**PH30030: Quantum Mechanics      Problems Sheet 1 Solutions**

1. a) We require $A^2 \int_0^a dx \sin^2\left(\frac{n\pi x}{a}\right) = 1$. From the useful integrals we get $\int_0^a dx \sin^2\left(\frac{n\pi x}{a}\right) = \left[\frac{x}{2} - \frac{a}{4n\pi}\sin\left(\frac{2n\pi x}{a}\right)\right]_0^a = \frac{a}{2}$. Therefore $A = \sqrt{\frac{2}{a}}$.

   b) We require $A^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dr\, r^2 \exp\left(-2r/a_0\right) = 1$. The $\theta$ and $\phi$ integrals give $4\pi$. From the useful integrals we get $\int_0^{\infty} dr\, r^2 \exp\left(-2r/a_0\right) = \frac{2}{\left(2/a_0\right)^3}$. Therefore $A = \sqrt{\frac{1}{\pi a_0^3}}$.

   c) We require $A^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \sin^2\theta = 1$. The $\phi$ integral gives $2\pi$. From the useful integrals we get $\int_0^{\pi} d\theta \sin^3\theta = \left[\frac{1}{3}\cos^3\theta - \cos\theta\right]_0^{\pi} = \frac{4}{3}$. Therefore $A = \sqrt{\frac{3}{8\pi}}$.

2. a) i), ii), iii) and vii) are linear. iv), v) and vi) are non-linear.

   b) i) & ii) do not commute; ii) & iii) commute; i) & vii) commute; ii) & vii) do not commute.

3. a) Follow the analysis we did in the lecture notes for $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$. You will find that $\frac{d}{dx}$ is not Hermitian, because we need the $i$ in the momentum operator to make the signs work out.

   b) The kinetic energy operator in 1D is $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$. We are trying to show (see the definition of an Hermitian operator in the lecture notes) that $\int dx\; f_1^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) f_2(x) = \int dx \left(\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) f_1(x)\right)^* f_2(x)$. I won't go through the details but, by integrating by parts twice, you can show that the two sides of this equation are the same.

4. a) The 3D momentum operator is $\underline{\hat{p}} = -i\hbar\underline{\nabla} = -i\hbar\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$. Operate with this on $\exp\left(i\underline{k}.\underline{r}\right) = \exp\left(i\left(k_x x + k_y y + k_z z\right)\right)$. We find $\frac{\partial}{\partial x}\exp\left(i\underline{k}.\underline{r}\right) = ik_x \exp\left(i\underline{k}.\underline{r}\right)$, and similarly for $y$ and $z$. Therefore $\underline{\hat{p}}\exp\left(i\underline{k}.\underline{r}\right) = \hbar\left(k_x, k_y, k_z\right)\exp\left(i\underline{k}.\underline{r}\right) = \hbar\underline{k}\exp\left(i\underline{k}.\underline{r}\right)$. This shows that $\exp\left(i\underline{k}.\underline{r}\right)$ is an eigenfunction of $\underline{\hat{p}}$.

b) From above, the eigenvalue is $\hbar\underline{k}$.

5. We want to show that $\frac{2}{a}\int_0^a dx \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right) = 0$ if $m \neq n$. The useful integrals can be used to show that this is the case.

6. We have $\psi = \sum_n c_n \phi_n$, so $\psi^* \psi = \sum_{m,n} c_m^* c_n \phi_m^* \phi_n$. Integrate both sides of this equation over the relevant region of space. The left hand side gives 1 because $\psi$ is normalised. Because the eigenfunctions $\phi$ are normalised and orthogonal, $\int \phi_m^* \phi_n = \delta_{mn}$, so the right hand side becomes $\sum_{m,n} c_m^* c_n \delta_{mn} = \sum_n \left|c_n\right|^2$. Therefore $\sum_n \left|c_n\right|^2 = 1$.

7. a) $\phi_1^* \phi_1 = \frac{1}{13}\left(2\chi_1^* + 3\chi_2^*\right)\left(2\chi_1 + 3\chi_2\right) = \frac{1}{13}\left(4\chi_1^*\chi_1 + 6\chi_1^*\chi_2 + 6\chi_2^*\chi_1 + 9\chi_2^*\chi_2\right)$. Integrate both sides over the relevant region of space and use the fact that $\chi_1$ and $\chi_2$ are normalised and orthogonal to each other. We then find that $\int \phi_1^* \phi_1 = 1$, as expected. In a similar way, we can show that $\int \phi_2^* \phi_2 = 1$ and $\int \phi_1^* \phi_2 = 0$.

b) We treat

$$\phi_1 = \frac{2}{\sqrt{13}}\chi_1 + \frac{3}{\sqrt{13}}\chi_2 \qquad (1)$$

$$\phi_2 = \frac{3}{\sqrt{13}}\chi_1 - \frac{2}{\sqrt{13}}\chi_2 \qquad (2)$$

as a pair of simultaneous equations for $\chi_1$ and $\chi_2$. Solving them, we find

$$\chi_1 = \frac{2}{\sqrt{13}}\phi_1 + \frac{3}{\sqrt{13}}\phi_2 \qquad (3)$$

$$\chi_2 = \frac{3}{\sqrt{13}}\phi_1 - \frac{2}{\sqrt{13}}\phi_2 \qquad (4)$$

c) We know that the state of the system after the first measurement is $\phi_1$, because $\alpha_1$ was measured. When the observable corresponding to $\hat{B}$ is measured, we know from equation (1) that the probability of measuring $\beta_1$ is $4/13$ and the probability of measuring $\beta_2$ is $9/13$. *If* the $\hat{B}$ measurement gives $\beta_1$, then the state of the system becomes $\chi_1$ and equation (3) shows that the probability of measuring $\alpha_1$ again is $4/13$. *If* the $\hat{B}$ measurement gives $\beta_2$, then the state of the system becomes $\chi_2$ and equation (4) shows that the probability of measuring $\alpha_1$ again is $9/13$. The total probability of measuring $\alpha_1$ again is therefore $\left(\frac{4}{13}\times\frac{4}{13}\right)+\left(\frac{9}{13}\times\frac{9}{13}\right)=\frac{97}{169}$.

8. a) In the lectures we found that $c_n = \frac{2\sqrt{2}}{n\pi}$ for $n$ odd, and $c_n = 0$ for $n$ even. The eigenvalues corresponding to the energy operator $\hat{H}$ are $E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}$. Therefore the first way of calculating $\langle \hat{H} \rangle$ gives $\langle \hat{H} \rangle = \sum_n |c_n|^2 \, E_n = \sum_{n \text{ odd}} \frac{8}{n^2\pi^2}\frac{\hbar^2\pi^2 n^2}{2ma^2} = \sum_{n \text{ odd}} \frac{4\hbar^2}{ma^2} = \infty$. The second way gives $\int_0^a dx\, \psi^* \, \hat{H}\, \psi$ where $\psi = \frac{1}{\sqrt{a}}$ and $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$. This method therefore gives zero.

b) I'll let you think about this!

9. For these observables to be compatible, the corresponding operators must commute. This is obviously the case for all these operators, because the $n^{\text{th}}$ power of an operator means that it operates $n$ times. For example, $\left[\hat{Q}^2, \hat{Q}^3\right] = \hat{Q}^2\hat{Q}^3 - \hat{Q}^3\hat{Q}^2 = \hat{Q}\hat{Q}\hat{Q}\hat{Q}\hat{Q} - \hat{Q}\hat{Q}\hat{Q}\hat{Q}\hat{Q} = 0$. The 1D momentum operator is $-i\hbar\frac{d}{dx}$ and the 1D kinetic energy operator is $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \equiv -\frac{\hbar^2}{2m}\frac{d}{dx}\frac{d}{dx}$. These obviously commute, which implies that momentum and kinetic energy can be measured simultaneously.