Homework Assignment #8

Math Methods

Due: Monday, Novermber 1st, midnight

Instructions:

Reading Quiz #6 is due by the start of class on Wednesday, November 10th. It covers the rest of chapter 4 (except normal modes).

Below is the a list of questions and problems from the texbook. It is not sufficient to simply obtain the correct answer. You must also explain your calculation, and each step so that it is clear that you understand the material.

Homework should be written legibly, on standard size paper. Do not write your homework up on scrap paper. If your work is illegible, it will be given a zero.

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1. Byron & Fuller, Chapter 4, problem 4.
2. Byron & Fuller, Chapter 4, problem 6.
3. Byron & Fuller, Chapter 4, problem 17.
4. Consider the three vectors

$$\begin{aligned}\vec{v}_1 &= \hat{\imath} + \hat{\jmath} + \hat{k} \\ \vec{v}_2 &= \hat{\imath} + 2\,\hat{\jmath} + 3\,\hat{k} \\ \vec{v}_3 &= \hat{\imath} + 2\,\hat{\jmath} + \hat{k}\end{aligned}$$

   Perform Gram-Schmidt orthonormalization on the set $\{\vec{v}_1, \vec{v}_2, \vec{v}_3\}$, starting with $\vec{v}_1$ as your first basis vector.

5. *Spinors:* Spin is often introduced in undergraduate physics courses simply as a 2-vector. This can be a bit confusing. Let's see why.

   In problem 28 from chapter 3 you learned that the operator $\hat{\mathcal{T}} \equiv e^{a\,\partial_x}$ is the *translation operator*, in that

$$\hat{\mathcal{T}}\,f(x) = f(x+a)$$

   In quantum mechanics this is written as:

$$\hat{\mathcal{T}} \equiv e^{ia\hat{p}_x/\hbar}$$

   since $\hat{p}_x = -i\hbar\partial_x$. This is stated as "the momentum operator is the *generator* of translations." In a similar fashion one can show that the generator of infinitesimal[1] rotations about the z axis is the operator $\hat{L}_z$, the operator which gives the z component of the angular momentum, so that to rotate something in quantum mechanics about the z-axis by an infinitesimal angle $\Delta\phi$ one can use the operator.

$$\hat{R}_z = e^{-i\hat{L}_z\Delta\phi/\hbar}$$

[1] We have to be a little careful since while translation operators are Abelian, rotation operators are not.

What about spin?

By analogy, the operator to rotate a spin about an arbitrary axis defined by the unit vector $\hat{n}$, is given by:

$$\hat{R}_{\hat{n}}(\Delta\phi) = \exp\left(\frac{-i\hat{\mathcal{S}}\cdot\hat{n}\,\Delta\phi,}{\hbar}\right) = \exp\left(\frac{-i\hat{\sigma}\cdot\hat{n}\,\Delta\phi}{2}\right)$$

where we have set the spin operator $\hat{\mathcal{S}} \to \hbar\hat{\sigma}/2$, the spin-1/2 operator made from the three Pauli matrices. Note that we have implicitly assumed our basis to the along the z-axis, with basis states:

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad\qquad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

(a) Show that

$$(\hat{\sigma}\cdot\hat{n})^k = \begin{cases} 1 & \text{k is even} \\ \hat{\sigma}\cdot\hat{n} & \text{k is odd} \end{cases}$$

(b) From the above prove that for the spin-1/2 case

$$\hat{R}_{\hat{n}}(\Delta\phi) = \cos\frac{\Delta\phi}{2} - i\,\sin\frac{\Delta\phi}{2}\hat{n}\cdot\hat{\sigma}$$

(c) If we repeatedly rotate about the same axis $\hat{n}$, then we know that rotations simply add, and we can write the general rotation matrix for an angle ϕ in the z-axis basis:

$$\begin{pmatrix} \cos\frac{\phi}{2} - i\,n_z\sin\frac{\phi}{2} & (-i\,n_x - n_y)\sin\frac{\phi}{2} \\ (-i\,n_x + n_y)\sin\frac{\phi}{2} & \cos\frac{\phi}{2} + i\,n_z\sin\frac{\phi}{2} \end{pmatrix}$$

(d) Using this matrix, what do you get if you rotate the state $|\uparrow\rangle$:

i. by $\pi/2$ about the x-axis?

ii. by π about the x-axis?

iii. by 2π about the x-axis?

(e) Does the state $|\uparrow\rangle$ rotate as a vector?

6. **Variational Calculations:** Consider the one dimensional Schrödinger equation, already converted to dimensionless units:

$$\mathcal{H}\psi(x) = \left\{-\frac{d^2}{dx^2} - \frac{1}{1+x^2}\right\}\psi(x) = E\,\psi(x)$$

with the boundary conditions $\psi(-\infty) = \psi(\infty) = 0$. We will assume a variational form for the groundstate:

$$\psi(x) = \sqrt{\frac{2\alpha^3}{\pi}}\frac{1}{x^2+\alpha^2}$$

where α is a constant that must be determined.

(a) Show that $\psi(x;\alpha)$ is normalized in the infinite interval.

(b) We wish to determine the value of α in a variational fashion so that:

$$\mathcal{I} \equiv \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

is a maximum. Evaluate an analytic expression for $\mathcal{I}(\alpha)$.

(c) Either plot your function and find its minimum, or take the dervivative and determine where it crosses zero. What is this value of α? Use this value of α to find an estimate of the smallest eigenvalue.

(d) Determine the groundstate eigenvalue directly by a numerical solution of the problem, using the eigenvalue solver for the Schrodinger equation that you developed in an earlier homework. Compare it to the value obtain from the variational calculation.

This problem is a bit tedious. You may question the wisdom of doing a variational calculation, since it required numerical evaluations only slightly simpler than writing an eigenvalue solver. On the other hand, eigenvalue solvers become much harder in two and three dimensions, whereas a good variational calculation is often much simpler.