PHYS : 516 Quantum Mechanics I

Homework #4

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1. Some authors define an *operator* to be real when every member of its matrix elements $\langle b'|A|b''\rangle$ is real in some representation. Is this concept representation independent? That is, do the matrix elements remain real even if some basis other than $\{|b'\rangle\}$ is used? Check your assertion using x and p_x.
Solution:
Let some other basis $|a'\rangle$ be used to represent the matrix then the new basis is related to the old basis by the transformation $|a'\rangle = U|b'\rangle$ where U is some unitary operator.

$$|a'\rangle = U|b'\rangle; \quad \Rightarrow \langle a'| = \langle b'| U^\dagger = \langle b'| U^{-1}$$

The matrix elements in this new basis then become

$$\langle a'|A|a''\rangle = \langle b'|U^{-1}AU|b'\rangle$$

If this has to remain real in the old $|b'\rangle$ basis then it must equal to the old matrix element

$$\langle b'|U^{-1}AU|b'\rangle = \langle b'|A|b''\rangle; \qquad \Rightarrow U^{-1}AU = A; \qquad \Rightarrow AU = UA; \qquad \Rightarrow [U, A] = 0$$

But it is not necessary that the operators U and A commute i.e.,$[U, A] = 0$. Thus the matrix element of an operator may not remain real in a different basis if it is real in one basis.

Checking this assertion with x and p_x. We know that operator x is hermitian in x basis so that the eigenvalues of x in position $|x'\rangle$ basis are real. Which means the the matrix elements $\langle x'|x|x''\rangle = x''\langle x'|x''\rangle = x''\delta(x'-x'')$ are all real because x'' is real eigenvalue of hermitian operator of x.

Now the matrix elements of x operator in p basis are

$$\begin{aligned}\langle p'|x|p''\rangle &= \int \langle p'|x|x'\rangle\langle x'|p''\rangle\, dx' = \int x'\langle p'|x'\rangle\langle x'|p''\rangle \\ &= \frac{1}{2\pi\hbar}\int x' \exp\left(-\frac{ip'x}{\hbar}\right)\exp\left(\frac{ip''x}{\hbar}\right)dx = \frac{1}{2\pi\hbar}\int x'\exp\left(i\frac{(p''-p')x'}{\hbar}\right)dx'\end{aligned}$$

making substitution $t = p'' - p'$ and $y = x'/\hbar$

$$= \frac{1}{2\pi\hbar}\int \hbar y e^{ity}\hbar dy = \frac{\hbar}{2\pi}\int y e^{ity} dy$$

and using differential under integral sign $\frac{d}{dt}\int e^{ity}dy = \int iye^{ity}dy \Rightarrow \int ye^{ity}dy = \frac{1}{i}\frac{d}{dt}\int e^{ity}dy$ we can write the above expression as

$$\langle p'|x|p''\rangle = \frac{\hbar}{2\pi}\frac{1}{i}\frac{d}{dt}\int e^{ity}dy = \frac{\hbar}{2\pi i}\frac{d}{dt}\int e^{i(p''-p')y}dy = \frac{\hbar}{2\pi i}\frac{d}{dt}2\pi\delta(p''-p') = \frac{\hbar}{i}\frac{d}{dt}\delta(p''-p')$$

This value is clearly imaginary as delta function is purely real. This shows that although the matrix elements of operator x in position basis are real the elements are no longer real in momentum basis. ■

2. (a) Suppose that $f(A)$ is a function of a Hermitian operator A with the property $A\left|a'\right\rangle = a'\left|a'\right\rangle$. Evaluate $\langle b''|f(A)|b'\rangle$ when the transformation matrix from the a' basis to the b' basis is known.
Solution:
The matrix element for the transformation matrix are $\left\langle b^{(i)}\middle|a^{(j)}\right\rangle$ for $i, j \in \{1, 2\cdots N\}$ where N is the no of independent state of system. The given expression can be written as

$$\begin{aligned}
\langle b''|f(A)|b'\rangle &= \sum_i \left\langle b''\middle|f(A)\middle|a^i\right\rangle\left\langle a^i\middle|b'\right\rangle && (\because \text{ Inserting } \sum_i \left|a^i\middle\rangle\middle\langle a^i\right| = 1)\\
&= \sum_i \left\langle b''\middle|f(a^i)\middle|a^i\right\rangle\left\langle a^i\middle|b'\right\rangle && (\because f(A)\left|a'\right\rangle = f(a')\left|a'\right\rangle)\\
&= \sum_i f(a^i)\left\langle b''\middle|a^i\right\rangle\left\langle a^i\middle|b'\right\rangle && (\because \langle\alpha|c|\beta\rangle = c\,\langle\alpha|\beta\rangle)
\end{aligned}$$

Since all the matrix elements $\left\langle b''\middle|a^i\right\rangle$ and $\left\langle a^i\middle|b'\right\rangle = \left\langle b'\middle|a^i\right\rangle^*$ are known the expression is completely known. ■

(b) Using the continuum analogue of the result obtained in (**??**), evaluate $\langle \mathbf{p}''|F(r)|\mathbf{p}'\rangle$. Simplify your expression as far as you can. Note that r is $\sqrt{x^2+y^2+z^2}$, where x, y, and z are *operators*.
Solution:
Since the position operators x, y and z are compatible operators (commutative i.e., $[x, y] = 0, [y, z] = 0$ and $[z, x] = 0$) we can represent the position eigenket as $|x', y', z'\rangle \equiv |\mathbf{r}'\rangle$. By problem (**??**) above we get

$$\langle \mathbf{p}''|F(\mathbf{r})|\mathbf{p}'\rangle = \int_{-\infty}^{\infty} F(r')\,\langle \mathbf{p}''|\mathbf{r}'\rangle\,\langle \mathbf{r}'|\mathbf{p}'\rangle\, d^3\mathbf{r}'$$

But we know the wavefunction of momentum in position basis as

$$\langle \mathbf{p}|\mathbf{r}\rangle = e^{-\dfrac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}} \qquad \Rightarrow \langle \mathbf{p}''|\mathbf{r}'\rangle = e^{-\dfrac{i\mathbf{p}''\cdot\mathbf{r}'}{\hbar}} \quad \text{and} \qquad \langle \mathbf{r}'|\mathbf{p}'\rangle = e^{-\dfrac{-i\mathbf{p}'\cdot\mathbf{r}'}{\hbar}}$$

Thus the expression becomes

$$\langle \mathbf{p}''|F(\mathbf{r})|\mathbf{p}'\rangle = \int_{-\infty}^{\infty} F(r')e^{-\dfrac{i(\mathbf{p}'-\mathbf{p}'')\cdot\mathbf{r}'}{\hbar}}\, d^3\mathbf{r}'$$

This integral gives the matrix element of the position operator $F(\mathbf{r})$ in the momentum $\mathbf{p}'$ basis. ■

3. The translation operator for a finite (spatial) displacement is given by

$$\mathfrak{T}(\mathbf{l}) = \exp\left(\frac{-i\mathbf{p}\cdot\mathbf{l}}{\hbar}\right),$$

where $\mathbf{p}$ is the momentum *operator*.

(a) Evaluate $[x_i, \mathfrak{T}(\mathbf{l})]$
Solution:
We can write the dot product of vectors $\mathbf{p}$ and displacement $\mathbf{l}$ as $\mathbf{p}\cdot\mathbf{l} = \sum_i p_i l_i$

$$[x_i, \mathfrak{T}(\mathbf{l})] = \left[x_i, \exp\left(\frac{-i\mathbf{p}\cdot\mathbf{l}}{\hbar}\right)\right] = i\hbar\frac{\partial}{\partial p_i}\exp\left(\frac{-i\sum_i p_i l_i}{\hbar}\right) = i\hbar l_i\left(\frac{-i}{\hbar}\right)\exp\left(-\frac{i\mathbf{p}\cdot\mathbf{l}}{\hbar}\right) = l_i\mathfrak{T}(\mathbf{l})$$

This gives the expression for $[x_i, \mathfrak{T}(\mathbf{l})]$. ■

(b) Using (**??**) (or otherwise), demonstrate how expectation value of $\langle \mathbf{x} \rangle$ changes under translation

Solution:

Let $|\alpha\rangle$ be any arbitrary position ket. Then the expectation value of for one of the component of position of the system (particle) is given by $\langle x_i \rangle = \langle \alpha | x_i | \alpha \rangle$. Let the position ket under translation be $|\beta\rangle \equiv \mathfrak{T}(\mathbf{l}) |\alpha\rangle$. The dual correspondence of this ket is $\langle \beta | = \langle \alpha | \mathfrak{T}(\mathbf{l})^\dagger$. Now the expectation value under translation is

$$\langle \beta | x_i | \beta \rangle = \langle \alpha | \mathfrak{T}(\mathbf{l})^\dagger x_i \mathfrak{T}(\mathbf{l}) | \alpha \rangle \tag{1}$$

But by the commutator relation (**??**) we have

$$[x_i, \mathfrak{T}(\mathbf{l})] = l_i \mathfrak{T}(\mathbf{l}); \qquad \Rightarrow x_i \mathfrak{T}(\mathbf{l}) - \mathfrak{T}(\mathbf{l}) x_i = l_i \mathfrak{T}(\mathbf{l})$$

Since we know that the translation operator is Unitary, $\mathfrak{T}(\mathbf{l})^\dagger \mathfrak{T}(\mathbf{l}) = 1$. Operating on both sides of this expression by $\mathfrak{T}(\mathbf{l})^\dagger$ we get

$$\begin{aligned} & \mathfrak{T}(\mathbf{l})^\dagger \{x_i \mathfrak{T}(\mathbf{l}) - \mathfrak{T}(\mathbf{l}) x_i\} = \mathfrak{T}(\mathbf{l})^\dagger l_i \mathfrak{T}(\mathbf{l}) \\ \Rightarrow \quad & \mathfrak{T}(\mathbf{l})^\dagger x_i \mathfrak{T}(\mathbf{l}) - \mathfrak{T}(\mathbf{l})^\dagger \mathfrak{T}(\mathbf{l}) x_i = l_i \mathfrak{T}(\mathbf{l})^\dagger \mathfrak{T}(\mathbf{l}) \\ \Rightarrow \quad & \mathfrak{T}(\mathbf{l})^\dagger x_i \mathfrak{T}(\mathbf{l}) = x_i + l_i \end{aligned}$$

Using this in (**??**) we get

$$\langle \beta | x_i | \beta \rangle = \langle \alpha | x_i + l_i | \alpha \rangle = \langle \alpha | x_i | \alpha \rangle + \langle \alpha | l_i | \alpha \rangle = \langle \alpha | x_i | \alpha \rangle + l_i$$

Now that we have found the expectation value of every component of $\mathbf{x}$ operator. The expression for this operator becomes

$$\langle \beta | x_i | \beta \rangle = \langle \alpha | x_i | \alpha \rangle + l_i; \qquad \Rightarrow \langle \mathbf{x} \rangle \xrightarrow{\mathfrak{T}(\mathbf{l})} \langle \mathbf{x} \rangle_{\text{old}} + \mathbf{l}$$

This gives the expectation value of position operator under translation. ■

4. For a Gaussian wave packet, whose wave function is position space is given by

$$\langle x' | \alpha \rangle = \left[\frac{1}{\sqrt{d\sqrt{\pi}}} \right] \exp \left[ikx' - \frac{x'^2}{2d^2} \right]$$

(a) Verify $\langle p \rangle = \hbar k$ and $\langle p^2 \rangle = \frac{\hbar^2}{2d^2} + \hbar^2 k^2$

Solution:

The expectation value of momentum p in the state $|\alpha\rangle$ is given by $\langle p \rangle = \langle \alpha | p | \alpha \rangle$. But by completeness of the position basis kets we can write the state $|\alpha\rangle$ as

$$\langle p \rangle = \langle \alpha | p | \alpha \rangle = \int dx' \, \langle \alpha | x' \rangle \, \langle x' | p | \alpha \rangle$$

But the operator identity

$$\langle x' | p | \alpha \rangle = -i\hbar \frac{\partial}{\partial x'} \langle x' | \alpha \rangle$$

Enables us to write

$$
\begin{aligned}
\langle p \rangle &= \int_{-\infty}^{\infty} dx' \, \langle \alpha | x' \rangle \left(-i\hbar \frac{\partial}{\partial x'} \right) \langle x' | \alpha \rangle \\
&= \int_{-\infty}^{\infty} dx' \left[\frac{1}{\sqrt{d\sqrt{\pi}}} \right] \exp\left[-ikx' - \frac{x'^2}{2d^2} \right] \left(-i\hbar \frac{\partial}{\partial x'} \right) \left[\frac{1}{\sqrt{d\sqrt{\pi}}} \right] \exp\left[ikx' - \frac{x'^2}{2d^2} \right] \\
&= \frac{1}{d\sqrt{\pi}} \int_{-\infty}^{\infty} dx' \left(-i\hbar \left(ik - \frac{x'}{d^2} \right) \right) \exp\left(-\frac{x'^2}{d^2} \right) \\
&= \frac{1}{d\sqrt{\pi}} \left[\hbar k \int_{-\infty}^{\infty} dx' \exp\left(-\frac{x'^2}{d^2} \right) + \frac{i\hbar}{d^2} \int_{-\infty}^{\infty} x' \exp\left(-\frac{x'^2}{d^2} \right) \right] \\
&= \frac{1}{d\sqrt{\pi}} \left[\hbar k \sqrt{\pi} d + \frac{i\hbar}{d^2} 0 \right] \\
&= \hbar k
\end{aligned}
$$

Smilarly the expectation value of operator p^2 can be written as

$$
\begin{aligned}
\langle p^2 \rangle &= \int_{-\infty}^{\infty} dx' \, \langle \alpha | x' \rangle \left(-i\hbar \frac{\partial}{\partial x'} \right)^2 \langle x' | \alpha \rangle \\
&= \int_{-\infty}^{\infty} dx' \left[\frac{1}{\sqrt{d\sqrt{\pi}}} \right] \exp\left[-ikx' - \frac{x'^2}{2d^2} \right] \left(-\hbar^2 \frac{\partial^2}{\partial x'^2} \right) \left[\frac{1}{\sqrt{d\sqrt{\pi}}} \right] \exp\left[ikx' - \frac{x'^2}{2d^2} \right] \\
&= \frac{1}{d\sqrt{\pi}} \int_{-\infty}^{\infty} dx' \left(\frac{\hbar^2}{d^2} - \hbar^2 \left(ik - \frac{x'}{d^2} \right)^2 \right) \exp\left(-\frac{x'^2}{d^2} \right) \\
&= \frac{1}{d\sqrt{\pi}} \int_{-\infty}^{\infty} dx' \left(\frac{\hbar^2}{d^2} + \hbar^2 k^2 + \frac{2ik\hbar^2}{d^2} - \frac{\hbar^2 x'^2}{d^4} \right) \exp\left(-\frac{x'^2}{d^2} \right) \\
&= \frac{1}{d\sqrt{\pi}} \left[\left(\frac{\hbar^2}{d^2} + \hbar^2 k^2 \right) \int_{-\infty}^{\infty} \exp\left(-\frac{x'^2}{d^2} \right) dx' + \frac{2ik\hbar^2}{d^2} \int_{-\infty}^{\infty} x' \exp\left(-\frac{x'^2}{d^2} \right) dx' - \frac{\hbar^2}{d^4} \int_{-\infty}^{\infty} x'^2 \exp\left(-\frac{x'^2}{d^2} \right) dx' \right] \\
&= \frac{1}{d\sqrt{\pi}} \left[\left(\frac{\hbar^2}{d^2} + \hbar^2 k^2 \right) \sqrt{\pi} d + \frac{2ik\hbar^2}{d^2} 0 - \frac{\hbar^2}{d^4} \left(\frac{\sqrt{\pi} d^3}{2} \right) \right] \\
&= \frac{\hbar^2}{d^2} + \hbar^2 k^2 - \frac{\hbar^2}{2d^2} \\
&= \frac{\hbar^2}{2d^2} + \hbar^2 k^2
\end{aligned}
$$

Thus the expectation values of the wavefunction is found as required. ■

(b) Evaluate the expectation value of p and p^2 usig the momentum-space wave functions as well.
Solution:
For the momentum space wave functions we can write

$$
\begin{aligned}
\langle p \rangle &= \int \langle \alpha | p | p' \rangle \langle p' | \alpha \rangle \, dp' = \int p' |\langle p' | \alpha \rangle|^2 dp' \\
&= \frac{d}{\hbar\sqrt{\pi}} \int p' \exp\left[-\frac{(p' - \hbar k)^2 d^2}{\hbar^2} \right] dp' \\
&= \frac{d}{\hbar\sqrt{\pi}} \left[\int p' \exp\left(-\frac{d^2}{\hbar^2} \right) dp' + \int p' \exp\left(\frac{(p - \hbar k)^2}{\hbar^2} \right) dp' \right] \\
&= \frac{d}{\hbar\sqrt{\pi}} \left[\frac{\hbar^2 k \sqrt{\pi}}{d} \right] = \hbar k
\end{aligned}
$$

Now for the expectation value of the square of momentum operator.

$$\begin{aligned}
\langle p^2 \rangle &= \int \langle \alpha | p | p' \rangle \langle p' | \alpha \rangle \, dp' = \int p'^2 |\langle p' | \alpha \rangle|^2 dp' \\
&= \frac{d}{\hbar\sqrt{\pi}} \int p'^2 \exp\left[-\frac{(p' - \hbar k)^2 d^2}{\hbar^2} \right] dp' \\
&= \frac{d}{\hbar\sqrt{\pi}} \left(\frac{\sqrt{\pi}}{2} \frac{\hbar^3}{d^3} + \frac{\hbar^3 k^2 \sqrt{\pi}}{d} \right) \\
&= \frac{\hbar^2}{2d^2} + \hbar^2 k^2
\end{aligned}$$

So the expectation value of the operators are the smae in the momentum state wave functions too. ■