

Quantum Mechanics (Physics 212A) Fall 2015 Assignment 2

Due 12:30pm Wednesday, October 14, 2015

1. Paulis

(a) Show (from the matrix representations) that

$$\sigma^i \sigma^j = i\epsilon_{ijk} \sigma^k + \delta_{ij} \mathbb{1} \quad (1)$$

where ϵ_{ijk} is the completely antisymmetric tensor in three indices, with

$$\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = +1, \epsilon_{231} = \epsilon_{132} = \epsilon_{321} = -1$$

and $\epsilon_{ijk} = 0$ if any two indices are equal. (On the right hand side of (1), we are using the Einstein summation convention.)

(b) Use (1) to show that

$$(\tilde{n} \cdot \vec{\sigma})^2 = \mathbb{1}$$

if \tilde{n} is a unit vector.

(c) Show by series expansion that

$$e^{i\tilde{n} \cdot \vec{\sigma} \theta} = \cos \theta \mathbb{1} + i \sin \theta \tilde{n} \cdot \vec{\sigma}.$$

2. Projector onto spin-up along \tilde{n} .

Show that the projector onto the state of a qbit $|\uparrow_{\tilde{n}}\rangle$ with spin up along an arbitrary unit vector \tilde{n} (defined by the relation $\tilde{n} \cdot \vec{\sigma} |\uparrow_{\tilde{n}}\rangle = |\uparrow_{\tilde{n}}\rangle$)¹ can be written as

$$|\uparrow_{\tilde{n}}\rangle \langle \uparrow_{\tilde{n}}| = \frac{1}{2} (1 + \tilde{n} \cdot \vec{\sigma}).$$

That is: check that the operator on the RHS is hermitian, squares to itself, and acts correctly on a basis.

3. Functions of operators.

Given a linear operator A , define the ‘superoperator’ ad_A , which implements the adjoint action of A , by

$$\text{ad}_A(B) = [A, B].$$

¹Sometimes it is called $|+\tilde{n}\rangle \equiv |\uparrow_{\tilde{n}}\rangle$.

(a) Show that this operator is a derivation,

$$\text{ad}_A(BC) = (\text{ad}_A B)C + B(\text{ad}_A C) . \quad (2)$$

That is: it satisfies a product rule, like a derivative.

(b) Show that (for finite-dimensional Hilbert spaces) one can “integrate by parts” under the trace:

$$\text{tr} [B \text{ad}_A C] = -\text{tr} [(\text{ad}_A B) C] .$$

(c) We are going to derive the formula

$$e^{A+B} = e^A e^{\hat{C}_A(B)} , \quad (3)$$

where

$$\hat{C}_A = \int_0^1 ds e^{-s \text{ad}_A} = \frac{e^{\text{ad}_A} - 1}{\text{ad}_A} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \text{ad}_A^n = 1 - \frac{1}{2} \text{ad}_A + \frac{1}{6} \text{ad}_A^2 + \dots .$$

To do this, consider the operator-valued function

$$G(s) = e^{-sA} e^{s(A+B)} .$$

Derive a first-order differential equation for $G(s)$ and solve it.

(d) For the special case where $[A, B] = c$ is a c -number show that (4) implies

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}c} . \quad (4)$$

4. Time evolution of a two-level system. [Le Bellac]

Consider the Hamiltonian

$$H = \hbar \begin{pmatrix} A & B \\ B & -A \end{pmatrix}$$

in the basis $|0\rangle \equiv |\uparrow\rangle, |1\rangle \equiv |\downarrow\rangle$, where A, B are real numbers. Set $\hbar = 1$. You know the eigensystem of this matrix from our discussion of Pauli gymnastics. It is useful to write it in terms of Ω, θ defined by

$$\Omega = 2\sqrt{A^2 + B^2}, \quad \tan \theta = \frac{B}{A} .$$

(a) The state vector at time t can be written as

$$|\varphi(t)\rangle = c_+(t)|0\rangle + c_-(t)|1\rangle .$$

Find a system of ODEs for the components $c_{\pm}(t)$ that follow from the Schrödinger equation.

- (b) Decompose the initial state $|\varphi(t=0)\rangle$ in the energy eigenbasis ($H|\epsilon_{\pm}\rangle = \epsilon_{\pm}|\epsilon_{\pm}\rangle$):

$$|\varphi(t=0)\rangle = \sum_{\pm} a_{\pm} |\epsilon_{\pm}\rangle .$$

Express $c_{+}(t)$ in terms of the coefficients a_{\pm} .

- (c) Suppose $c_{+}(0) = 0$. Find a_{\pm} (up to a phase) in terms of A, B (or rather, Ω and θ). Find the probability of finding the system in the state $|\uparrow\rangle$ at time t .

5. **The variational method.** [Le Bellac]

- (a) Let $|\varphi\rangle$ be a vector (not necessarily normalized) in the Hilbert space of states, and let \mathbf{H} be a Hamiltonian of interest. The expectation value $\langle \mathbf{H} \rangle_{\varphi}$ is

$$\langle \mathbf{H} \rangle_{\varphi} = \frac{\langle \varphi | \mathbf{H} | \varphi \rangle}{\langle \varphi | \varphi \rangle} .$$

Show that if the minimum and maximum of this quantity on the space of states are obtained for $|\varphi\rangle = |\varphi_m\rangle$ and $|\varphi\rangle = |\varphi_M\rangle$ respectively, then $|\varphi_{m,M}\rangle$ are eigenvectors of \mathbf{H} with the smallest and largest eigenvalues in the spectrum, E_m, E_M .

- (b) Suppose the vector $|\varphi\rangle$ depends on a parameter α : $|\varphi\rangle = |\varphi(\alpha)\rangle$. Show that if

$$\partial_{\alpha} \langle \mathbf{H} \rangle_{\varphi(\alpha)} |_{\alpha=\alpha_0} = 0$$

then $E_m \leq \langle \mathbf{H} \rangle_{\varphi(\alpha_0)}$ if α_0 is a minimum of $\langle \mathbf{H} \rangle_{\varphi(\alpha)}$. Similarly, show that $E_M \geq \langle \mathbf{H} \rangle_{\varphi(\alpha_0)}$ if α_0 is a maximum of $\langle \mathbf{H} \rangle_{\varphi(\alpha)}$.

This fact forms the basis of an approximation method called the variational method. If you have a good guess for the form of the groundstate, you can find the best approximation within that family of states, and it produces a bound on the correct groundstate energy.

- (c) Consider the special case of $\dim \mathcal{H} = 2$, with Hamiltonian

$$\mathbf{H} = \begin{pmatrix} a + c & b \\ b & a - c \end{pmatrix}$$

with a, b, c real. Parametrizing the variational state as

$$|\varphi(\alpha)\rangle = \begin{pmatrix} \cos \alpha/2 \\ \sin \alpha/2 \end{pmatrix} ,$$

find the values of $\alpha = \alpha_0$ which extremize the expectation value of the Hamiltonian. Show that this reproduces the eigenstates:

$$|\chi_{+}\rangle = \begin{pmatrix} \cos \theta/2 \\ \sin \theta/2 \end{pmatrix} , \quad |\chi_{-}\rangle = \begin{pmatrix} -\sin \theta/2 \\ \cos \theta/2 \end{pmatrix} .$$

where $\tan \theta = b/c$.

6. **The Feynman-Hellmann theorem.** Suppose the Hamiltonian depends on a parameter s , $\mathbf{H} = \mathbf{H}(s)$. Suppose $E(s)$ is a non-degenerate eigenvalue with normalized eigenvector $|\phi(s)\rangle$. Show that

$$\partial_s E(s) = \langle \phi(s) | \partial_s \mathbf{H}(s) | \phi(s) \rangle.$$