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## Quantum Mechanics I

1st Midterm Exam Solutions

DISCLAIMER: This solution set presents more detail than was required of the Student, and is meant as an additional resource for learning. Please do study not just the solutions as presented, but try also to understand the rationale behind the approach.

**1.** Given the two state vectors, 
$$|u_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix}$$
, and  $|u_2\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$ ,

a. prove that they form a complete basis for 2-dimensional vectors. Solution\_

For them to form a (complete) basis for 2-dimensional vectors, the two  $|u_i\rangle$ 's must be linearly independent. This we prove by showing that the requirement

$$\sum_{i=1}^{2} c_i \left| u_i \right\rangle = \frac{c_1}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix} + c_2 \begin{bmatrix} 0\\1 \end{bmatrix} = 0 , \qquad \Rightarrow \qquad \begin{cases} c_1 \stackrel{!}{=} 0 , \\ \frac{c_1}{\sqrt{2}} + c_2 \stackrel{!}{=} 0 , \\ \frac{c_1}{\sqrt{2}} + c_2 \stackrel{!}{=} 0 , \end{cases}$$

which would hold only if both  $c_1$  and  $c_2$  vanish.

b. Specify the  $\langle u_i |, i = 1, 2$  and show that this basis it not orthonormal. Solution\_

For the  $\langle u_i |$  to act on the column-vectors  $|u_i\rangle$  and to produce (in general, complex) numbers, they must be hermitian-conjugate row-vectors:

$$\langle u_1 | = \frac{1}{\sqrt{2}} [1, 1] , \quad \langle u_2 | = [0, 1] .$$

Non-orthogonality is proven by finding  $\langle u_i | u_i \rangle \neq 0$  for any  $i \neq j$ . In this case:

$$\langle u_1 | u_2 \rangle = \frac{1}{\sqrt{2}} [1,1] \begin{bmatrix} 0\\1 \end{bmatrix} = \frac{1}{\sqrt{2}} (1 \cdot 0 + 1 \cdot 1) = \frac{1}{\sqrt{2}} \neq 0.$$

Since  $\langle u_i | u_i \rangle \neq 0$  when  $i \neq j$ , this basis, albeit complete, is not orthogonal.

c. Construct an orthonormal basis  $\{|v_1\rangle = |u_1\rangle, |v_2\rangle = ?\}$ . Solution\_

We start with the  $|v_1\rangle = |u_1\rangle$ , as instructed, write  $|v_2\rangle = a |u_1\rangle + b |u_2\rangle$ , and require orthogonality:

$$0 \stackrel{!}{=} \langle v_1 | v_2 \rangle = \langle u_1 | \left[ a | u_1 \rangle + b | u_2 \rangle \right] = a + \frac{b}{\sqrt{2}} , \quad \Rightarrow \quad b = -\sqrt{2}a ,$$

and so

$$|v_1\rangle = \frac{a}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix} - \sqrt{2}a \begin{bmatrix} 0\\1 \end{bmatrix} = \frac{a}{\sqrt{2}} \begin{bmatrix} 1\\-1 \end{bmatrix}$$
, and  $\langle v_2| = \frac{a}{\sqrt{2}} [1, -1]$ .

Don't Panic !

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8th Oct. '03.

T. Hübsch

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## 1st Mid-Term Exam

Instructor's Solution

Finally, we normalize:

$$1 \stackrel{!}{=} \langle v_2 | v_2 \rangle = \frac{|a|^2}{2} [1, -1] \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{|a|^2}{2} \cdot 2, \quad \Rightarrow \quad |v_2 \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

d. Construct the projection operators  $\hat{P}_i = |v_i\rangle \langle v_i|$  and prove that  $\sum_{i=1}^{2} \hat{P}_i = 1$ , and that  $\hat{P}_i \hat{P}_j = \delta_{ij} \hat{P}_j$ ,  $\forall i, j = 1, 2$ . Solution\_\_\_\_\_\_

Straightforwardly:

$$\hat{\mathsf{P}}_{1} = |v_{1}\rangle \langle v_{1}| = \frac{1}{2} \begin{bmatrix} 1\\1 \end{bmatrix} [1,1] = \begin{bmatrix} 1/2 & 1/2\\1/2 & 1/2 \end{bmatrix} ,$$

and

$$\hat{\mathsf{P}}_2 = |v_2\rangle \langle v_2| = \frac{1}{2} \begin{bmatrix} 1\\-1 \end{bmatrix} [1, -1] = \begin{bmatrix} 1/2 & -1/2\\-1/2 & 1/2 \end{bmatrix} .$$

And, with these, indeed:

$$\begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} + \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} ,$$

and, similarly,

$$\begin{bmatrix} 1/_2 & \pm 1/_2 \\ \pm 1/_2 & 1/_2 \end{bmatrix} \begin{bmatrix} 1/_2 & \pm 1/_2 \\ \pm 1/_2 & 1/_2 \end{bmatrix} = \begin{bmatrix} 1/_2 & \pm 1/_2 \\ \pm 1/_2 & 1/_2 \end{bmatrix}, \quad \text{but} \quad \begin{bmatrix} 1/_2 & 1/_2 \\ 1/_2 & 1/_2 \end{bmatrix} \begin{bmatrix} 1/_2 & -1/_2 \\ -1/_2 & 1/_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

**2.** An observable of the system in problem 1 is represented by  $\hat{F} = \begin{bmatrix} 2 & 2 \\ 2 & -1 \end{bmatrix}$ .

a. Determine all possible results of (single attempts of) measuring  $\hat{F}$ . Solution\_\_\_\_\_

Possible outcomes of single measurements are the eigenvalues of  $\hat{F}$ . These we obtain by solving the secular equation:

$$0 \stackrel{!}{=} \det[\hat{F} - f\mathbf{1}] = \begin{vmatrix} 2-f & 2\\ 2 & -1-f \end{vmatrix} = -(2-f)(1+f) - 4 = (f+2)(f-3) ,$$

so the possible single measurement results are f = -2, +3.

b. Determine all eigenvectors of  $\hat{F}$ . Solution\_\_\_\_\_

Writing 
$$\hat{F} |f\rangle = f |f\rangle$$
 as  $[\hat{F} - f\mathbf{1}] |f\rangle = 0$ , we calculate for each of  $f = -2, +3$ : [=8pt]  
 $0 \stackrel{!}{=} [\hat{F} + 2\mathbf{1}] |-2\rangle = \begin{bmatrix} 4 & 2\\ 2 & 1 \end{bmatrix} \begin{bmatrix} x\\ y \end{bmatrix}$ ,  $\Rightarrow \quad 4x + 2y = 0\\ 2x + y = 0 \end{bmatrix} \Rightarrow \quad |-2\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 1\\ -2 \end{bmatrix}$ .  
 $0 \stackrel{!}{=} [\hat{F} - 3\mathbf{1}] |+3\rangle = \begin{bmatrix} -1 & 2\\ 2 & -4 \end{bmatrix} \begin{bmatrix} x\\ y \end{bmatrix}$ ,  $\Rightarrow \quad -x + 2y = 0\\ 2x - 4y = 0 \end{bmatrix} \Rightarrow \quad |+3\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 2\\ 1 \end{bmatrix}$ .

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c. Calculate the expectation value of  $\hat{F}$  in the pure state  $v_1$ . Solution\_\_\_\_\_

This expectation value equals  $\text{Tr}[\hat{\rho}_{u_1}\hat{F}] = \langle u_1 | \hat{F} | u_1 \rangle$ , and we can calculate it directly:

$$\langle \hat{F} \rangle_{u_1} = \operatorname{Tr} \left[ \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} \cdot \begin{bmatrix} 2 & 2 \\ 2 & -1 \end{bmatrix} \right] = \operatorname{Tr} \begin{bmatrix} 2 & 1/2 \\ 2 & 1/2 \end{bmatrix} = \frac{5}{2} ,$$

or

$$\langle \hat{F} \rangle_{u_1} = \frac{1}{2} [1,1] \begin{bmatrix} 2 & 2\\ 2 & -1 \end{bmatrix} \begin{bmatrix} 1\\ 1 \end{bmatrix} = \frac{1}{2} [1,1] \begin{bmatrix} 4\\ 1 \end{bmatrix} = \frac{5}{2} ,$$

d. Calculate the expectation value of  $\hat{F}$  in the impure state  $\hat{\rho} = \frac{1}{4}\hat{P}_1 + \frac{3}{4}\hat{P}_2$ . Solution\_\_\_\_\_

Doing the straightforward matrix algebra:

$$\hat{\rho} = \frac{1}{4}\hat{P}_1 + \frac{3}{4}\hat{P}_2 = \frac{1}{4}\begin{bmatrix} 1/2 & 1/2\\ 1/2 & 1/2\\ 1/2 & 1/2 \end{bmatrix} + \frac{3}{4}\begin{bmatrix} 1/2 & -1/2\\ -1/2 & 1/2\\ -1/2 & 1/2 \end{bmatrix} = \begin{bmatrix} 1/2 & -1/4\\ -1/4 & 1/2\\ 1/2 \end{bmatrix},$$

we have that

$$\langle \hat{F} \rangle_{\rho} = \operatorname{Tr} \left[ \begin{bmatrix} 1/2 & -1/4 \\ -1/4 & 1/2 \end{bmatrix} \cdot \begin{bmatrix} 2 & 2 \\ 2 & -1 \end{bmatrix} \right] = \operatorname{Tr} \begin{bmatrix} 1/2 & 5/4 \\ 1/2 & -1 \end{bmatrix} = -\frac{1}{2}.$$

Alternatively, using the linearity of Tr[], we have that

$$\langle \hat{F} \rangle_{\rho} = \operatorname{Tr}\left[ \left( \frac{1}{4} \hat{P}_{1} + \frac{3}{4} \hat{P}_{2} \right) \hat{F} \right] = \frac{1}{4} \operatorname{Tr}\left[ \hat{P}_{1} \hat{F} \right] + \frac{3}{4} \operatorname{Tr}\left[ \hat{P}_{2} \hat{F} \right] = \frac{1}{4} \langle v_{1} | \hat{F} | v_{1} \rangle + \frac{3}{4} \langle v_{2} | \hat{F} | v_{2} \rangle ,$$

$$= \frac{1}{4} \left( \frac{1}{2} [1, 1] \begin{bmatrix} 2 & 2 \\ 2 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right) + \frac{3}{4} \left( \frac{1}{2} [1, -1] \begin{bmatrix} 2 & 2 \\ 2 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right) = \frac{1}{4} \left( \frac{5}{2} \right) + \frac{3}{4} \left( -\frac{3}{2} \right) = -\frac{1}{2} .$$

Notice that this is not a pure state, so that there exists no  $|\psi\rangle$  such that  $\langle \hat{F} \rangle_{\rho}$  would be calculable as  $\langle \psi | \hat{F} | \psi \rangle$  for all hermitian  $\hat{F}$ 's. [=10pt]

e. Calculate the probability that the measurement of the observable  $\hat{F}$  in the system in state pure state  $v_1$  would turn out to be 3. Solution\_\_\_\_\_.

As given in the text, and used in the homework solution,  $\operatorname{Prob}(\hat{F}=f|\hat{\rho}) = \operatorname{Tr}[\hat{\rho}\,\hat{\mathsf{P}}_{f}].$ Since  $\hat{\mathsf{P}}_{f} \stackrel{\text{def}}{=} |f\rangle \langle f|$ , and for the pure state  $\hat{\rho}_{v_{1}} = |v_{1}\rangle \langle v_{1}|$ , we have that

$$\operatorname{Prob}(\hat{F}=f|\hat{\rho}) = \operatorname{Tr}\left[\hat{\rho}|f\rangle\langle f|\right] = \langle f|\hat{\rho}|f\rangle, \quad = \operatorname{Tr}\left[|v_1\rangle\langle v_1||\hat{P}_f\right] = \langle v_1|\hat{P}_f|v_1\rangle$$

that is,

$$\operatorname{Prob}(\hat{F}=f|\hat{\rho}) = \operatorname{Tr}\left[\left|v_{1}\right\rangle\left\langle v_{1}\right|\left|f\right\rangle\left\langle f\right|\right] = \left\langle f|v_{1}\right\rangle\left\langle v_{1}|f\right\rangle = \left|\left\langle v_{1}|f\right\rangle\right|^{2}.$$

Alternatively (as done in other texts focusing on the wave-functions), we can expand  $|v_1\rangle = c_{-2} |-2\rangle + c_{+3} |+3\rangle$ , use the orthonormalization of the  $|f\rangle$  to obtain that  $\langle +3|v_1\rangle = c_{+3}$  is

the probability amplitude, and deduce that  $\operatorname{Prob}(\hat{F}=f|\hat{\rho}) = |c_f|^2 = |\langle f|v_1\rangle|^2$ , in agreement with the above, more direct calculation.

For our case at hand,

$$\operatorname{Prob}(\hat{F}=3|\hat{\rho}_{v_1}) = \left|\langle v_1|+3\rangle\right|^2 = \left|\frac{1}{\sqrt{2}}[1,1]\cdot\frac{1}{\sqrt{5}}\begin{bmatrix}2\\1\end{bmatrix}\right|^2 = \left|\frac{3}{\sqrt{10}}\right|^2 = \frac{9}{10}.$$

f. Calculate the probability that the measurement of the observable  $\hat{F}$  in the system in impure state with  $\hat{\rho} = \frac{1}{4}\hat{P}_1 + \frac{3}{4}\hat{P}_2$  would turn out to be 3. Solution\_\_\_\_\_.

Using above results, we have that  $\operatorname{Prob}(\hat{F}=f|\hat{\rho})=\langle f|\hat{\rho}|f\rangle$  now is:

$$\operatorname{Prob}(\hat{F}=3|\hat{\rho}) = \frac{1}{5}[2,1] \begin{bmatrix} 1/2 & -1/4 \\ -1/4 & 1/2 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \frac{3}{10}$$

We could have also calculated this using the linearity of Tr[]:

$$\begin{aligned} \operatorname{Prob}(\hat{F}=f|\hat{\rho}) &= \operatorname{Tr}[(\frac{1}{4}\hat{\mathsf{P}}_{1} + \frac{3}{4}\hat{\mathsf{P}}_{2})\hat{\mathsf{P}}_{f}] = \frac{1}{4}\operatorname{Tr}[\hat{\mathsf{P}}_{1}\hat{\mathsf{P}}_{f}] + \frac{3}{4}\operatorname{Tr}[\hat{\mathsf{P}}_{2}\hat{\mathsf{P}}_{f}] ,\\ &= \frac{1}{4}|\langle v_{1}|f\rangle|^{2} + \frac{3}{4}|\langle v_{2}|f\rangle|^{2} \end{aligned}$$

Thus,  $\operatorname{Prob}(\hat{F}=3|\hat{\rho}) = \frac{1}{4} |\langle v_1|+3\rangle|^2 + \frac{3}{4} |\langle v_2|+3\rangle|^2 = \frac{1}{4} |\frac{1\cdot 2+1\cdot 1}{\sqrt{2\cdot 5}}|^2 + \frac{3}{4} |\frac{1\cdot 2-1\cdot 1}{\sqrt{2\cdot 5}}|^2 = \frac{3}{10}.$  [=20pt]

**3.** Consider a particle under the influence of the potential:  $W(x) = W_0$  for x < 0, W(x) = 0 for 0 < x < a, and  $W(x) = +\infty$  for a < x, with  $W_0, a > 0$ .

a. Sketch potential and determine the allowed values of the total energy. Solution\_\_\_\_\_



b. State/specify all boundary conditions for stationary states with  $0 < E < W_0$ .

Besides the mathcing condition at x = 0:

$$\lim_{\epsilon \to 0} \psi(-\epsilon) = \lim_{\epsilon \to 0} \psi(+\epsilon) , \quad \text{and} \quad \lim_{\epsilon \to 0} \psi'(-\epsilon) = \lim_{\epsilon \to 0} \psi'(+\epsilon) ,$$

[=10pt]

we also have that  $\psi(a) = 0$  and  $\lim_{x \to -\infty} \psi(x) = 0$ . [=10pt] c. Sketch the wave-function of a stationary state with  $0 < E < W_0$ . Solution\_\_\_\_\_.

A wave-function is sketched in the figure on the previous page. Note that it satisfies the boundary conditions spelled out in the previous part. Furthermore, it identically vanishes in the region x > a, where  $W(x) = +\infty$ . Finally, note that it is oscillatory for 0 < x < a, where E > W(x), but that it decays (to the left) for x < 0 where E < W(x). [=10pt] Now let  $W_0 \to \infty$ .

d. Sketch potential and determine the allowed values of the total energy.



e. State all boundary conditions and sketch the wave-function of a stationary state. Solution\_\_\_\_\_

This time,  $W(x) = +\infty$  both when x < 0 and when x > a: there  $\psi(x) \equiv 0$ . For 0 < x < a, allowed, positive values of E are always bigger than W(x), and the solution is oscillatory, as sketched in the figure above. Thus,  $\psi(0) = 0 = \psi(a)$  are the only boundary conditions.[=10pt]

f. Calculate the wave-number, k, and thus the energy of all stationary states. Solution\_\_\_\_\_

Writing the solution as  $\psi(x) = A \sin(kx+\delta)$ , we find that:

$$@x=0: \quad \psi(0) = A\sin(\delta) \stackrel{!}{=} 0 , \quad \Rightarrow \quad \delta = 0 ,$$

and then:

$$@x=a: \psi(a)\Big|_{\delta=0} = A\sin(ka) \stackrel{!}{=} 0, \Rightarrow ka = n\pi, \text{ for } n = 1, 2, 3, \dots$$

so that  $k = n\pi/a$ . Since  $k^2 = \frac{2m}{\hbar^2}E$ , we have that

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$
,  $n = 1, 2, 3, \dots$ 

are all the allowed values of the energy, corresponding to the stationary states with the wave-functions  $\psi_n(x) = A \sin\left(\frac{n\pi\hbar}{a}x\right)$ . [=10pt]