PHYS30201 Mathematical Fundamentals of Quantum Mechanics 2016-17: Examples 2

You may use the following result for Gaussian integrals:
$\int_{-\infty}^{\infty} \mathrm{e}^{-\alpha x^2}\,\mathrm{d}x = \sqrt{\pi/\alpha}$, and $\int_{-\infty}^{\infty} x^{2n}\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\alpha^n}\sqrt{\frac{\pi}{\alpha}}$.

1. Which of the following are well-constructed expressions? State whether they are scalars, kets, bras or operators. Assume the usual notation is being used to distinguish between, say, an operator $\hat{A}$ and a scalar β. If it is a ket, write down the corresponding bra and vice versa; if an operator, write down its adjoint (for $\hat{A}$, that will just be $\hat{A}^\dagger$).

   (i) $\hat{A}|b\rangle + \beta|d\rangle$ (ii) $\beta\langle d| + \langle c|\alpha^*$ (iii) $|a\rangle\langle b| + \hat{A} + \beta$ (iv) $\langle b|a\rangle\hat{G}$ (v) $|a\rangle\langle b|\hat{G}$
   (vi) $|a\rangle\hat{G}\langle b|$ (vii) $|a\rangle|b\rangle\langle c|$ (viii) $\big(\hat{F}\otimes\hat{G}\big)\big(|a\rangle\otimes|b\rangle\big)$ (ix) $\hat{Q}\big(|a\rangle\otimes|b\rangle + |\heartsuit\rangle\big)$

2. Consider the set of orthogonal normalised basis functions

$$\{\phi_0(x) = N_0\mathrm{e}^{-x^2/2},\ \phi_1(x) = N_1 x\mathrm{e}^{-x^2/2},\ \phi_2(x) = N_2(2x^2-1)\mathrm{e}^{-x^2/2},\ \phi_3(x) = N_3(2x^3-3x)\mathrm{e}^{-x^2/2}\ldots\}.$$

   which can also be considered the representations of the vectors $\{|n\rangle\}$, noting that $|0\rangle$ is NOT the zero vector!
   i) Find N_0, N_1 and N_2.
   ii) Verify that $\langle 0|2\rangle = 0$
   iii) If $f(x) = 2i\phi_0(x) + 3\phi_2(x)$ and $g(x) = 4\phi_0(x) - i\phi_2(x)$, find $\langle f|g\rangle$.
   iv) If we expand $f(x) = x^2\mathrm{e}^{-x^2/2}$ in this basis, $f(x) = \sum_{n=0}^{\infty} f_n\phi_n(x)$, find the first four coefficients $f_0, ..f_3$.

3. Verify that $-i\frac{\mathrm{d}}{\mathrm{d}x}$ and $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ are Hermitian operators in the space of functions which vanish at $\pm\infty$.

4. Show that if we write $\phi(x) \equiv f(x)\mathrm{e}^{-x^2/2}$, the first of the following two differential eigenvalue equations implies the second:

$$-\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} + x^2\phi = \mathcal{E}\phi \quad\Rightarrow\quad \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}f}{\mathrm{d}x} + (\mathcal{E}-1)f = 0$$

   Hence verify that the square-integrable solutions $\phi(x)$ of the first equation are obtained if $f(x)$ is a Hermite polynomial, with the allowed values of $\mathcal{E}$ being the positive odd integers.

5. Find the matrix elements $\langle 1|\hat{D}|0\rangle$ and $\langle 2|\hat{D}^2|0\rangle$ where $|n\rangle$ refers to the basis functions of qu. 2.

6. If $|f\rangle$ corresponds to some square-integrable function $f(x)$, $|n\rangle$ corresponds to the basis functions of qu. 2, and $|f\rangle = \sum_{n=0}^{\infty} f_n|n\rangle$, show that

$$\text{(i) } f_n = \langle n|f\rangle \qquad \text{(ii) } \langle f|g\rangle = \sum_{n=0}^{\infty} f_n^* g_n; \qquad \text{(iii) } \langle f|f\rangle = \sum_{n=0}^{\infty}|f_n|^2 < \infty.$$

7. In this question, $\hat{A}$, $\hat{B}$ and $\hat{C}$ are arbitrary operators in any space. $\hat{K}(\equiv \hat{K}_x)$ and $\hat{X}$ are the operators in function space defined in lectures, as are $\hat{Y}$, $\hat{Z}$, $\hat{K}_y$, $\hat{K}_z$ and the vector operators $\hat{\mathbf{X}}$ and $\hat{\mathbf{K}}$ of which these are components.

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

   ii) Show that $[\hat{A}, \hat{A}^n] = 0$.

   iii) If $[\hat{A}, \hat{B}] = c\hat{I}$, where c is a number, show that $[\hat{A}, \hat{B}^n] = cn\hat{B}^{n-1}$

   iv) Let $Q(x)$ be a polynomial with derivative $R(x)$, and let $\hat{Q} = Q(\hat{X})$ and $\hat{R} = R(\hat{X})$. Show that $[\hat{K}, \hat{Q}] = -i\hat{R}$.
   (Hint: in this part and the following one, you should only use the commutation rules, not the representations of the operators.)

   v) Defining $\hat{L}_x = \hbar(\hat{Y}\hat{K}_z - \hat{Z}\hat{K}_y)$, show that

   $$\text{(a) } [\hat{L}_x, \hat{X}] = [\hat{L}_x, \hat{K}_x] = 0; \qquad \text{(b) } [\hat{L}_x, \hat{Y}] = i\hbar\hat{Z} \qquad \text{(c) } [\hat{L}_x, \hat{K}_z] = -i\hbar\hat{K}_y.$$

   vi) Given a function of x, y and z, $V(\mathbf{r})$, show that in the position representation

   $$[\hat{\mathbf{K}}, V(\hat{\mathbf{X}})] \underset{x}{\longrightarrow} -i\,\nabla V(\mathbf{r}).$$

   (Hint: consider the commutator acting on some arbitrary state $|f\rangle \underset{x}{\longrightarrow} f(\mathbf{r})$.)
   Hence for a spherically symmetric function $V(\mathbf{r}) \equiv V(r)$, with (as usual) $r = |\mathbf{r}|$, show that $[\hat{\mathbf{K}}, V(\hat{\mathbf{X}}))] \underset{x}{\longrightarrow} -i\,\hat{\mathbf{r}}\dfrac{\mathrm{d}V}{\mathrm{d}r}$ (where $\hat{\mathbf{r}} \equiv \mathbf{r}/r$ is a unit vector, not an operator!).

8. Write down the representations in the x- and k-bases of the particular eigenstate of $\hat{\mathbf{K}}$, $|\mathbf{k}_0\rangle$, for which $\mathbf{k}_0 = \big(2\,\mathbf{e}_x - \mathbf{e}_z\big)$.

9. Verify the result from lectures, that $f(x)$ is the inverse Fourier transform of $F(k) = \langle k|f\rangle$. (Hint: Start with $f(x) = \langle x|f\rangle$ and insert the representation of the identity operator in the k-basis.)

10. Since $\hat{K}$ is Hermitian, $\langle k|\hat{K}|f\rangle = k\langle k|f\rangle$. Show that this still works in x-representation, by inserting $\hat{I} = \int |x\rangle\langle x|\mathrm{d}x$ before the $\hat{K}$. (This demonstrates that if $F(k)$ is the Fourier transform of $f(x)$, $kF(k)$ is the Fourier transform of $-i\dfrac{\mathrm{d}f}{\mathrm{d}x}$.)

11. Find $\Phi_0(k) \equiv \langle k|0\rangle$, if $\langle x|0\rangle = \phi_0(x)$ from qu. 2. Check that $\Phi_0(k)$ is normalised. Without calculation, but with reference the fact that the $|n\rangle$ are eigenstates of $\hat{K}^2 + \hat{X}^2$, write down $\Phi_n(k) \equiv \langle k|n\rangle$.