Quantum Mechanics: Take-home Assignment 1

IUCAA-NCRA Graduate School

August - September 2016

09 August 2016

To be returned in the class on 18 August 2016

- The deadline for the submission of the solutions of this assignment will be strictly enforced. No marks will be given if the assignment is not returned in time.
- You are free to discuss the solutions with friends, seniors and consult any books. However, you should understand and be clear about every step in the answers. Marks may be reduced if you have not understood what you have written even though the answer is correct.
- Let me know if you find anything to be unclear or if you think that something is wrong in any of the questions.

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1. **Gram-Schmidt algorithm:** Let $|\alpha_i\rangle$, $i = 1, 2, \ldots, N$ be a set of basis vectors (not necessarily orthogonal) in an N-dimensional vector space. According to the Gram-Schmidt algorithm, one can form a set of orthogonal basis vectors $|f_i\rangle$ using the relations

$$
\begin{aligned}
|f_1\rangle &= |\alpha_1\rangle\,, \\
|f_2\rangle &= |\alpha_2\rangle - \frac{\langle f_1|\alpha_2\rangle}{\langle f_1|f_1\rangle}\,|f_1\rangle\,, \\
|f_3\rangle &= |\alpha_3\rangle - \frac{\langle f_1|\alpha_3\rangle}{\langle f_1|f_1\rangle}\,|f_1\rangle - \frac{\langle f_2|\alpha_3\rangle}{\langle f_2|f_2\rangle}\,|f_2\rangle\,, \\
&\vdots \\
|f_N\rangle &= |\alpha_N\rangle - \frac{\langle f_1|\alpha_N\rangle}{\langle f_1|f_1\rangle}\,|f_1\rangle - \frac{\langle f_2|\alpha_N\rangle}{\langle f_2|f_2\rangle}\,|f_2\rangle - \ldots - \frac{\langle f_{N-1}|\alpha_N\rangle}{\langle f_{N-1}|f_{N-1}\rangle}\,|f_{N-1}\rangle\,.
\end{aligned}
$$

   (a) Show that $\langle f_i|f_j\rangle = 0$ for $i \neq j$, $i, j = 1, 2, \ldots, N$.

   (b) Consider the vector space of real polynomials $|A(t)\rangle$ of degree ≤ 2. What is the dimension of this space?

   (c) Consider the set of polynomials $\{1, t, t^2\}$. Since any polynomial of degree ≤ 2 can be written as a linear combination of these three polynomials, they form a basis in the vector space. Let the inner product in this space be defined as

$$\langle A|B\rangle = \int_{-1}^{1} \mathrm{d}t\; A(t)\; B(t).$$

   Starting with the basis $\{1, t, t^2\}$, use the Gram-Schmidt procedure to form an orthogonal basis $|f_i(t)\rangle$. Normalize the basis vectors such that $|f_i(t = 1)\rangle = 1$. Can you identify the polynomials thus obtained?

[5+1+9]

2. The quantum mechanical angular momentum operator is defined as

$$\boldsymbol{L} = \boldsymbol{X} \times \boldsymbol{P} = -\mathrm{i}\hbar \boldsymbol{X} \times \boldsymbol{\nabla}.$$

   (a) Show that

$$[L_x, L_y] = \mathrm{i}\hbar L_z.$$

   Write down the results for $[L_y, L_z]$ and $[L_z, L_x]$ as well (you need not prove them).

   (b) Show that

$$[\boldsymbol{L}^2, L_z] = 0.$$

   (c) Let us define two new operators as

$$L_\pm \equiv L_x \pm \mathrm{i}L_y.$$

   Show that

$$\boldsymbol{L}^2 = L_+ L_- + L_z^2 - \hbar L_z.$$

(d) Let $R(\boldsymbol{\theta})$ be the rotation operator which rotates the position basis ket $|\boldsymbol{x}\rangle$ by an angle $\theta \equiv |\boldsymbol{\theta}|$ about the axis $\hat{\theta} \equiv \boldsymbol{\theta}/\theta$. Show that for an infinitesimal rotation $\delta\boldsymbol{\theta}$, we can write

$$R(\delta\boldsymbol{\theta})\,|\boldsymbol{x}\rangle = |\boldsymbol{x} + \delta\boldsymbol{\theta} \times \boldsymbol{x}\rangle\,.$$

Hence show that the rotation operator for any arbitrary $\boldsymbol{\theta}$ is given by

$$R(\boldsymbol{\theta}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}\cdot\boldsymbol{L}/\hbar}.$$

[5+5+3+12]

3. **Spin-1/2 particle in an electromagentic field:**

(a) Show that the Lagrangian of a (classical) charged particle of mass m and charge q in presence of an external electromagnetic field is

$$L = \frac{1}{2}m\dot{\boldsymbol{x}}^2 - q\phi(\boldsymbol{x},t) + q\frac{\dot{\boldsymbol{x}}}{c}\cdot\boldsymbol{A}(\boldsymbol{x},t),$$

where ϕ is the electric scalar potential and $\boldsymbol{A}$ is the magnetic vector potential. It is sufficient to show that the above Lagrangian gives the correct equation of motion.

(b) Hence show that the Hamiltonian is

$$H = \frac{1}{2m}\left[\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}(\boldsymbol{x},t)\right]^2 + q\phi(\boldsymbol{x},t).$$

(Thus one can incorporate the effects of the electromagnetic field into the Hamiltonian by replacing $\boldsymbol{p} \to \boldsymbol{p} - (q/c)\boldsymbol{A}$ and $H \to H - q\phi$.)

(c) We know that the state of a spin-1/2 particle can be written as

$$\langle\boldsymbol{x}|\psi\rangle = \psi_+(\boldsymbol{x})\ \ |\chi_+\rangle + \psi_-(\boldsymbol{x})\ \ |\chi_-\rangle = \begin{pmatrix} \psi_+(\boldsymbol{x}) \\ \psi_-(\boldsymbol{x}) \end{pmatrix}$$

Since the wave functions $\psi_\pm(\boldsymbol{x})$ satisfy the Schrödinger equation, we can write

$$\mathrm{i}\hbar\frac{\partial\langle\boldsymbol{x}|\psi\rangle}{\partial t} = \langle\boldsymbol{x}|H|\psi\rangle\,,$$

which, in absence of any external field or potential, becomes

$$\mathrm{i}\hbar\frac{\partial\langle\boldsymbol{x}|\psi\rangle}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\langle\boldsymbol{x}|\psi\rangle\,.$$

Show that the above equation is equivalent to

$$\mathrm{i}\hbar\frac{\partial\langle\boldsymbol{x}|\psi\rangle}{\partial t} = -\frac{\hbar^2}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\nabla})^2\langle\boldsymbol{x}|\psi\rangle\,,$$

where the components of $\boldsymbol{\sigma}$ are the 2×2 Pauli matrices. This is a simple way of introducing spin (by hand) into the non-relativistic Schrödinger equation.

(d) Argue that in the presence of electromagnetic fields, the above equation modifies to

$$\mathrm{i}\hbar\frac{\partial\langle\boldsymbol{x}|\psi\rangle}{\partial t} = \frac{1}{2m}\left[\boldsymbol{\sigma}\cdot\left(-\mathrm{i}\hbar\boldsymbol{\nabla} - \frac{q}{c}\boldsymbol{A}\right)\right]^2\langle\boldsymbol{x}|\psi\rangle + q\phi\,\langle\boldsymbol{x}|\psi\rangle\,,$$

where $\boldsymbol{A}$ and ϕ should be treated as quantum mechanical operators (in the coordinate basis).

(e) Show that the above equation can be written as

$$\mathrm{i}\hbar\frac{\partial\langle\boldsymbol{x}|\psi\rangle}{\partial t} = \frac{1}{2m}\left(-\mathrm{i}\hbar\boldsymbol{\nabla} - \frac{q}{c}\boldsymbol{A}\right)^2\langle\boldsymbol{x}|\psi\rangle - \frac{q\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{B}\,\langle\boldsymbol{x}|\psi\rangle + q\phi\,\langle\boldsymbol{x}|\psi\rangle\,,$$

where $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$ is the magnetic field. Can you interpret the significance of this equation?

[6+2+3+2+7]