

If $[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0$ we recover the standard Baker-Hausdorff formula.

a) Use the above formulate to prove the *Trotter decomposition* (3p)

$$e^{-i\left(\hat{A}+\hat{B}\right)t} = \lim_{n\to\infty}\left[e^{-i\frac{\hat{A}t}{n}}e^{-i\frac{\hat{B}t}{n}}\right]^n. \tag{15}$$

b) If we consider n to be finite, but still $n \gg 1$ we can use the Trotter decomposition as an approximation for numerically simulating time-evolution;

$$\hat{U}(t) \approx \left[e^{-i\frac{\hat{A}t}{n}}e^{-i\frac{\hat{B}t}{n}}\right]^n. \tag{16}$$

For example, let $dt = t/n$ and the final time of the simulation is thereby $T = ndt = t$, and take $\hat{A} = \frac{\hat{p}^2}{2m}$ and $\hat{B} = V(\hat{x})$. Then we have $\psi(x,dt) = \exp\left(-i\frac{\hat{p}^2}{2m}dt\right)\exp(-iV(\hat{x})dt)\psi(x,0)$, and since the operator $V(\hat{x})$ is diagonal in the x-representation it is easy to apply, and the operator $\hat{p}$ is diagonal in the p-representation one applies the Fourier transform before applying $\exp\left(-i\frac{\hat{p}^2}{2m}dt\right)\exp(-iV(\hat{x})dt)$.

Show, however, that a slightly better approximation, for finite n, is to split the exponential as (4p)

$$\hat{U}(t) \approx \left[e^{-i\frac{\hat{B}t}{2n}}e^{-i\frac{\hat{A}t}{n}}e^{-i\frac{\hat{B}t}{2n}}\right]^n. \tag{17}$$