Some hints/solutions to problem set 04.

Please use responsibly — there might be misprints and typos.

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1. Matrices (or operators) might not commute with each other. This means, it $\hat{A}$ and $\hat{B}$ are matrices (or operators), $\hat{A}\hat{B}$ might be unequal to $\hat{B}\hat{A}$. We define the **commutator** of two matrices (or oberators) $\hat{A}$ and $\hat{B}$ as

$$[\hat{A}, \hat{B}] \;=\; \hat{A}\hat{B} - \hat{B}\hat{A}$$

Sometimes operators acting on functions are written with a hat, as I've done here. Operators acting on finite vectors, i.e., matrices, are usually written without a hat. Let's use the hat notation for this problem.

(a) Show that $[\hat{B}, \hat{A}] = -[\hat{A}, \hat{B}]$.

Hints / Solution / Discussion →
trivial

(b) Show that $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$.
Typing hats is painful, so I write the answers without hats.

$$\begin{aligned} [A, B + C] \;&=\; A(B + C) - (B + C)A \;=\; AB + AC - BA - CA \\ &=\; (AB - BA) + (AC - CA) \;=\; [A, B] + [A, C] \end{aligned}$$

Hints / Solution / Discussion →

(c) Show that $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$.

Hints / Solution / Discussion →

$$\text{Left side} \;=\; [A, BC] \;=\; ABC - BCA$$

$$\begin{aligned} \text{Right side} \;&=\; [A, B]C + B[A, C] \;=\; (AB - BA)C \;+\; B(AC - CA) \\ &=\; ABC - BAC + BAC - BCA \;=\; ABC - BCA \end{aligned}$$

Hence the two sides are equal.

2. (a) Look up the three Pauli matrices, denoted as σ_x, σ_y, σ_z, and write them down, (Each one is a 2×2 matrix.)

Hints / Solution / Discussion $\rightarrow$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \qquad \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(b) Calculate $[\sigma_x, \sigma_y]$ and express it in terms of σ_z.

Hints / Solution / Discussion $\rightarrow$

$$\begin{aligned} [\sigma_x, \sigma_y] &= \sigma_x\sigma_y - \sigma_y\sigma_x \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} \\ &\qquad\qquad = 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2i\sigma_z \end{aligned}$$

(c) Look up (or calculate or guess correctly) $[\sigma_y, \sigma_z]$ in terms of σ_x, and $[\sigma_z, \sigma_x]$ in terms of σ_y. No need to show calculations; just report the results.

Hints / Solution / Discussion $\rightarrow$

$$[\sigma_y, \sigma_z] = 2i\sigma_x \qquad [\sigma_z, \sigma_x] = 2i\sigma_y$$

(d) Find the eigenvalues and eigenvectors of σ_x.

Hints / Solution / Discussion $\rightarrow$
To calculate eigenvalues, could write the equation

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

and try looking for solutions for λ, α, β. Probably easier to use the determinant condition for eigenvalues:

$$\begin{vmatrix} 0-\lambda & 1 \\ 1 & 0-\lambda \end{vmatrix} = 0$$

The solutions are $\lambda = \pm 1$.

Eigenvector corresponding to $\lambda = 1$: substituting this value in the eigenvalue equation,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \qquad \Longrightarrow \qquad \alpha = \beta$$

so the corresponding eigenvector is $\begin{pmatrix} \alpha \\ \alpha \end{pmatrix}$, or, normalizing, $\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$ **times an arbitrary phase factor**.

The unknown phase factor is an important qualifier. This means that

$$-\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = e^{i\pi} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

and

$$e^{i\pi/2} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} i/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix}$$

and

$$e^{i\pi/4} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} + \frac{i}{2} \\ \frac{1}{2} + \frac{i}{2} \end{pmatrix}$$

are all equally valid normalized eigenvectors corresponding to the eigenvalue $\lambda = 1$.

Similarly, eigenvector corresponding to $\lambda = -1$ can be found to be $\begin{pmatrix} \alpha \\ -\alpha \end{pmatrix}$, or, normalizing, $\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$ times an arbitrary phase factor.

(e) Find the eigenvalues and eigenvectors of σ_z.

Hints / Solution / Discussion →

The eigenvalues are ± 1. Corresponding normalized eigenvectors are

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{corresponding to eigenvalue } +1 \tag{1}$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{corresponding to eigenvalue } -1 \tag{2}$$

.... times arbitrary phase factors, of course.

(f) Is it easier to find eigenvalues & eigenvectors if the matrix is diagonal? Why?

Hints / Solution / Discussion →
Because, if diagonal, the diagonal matrix elements are themselves the eigenvalues. No additional calculation required for eigenvalues, if the matrix is 'already' diagonal.

3. (a) In Charles Nash's notes (linked on module webpage): Read Section 5 of Chapter III, on 'Expectation Values'. Begins on page 42.

   (b) Define the expectation value of an observable represented by operator $\hat{A}$, when the system state is $|\psi\rangle$.

   Hints / Solution / Discussion →

$$\langle\psi|\,\hat{A}\,|\psi\rangle$$

   (c) The state $|\phi\rangle$ is a normalized eigenstate of $\hat{A}$, with the corresponding eigenvalue being λ. What is the expectation value of $\hat{A}$ in this state? (Prove/derive your answer.)

   Hints / Solution / Discussion →
   Since $\hat{A}\,|\phi\rangle = \lambda\,|\phi\rangle$, we get

$$\langle\phi|\,\hat{A}\,|\phi\rangle \;=\; \langle\phi|\,\lambda\,|\phi\rangle \;=\; \langle\phi|\,\lambda\,|\phi\rangle \;=\; \lambda\langle\phi\big|\phi\rangle \;=\; \lambda\cdot 1 \;=\; \lambda$$

   We have used the fact that $|\phi\rangle$ is **normalized**, $\langle\phi\big|\phi\rangle = 1$.

4. For a spin-1/2 system, the operators for the components of spin are

$$S_x \;=\; \frac{\hbar}{2}\sigma_x \qquad S_z \;=\; \frac{\hbar}{2}\sigma_z \qquad S_z \;=\; \frac{\hbar}{2}\sigma_z$$

   (a) Find the eigenvalues and eigenvectors of S_z. How are they related to the eigenvalues and eigenvectors of σ_z?

   Hints / Solution / Discussion →
   One can re-do an eigenproblem calculation. Alternatively, since we know the eigenvalues and eigenvectors of σ_z, we can use that information.

Since $S_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$, the eigenvalues of S_z are $\hbar/2$ times the eigenvalues of σ_z, i.e.,

$$+\frac{\hbar}{2} \qquad \text{and} \qquad -\frac{\hbar}{2}$$

The corresponding eigenvectors are the same as the eigenvectors of σ_z.

(b) If our two-level system is in the state $|\psi\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, then find the expectation values of S_z and S_x.

Hints / Solution / Discussion →

$$\langle\psi|\, S_z\,|\psi\rangle \;=\; \begin{pmatrix}1 & 0\end{pmatrix}\left[\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right]\begin{pmatrix}1\\0\end{pmatrix} \;=\; \frac{\hbar}{2}\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} \;=\; \frac{\hbar}{2}$$

$$\langle\psi|\, S_x\,|\psi\rangle \;=\; \begin{pmatrix}1 & 0\end{pmatrix}\left[\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right]\begin{pmatrix}1\\0\end{pmatrix} \;=\; \frac{\hbar}{2}\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \;=\; 0$$

(c) Which one of the expectation values could you have guessed?

Hints / Solution / Discussion →
Since the state is an eigenvector of S_z, one could have known that the expectation value is the corresponding eigenvalue, hance $\hbar/2$.

The S_x eigenvalue being zero could also be guessed from physical considerations. In a measurement of S_x, one can only obtain the result $\hbar/2$ or $-\hbar/2$, because those are the eigenvalues of S_x. One could guess that an eigenvector of S_z will not prefer one of the S_x values over the other. (Very roughly, this reflects the intuition that that the z direction should not have a preference between $+x$ and $-x$ directions.) Hence, one could guess equal probabilities to find the values $\hbar/2$ or $-\hbar/2$. This means the expectation value is midway between these values, hence zero.

(d) Find the commutation relations between the operators S_x, S_y and S_z. (You may use the results for commutators of Pauli matrices.)

Hints / Solution / Discussion →

$$[S_x, S_y] \;=\; i\hbar S_z\ , \quad [S_y, S_x] \;=\; i\hbar S_x\ , \quad [S_z, S_x] \;=\; i\hbar S_y$$

5. When electromagnetic radiation of frequency 2×10^{15} Hz shines on a sample of gold, the emitted electrons have a kinetic energy of 3.0 eV. When this frequency is increased to 10^{16} Hz, the electron kinetic energy is 36.1 eV. (This is the photoelectric effect.)

   (a) How much is 1 eV of energy, in SI units? (Look up.)

   Hints / Solution / Discussion →
   1eV is approximately $1,6\times10^{-19}$J. (More digits: $1,60218\times10^{-19}$J.)

   (b) Pretending that we do not know the value of Planck's constant (h), use the above data to estimate h in units of SI units (J-s), Use Einstein's energy conservation equation for the photoelectric effect.

   Hints / Solution / Discussion →
   Einstein's equation:
   $$\text{K.E.} \;=\; W \;+\; hf$$
   so that h is the slope of the K.E. versus f line:
   $$h \approx \frac{(\text{K.E.})_2-(\text{K.E.})_1}{f_2-f_1} \;=\; \frac{(36.1-3.0)\text{eV}}{(10^{16}-2\times10^{15})\text{Hz}}$$
   $$= \frac{(33.1)\times1.6\times10^{-19}\text{J}}{(8\times10^{15})\text{s}^{-1}} \;=\; 6.62\times10^{-34}\text{J.s}$$

   (c) Use the above data to find the work function of gold, in eV and also in Joules. (You don't necessarily need the value of h for this, but if you want you can use $h=6.626\times10^{-34}$ J-s.) What does the work function physically represent?

   Hints / Solution / Discussion →
   Calculation left as an exercise.
   Physically, the work function represents the minimal amount of energy required by an electron to be able to leave the surface of the metal.

6. Look up the properties of the Dirac delta function. If a is a positive real number, write down the values of the following integrals.

$$\text{(a)} \int_{-a}^{a} dx\ \delta(x) \qquad \text{(b)} \int_{a}^{2a} dx\ \delta(x) \qquad \text{(c)} \int_{-a}^{a} dx\ \delta(x)f(x)$$

$$\text{(d)} \int_{a}^{2a} dx\ \delta(x)f(x) \qquad \text{(e)} \int_{-a}^{a} dx\ \delta(x-2a)$$

$$\text{(f)} \int_{-a}^{a} dx\ \delta(x-2a)f(x) \qquad \text{(g)} \int_{0}^{3a} dx\ \delta(x-2a)f(x)$$

Hint: plotting the integrand in the region within the limits of integration is often helpful.

Hints / Solution / Discussion →

The Dirac delta function is zero everywhere except when it's argument is zero. Thus, $\delta(x)$ is zero everywhere except for at $x = 0$, and $\delta(x - 2a)$ is zero everywhere except for the point $x = 2a$. If the integration interval does not include this point, then the integral should be zero.

At the point where its argument vanishes, the delta function is difficult to describe. You can think of it as being infinite at that point only, in a way that integration over the function gives 1. There are various ways to think about the delta function — please do some reading about it.

$$\int_{-a}^{a} dx\ \delta(x) = 1$$

$$\int_{a}^{2a} dx\ \delta(x) = 0$$

In this case, the nonzero part of the Dirac delta function falls outside the range of integration. Draw a cartoon of the delta function, and mark the region of integration on the same plot, to convince yourself of this.

$$\int_{-a}^{a} dx\ \delta(x)f(x) = f(0)$$

$$\int_{a}^{2a} dx\ \delta(x)f(x) = 0$$

$$\int_{-a}^{a} dx\ \delta(x-2a) = 0$$

In this case again, the nonzero part of the Dirac delta function falls outside the range of integration. Draw a cartoon of the delta function: the infinite peak should be at $x = 2a$. This falls outside the region of integration, which is $(-a, a)$.

$$\int_{-a}^{a} dx\ \delta(x-2a) f(x) \ = \ 0$$

$$\int_{0}^{3a} dx\ \delta(x-2a) f(x) \ = \ f(2a)$$