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

1. i) Ket; bra is $\langle b|\hat{A}^\dagger + \langle d|\beta^*$.
   ii) Bra; ket is $\beta^*|d\rangle + \alpha|c\rangle$. Note the placement of the scalars is purely conventional.
   iii) Strictly, nothing. Assuming $\beta\hat{I}$ is meant, it is an operator with adjoint $|b\rangle\langle a| + \hat{A}^\dagger + \beta^*\hat{I}$.
   iv) Operator with adjoint $\hat{G}^\dagger\langle a|b\rangle$
   v) Operator with adjoint $\hat{G}^\dagger|b\rangle\langle a|$
   vi) Nothing. An operator $\hat{G}$ cannot sit to the left of a bra or the right of a ket. (Example (iv) doesn't contradict this, as $\hat{G}$ is on the right of an inner product, not a ket.)
   vii) Nothing
   viii) Ket; bra is $\big(\langle a|\otimes\langle b|\big)\big(\hat{F}^\dagger\otimes\hat{G}^\dagger\big) = \big(\langle a|\hat{F}^\dagger\big)\otimes\big(\langle b|\hat{G}^\dagger\big)$
   ix) We can't tell. IF $|\heartsuit\rangle$ is in the product space (while $|a\rangle$ and $|b\rangle$ are in the individual spaces), and if $\hat{Q}$ is an operator in the product space, then this is a ket in the product space with bra $\big(\langle a|\otimes\langle b| + \langle\heartsuit|\big)\hat{Q}^\dagger$. If $\hat{Q}$ is an operator in one of the individual spaces and it is clear which, i.e. $\hat{Q}\otimes\hat{I}$ or $\hat{I}\otimes\hat{Q}$ is implied, the expression would still make sense as a ket. However there is no acceptable interpretation in which $|\heartsuit\rangle$ is not in the product space.

2. i) $N_0 = 1/\sqrt[4]{\pi}$, $N_1 = \sqrt{2}N_0$, $N_2 = N_0/\sqrt{2}$, $N_3 = N_0/\sqrt{3}$
   ii) $\langle 0|2\rangle = N_0N_2\int_{-\infty}^{\infty}\phi_0^*(x)\phi_2(x)\mathrm{d}x = N_0N_2\int_{-\infty}^{\infty}(2x^2-1)\mathrm{e}^{-x^2}\mathrm{d}x = 0$.
   iii) $\langle f|g\rangle = \big(-2i\langle 0| + 3\langle 2|\big)\big(4|0\rangle - i|2\rangle + 4i|3\rangle\big) = -11i$. Note the need to take the complex conjugate of the coefficients of $|f\rangle$. We have used $\langle m|n\rangle = \delta_{mn}$.
   iv) By inspection we see that $f(x) = \phi_2(x)/(2N_2) + \phi_0(x)/(2N_0)$. So $f_0 = \pi^{1/4}/2$, $f_2 = \pi^{1/4}/\sqrt{2}$, $f_1 = f_3 = 0$ (and indeed $f_n = 0$ for all other n).

3.
$$\begin{aligned}
\langle f|\hat{K}|g\rangle = -i\int_{-\infty}^{\infty} f^*(x)\frac{\mathrm{d}g}{\mathrm{d}x}\,\mathrm{d}x &= \Big[-if^*g\Big]_{-\infty}^{\infty} + i\int_{-\infty}^{\infty}\frac{\mathrm{d}f^*}{\mathrm{d}x}g(x)\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\left(-i\frac{\mathrm{d}f}{\mathrm{d}x}\right)^* g(x)\,\mathrm{d}x = \langle g|\hat{K}|f\rangle^* \\
\langle f|\hat{D}^2|g\rangle = \int_{-\infty}^{\infty} f^*(x)\frac{\mathrm{d}^2g}{\mathrm{d}x^2}\,\mathrm{d}x &= \Big[f^*g'\Big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\mathrm{d}f^*}{\mathrm{d}x}\frac{\mathrm{d}g}{\mathrm{d}x}\,\mathrm{d}x \\
&= -\Big[f^{*\prime}g\Big]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{\mathrm{d}^2f^*}{\mathrm{d}x^2}g(x)\,\mathrm{d}x = \langle g|\hat{D}^2|f\rangle^*
\end{aligned}$$

   where we have used the fact that f and g vanish at $x = \pm\infty$ to drop the boundary terms.

4. The equation for f would be Hermite's equation if $\mathcal{E} - 1$ were replaced by $2n$. The finite solutions of Hermite's equation (those in which the recursion relation for the coefficients of a series solution terminates) are those for which n is an non-negative integer. Hence we need $\mathcal{E} - 1 = 2n$, i.e. $\mathcal{E}$ is a positive odd integer. (See the course notes appendix.)

5. We can do this question with Gaussian integrals: $\langle 1|\hat{D}|0\rangle = \int_{-\infty}^{\infty}\phi_1(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi_0(x)\mathrm{d}x$ etc. However an easier way is to use orthogonality of the basis functions as follows.
   By explicit differentiation of the corresponding function $\phi_0(x)$, we find $\hat{D}|0\rangle = -N_0/N_1|1\rangle$ and $\hat{D}|1\rangle = N_1/(2N_0)|0\rangle - N_1/(2N_2)|2\rangle$. So:
   $\langle 1|\hat{D}|0\rangle = -N_0/N_1 = -1/\sqrt{2}$ and $\langle 2|\hat{D}^2|0\rangle = N_0/(2N_2) = 1/\sqrt{2}$.

6. i) If $|f\rangle = \sum_{n=0}^{\infty} f_n|n\rangle$, then $\langle n|f\rangle = \sum_{m=0}^{\infty} f_m\langle n|m\rangle = \sum_{m=0}^{\infty} f_m\delta_{mn} = f_n$ as required. (Note the need to choose another dummy variable if we are using n as our free varible.)

   ii) Inserting the identity operator, we have $\langle f|g\rangle = \sum_{n=0}^{\infty}\langle f|n\rangle\langle n|g\rangle = \sum_{n=0}^{\infty} f_n^* g_n$.

   iii) From (ii) $\langle f|f\rangle = \sum_{n=0}^{\infty}|f_n|^2$. But $\langle f|f\rangle = \int_{-\infty}^{\infty} f^*(x)f(x)\,\mathrm{d}x$ also, and that must be finite if f is square integrable. So $\sum_{n=0}^{\infty}|f_n|^2 < \infty$.

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

   ii) $[\hat{A},\hat{A}^n] = \hat{A}(\hat{A}\hat{A}\ldots\hat{A}) - (\hat{A}\hat{A}\ldots\hat{A})\hat{A} = \hat{A}^{n+1} - \hat{A}^{n+1} = 0$.

   iii) First note that $\hat{A}\hat{B} = \hat{B}\hat{A} + c\hat{I}$, so $\hat{B}^m\hat{A}\hat{B}^{n-m} = \hat{B}^{m+1}\hat{A}\hat{B}^{n-m-1} + c\hat{B}^{n-1}$. Using this repeatedly, we can take $\hat{A}$ through the list of $\hat{B}$s in n steps, picking up a term $c\hat{B}^{n-1}$ at each step. So $\hat{A}\hat{B}^n = \hat{B}^n\hat{A} + nc\hat{B}^{n-1}$.
   We can also do it by induction: *assume* it is true for some k: $[\hat{A},\hat{B}^k] = ck\hat{B}^{k-1}$. Then

$$[\hat{A},\hat{B}^{k+1}] = [\hat{A},\hat{B}^k\hat{B}] = [\hat{A},\hat{B}^k]\hat{B} + \hat{B}^k[\hat{A},\hat{B}] = ck\hat{B}^{k-1}\hat{B} + c\hat{B}^k = c(k+1)\hat{B}^k;$$

   so if it holds for $n = k$ it also holds for $n = k+1$. But it is true by definition for $n = 1$, so it is true for all $n \geq 1$.

   iv) Let $Q(x) = \sum_m q_m x^m$, so $R(x) = \sum_m m q_m x^{m-1}$. Then from the result above, with $c = -i$, $[\hat{K},\hat{Q}] = -i\sum_m q_m[\hat{K},\hat{X}^m] = -i\sum_m m q_m\hat{X}^{m-1} = -i\hat{R}$.
   An alternative approach is as follows. Let $|f\rangle$ be an arbitrary vector; then in the x-representation, $\langle x|\hat{Q}|f\rangle = Q(x)f(x)$. Then

$$\begin{aligned}[\hat{K},\hat{Q}]|f\rangle \underset{x}{\longrightarrow} \langle x|\hat{K}\hat{Q} - \hat{Q}\hat{K}|f\rangle &= \int \langle x|\hat{K}|x'\rangle\langle x'|\hat{Q}|f\rangle - \langle x|\hat{Q}|x'\rangle\langle x'|\hat{K}|f\rangle \mathrm{d}x' \\ &= -i\int \delta(x-x')\Big(\frac{\mathrm{d}}{\mathrm{d}x'}(Q(x')f(x')) - Q(x')\frac{\mathrm{d}}{\mathrm{d}x'}f(x')\Big) = -i\frac{\mathrm{d}Q}{\mathrm{d}x}f(x) = -iR(x)f(x)\end{aligned}$$

   With experience, we can just write

$$[\hat{K},\hat{Q}]|f\rangle \underset{x}{\longrightarrow} -i\left(\frac{\mathrm{d}Qf}{\mathrm{d}x} - Q(x)\frac{\mathrm{d}f}{\mathrm{d}x}\right) = -i\frac{\mathrm{d}Q}{\mathrm{d}x}f(x) = -iR(x)f(x).$$

   Since $|f\rangle$ and hence $f(x)$ is arbitrary, this must imply the operator relation $[\hat{K},\hat{Q}] = -i\hat{R}$.

   v) We can use $[\hat{A},\hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}] + [\hat{A},\hat{B}]\hat{C}$ and $[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$ to reduce the compound commutators to simple ones, without ever writing expressions like $\hat{A}\hat{B} - \hat{B}\hat{A}$. Clearly if $\hat{A}$ commutes with $\hat{B}$ and $\hat{C}$, it commutes with the product $\hat{B}\hat{C}$.
   Furthermore we use the fact that the only non-vanishing commutators among the $\hat{X}_i$ and $\hat{K}_j$ are $[\hat{X}_i,\hat{K}_i] = i\hat{I}$.
   (a) $[\hat{L}_X,\hat{X}] = [\hat{L}_X,\hat{K}_X] = 0$ because $\hat{X}$ and $\hat{K}_X$ commute with all of $\hat{Y}$, $\hat{K}_Z$, $\hat{Z}$ and $\hat{K}_Y$.
   (b) $[\hat{L}_X,\hat{Y}] = \hbar[\hat{Y}\hat{K}_Z,\hat{Y}] - \hbar[\hat{Z}\hat{K}_Y,\hat{Y}] = 0 - \hbar\hat{Z}[\hat{K}_Y,\hat{Y}] - \hbar[\hat{Z},\hat{Y}]\hat{K}_Y = i\hbar\hat{Z}$.
   (c) $[\hat{L}_X,\hat{K}_Z] = -\hbar[\hat{Z}\hat{K}_Y,\hat{K}_Z] = -\hbar[\hat{Z},\hat{K}_Z]\hat{K}_Y = -i\hbar\hat{K}_Y$.

   The full set of relations like these are

$$[\hat{L}_i,\hat{X}_j] = i\hbar\sum_k \epsilon_{ijk}\hat{X}_k \qquad [\hat{L}_i,\hat{K}_j] = i\hbar\sum_k \epsilon_{ijk}\hat{K}_k$$

   where $\epsilon_{ijk} = 1$ if i,j,k is a cyclic permutation of $1,2,3$, -1 if an anticylic permutation such as $2,1,3$ and 0 if any two indices are the same, and we have defined $\{\hat{X}_1,\hat{X}_2,\hat{X}_3\} \equiv \{\hat{X},\hat{Y},\hat{Z}\}$.

vi) In the x-representation (see part (iv)), we have

$$[\hat{\mathbf{K}}, V(\hat{\mathbf{X}})]|f\rangle \underset{\mathbf{x}}{\longrightarrow} -i\Big(\nabla\big(V(\mathbf{r})f(\mathbf{r})\big) - V(\mathbf{r})\nabla f(\mathbf{r})\Big) = \big(-i\nabla V(\mathbf{r})\big)f(\mathbf{r}).$$

However since $|f\rangle$ is arbitrary, the relation must hold for the operators:
$[\hat{\mathbf{K}}, V(\hat{\mathbf{X}})] \underset{x}{\longrightarrow} -i\,\nabla V(\mathbf{r})$.
If $V = V(r)$,

$$\nabla V = \sum_i \mathbf{e}_i \frac{\partial}{\partial x_i} V(r) = \sum_i \mathbf{e}_i \frac{\partial r}{\partial x_i}\frac{\mathrm{d}V(r)}{\mathrm{d}r} = \sum_i \mathbf{e}_i \frac{x_i}{r}\frac{\mathrm{d}V(r)}{\mathrm{d}r} = \hat{\mathbf{r}}\frac{\mathrm{d}V}{\mathrm{d}r}.$$

8. If $\mathbf{k}_0 = \big(2\,\mathbf{e}_x - \mathbf{e}_z\big)$—or $(2, 0, -1)$ in coordinate notation,

$\langle \mathbf{r}|\mathbf{k}_0\rangle = (\frac{1}{2\pi})^{3/2}\mathrm{e}^{i\mathbf{k}_0\cdot\mathbf{r}} = (\frac{1}{2\pi})^{3/2}\mathrm{e}^{i(2x-z)}$ and $\langle \mathbf{k}|\mathbf{k}_0\rangle = \delta(\mathbf{k}-\mathbf{k}_0) = \delta(k_x-2)\delta(k_y-0)\delta(k_z+1)$

9. $f(x) \equiv \langle x|f\rangle = \int_{-\infty}^{\infty}\langle x|k\rangle\langle k|f\rangle\,\mathrm{d}k = \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{ikx}F(k)\,\mathrm{d}k$, so $f(x)$ is the inverse F. T. of $F(k)$.

10.
$$\begin{aligned}\langle k|\hat{K}|f\rangle &= \int_{-\infty}^{\infty}\langle k|x\rangle\langle x|\hat{K}|f\rangle\,\mathrm{d}x = -i\sqrt{\tfrac{1}{2\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-ikx}\frac{\mathrm{d}f}{\mathrm{d}x}\,\mathrm{d}x\\ &= i\sqrt{\tfrac{1}{2\pi}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\mathrm{e}^{-ikx}}{\mathrm{d}x}f(x)\,\mathrm{d}x = k\sqrt{\tfrac{1}{2\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-ikx}f(x)\,\mathrm{d}x = kF(k)\end{aligned}$$

11.
$$\begin{aligned}\Phi_0(k) = \langle k|0\rangle &= \int_{-\infty}^{\infty}\langle k|x\rangle\langle x|0\rangle\,\mathrm{d}x = N_0(2\pi)^{-1/2}\int_{-\infty}^{\infty}\mathrm{e}^{-ikx}\mathrm{e}^{-x^2/2}\mathrm{d}x\\ &= N_0(2\pi)^{-1/2}\mathrm{e}^{-k^2/2}\int_{-\infty}^{\infty}\mathrm{e}^{-(x+ik)^2/2}\mathrm{d}x = N_0\,\mathrm{e}^{-k^2/2}\end{aligned}$$

where to obtain the second-last expression we used the trick of completing the square, and then to perform the Gaussian integral we have changed variable $x = x' - ik$; those who have done the “complex variables” course know that this is legitimate. (See the course notes appendix.) It is easy to see that $\Phi_0(k)$ is normalised.

The states $|n\rangle$ are eigenstates of $\hat{K}^2 + \hat{X}^2$. The symmetry between k and x is obvious; the differential equation in the k-basis is identical in form to that in the x-representation, and the solutions are $\Phi_n(k) = N_n H_n(k)\mathrm{e}^{-k^2/2}$. (If one carries out the Fourier transform, the result may differ by a phase such as i or -1.)