PH30030: Quantum Mechanics   Problems Sheet 1

Some useful integrals. I want the problems sheets to be more about developing your understanding of the fundamentals of quantum mechanics than exercises in algebra. The integrals given below should help in doing these problems. Having said that, quantum mechanics is a rather theoretical and mathematical area of physics, so you can't avoid tedious algebra altogether…..

In these integrals, α and a are constants, and m and n are integers.

$$\int dx \sin^2(\alpha x) = \frac{x}{2} - \frac{1}{4\alpha}\sin(2\alpha x)$$

$$\int dx \sin(\alpha x)\cos(\alpha x) = -\frac{1}{4\alpha}\cos(2\alpha x)$$

$$\int dx \sin^3(\alpha x) = \frac{1}{\alpha}\left(\frac{1}{3}\cos^3(\alpha x) - \cos(\alpha x)\right)$$

$$\int dx \sin(\alpha_1 x)\sin(\alpha_2 x) = -\frac{\sin(\alpha_1 x + \alpha_2 x)}{2(\alpha_1 + \alpha_2)} + \frac{\sin(\alpha_1 x - \alpha_2 x)}{2(\alpha_1 - \alpha_2)}$$

$$\int_0^a dx\, x \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right) = \frac{2a^2 mn\left(-1+(-1)^{m+n}\right)}{\pi^2\left(m^2-n^2\right)^2}$$

$$\int_0^a dx\, x \sin^2\left(\frac{m\pi x}{a}\right) = \frac{a^2}{4}$$

$$\int_0^a dx\, x^2 \sin^2\left(\frac{m\pi x}{a}\right) = \frac{a^3\left(2m^2\pi^2-3\right)}{12m^2\pi^2}$$

$$\int_0^a dx \exp(-ikx)\sin\left(\frac{m\pi x}{a}\right) = \frac{m\pi a\left(-1+(-1)^m \exp(-ika)\right)}{k^2a^2 - m^2\pi^2}$$

$$\int_0^\infty dx\, x^n \exp(-\alpha x) = \frac{n!}{\alpha^{n+1}}$$

1. Normalise the following wavefunctions (i.e. find the normalisation constant A).

   a) The n^{th} level of the infinite square well in 1D, between $x=0$ and $x=a$: $\psi(x) = A\sin\left(\frac{n\pi x}{a}\right)$.

   b) The $1s$ state of the hydrogen atom (in 3D spherical polars): $\psi(r) = A\exp(-r/a_0)$.

   c) A spherical harmonic (also in 3D spherical polars): $Y_{11}(\theta,\phi) = A\sin\theta\exp(i\phi)$.

   Note: This question is for revision of year 2 work, and to remind you what some important wavefunctions look like. Be careful with the integrations in parts (b) and (c); in part (c), ignore the r integration.

2. An operator operates on the function $f(x)$ to produce the following functions (c is a constant):

i) $x\,f(x)$ ii) $\dfrac{df}{dx}$ iii) $c\,f(x)$ iv) $f(x)+c$

v) $f^2(x)$ vi) $f\dfrac{df}{dx}$ vii) $p(x)\,f(x)$ (where $p(x)$ is an arbitrary function)

a) Which of these operators are linear?

b) Which of the following pairs of operators commute: i) & ii); ii) & iii); i) & vii); ii) & vii)?

3. a) Show that the 1D operator $\dfrac{d}{dx}$ is not Hermitian.

b) Show that the kinetic energy operator in 1D is Hermitian.

Note: As in the lecture notes, you can assume that the function operated on by these operators is "well behaved" at the boundaries of the relevant region (i.e., it has the properties you want it to have!).

4. In the lecture notes we showed that the un-normalised eigenfunctions of the momentum operator in 1D are $\exp(ikx)$ with eigenvalues $\hbar k$.

a) Show that the un-normalised eigenfunctions of the 3D momentum operator are 3D plane waves: $\exp(i\underline{k}.\underline{r})$ (where $\underline{k}$ is a constant vector called the wavevector).

b) What are the eigenvalues?

Note: It is easiest to express $\underline{k}.\underline{r}$ in Cartesian coordinates.

5. Confirm that the energy eigenfunctions of the infinite square well, $\phi_n(x)=\sqrt{\dfrac{2}{a}}\sin\left(\dfrac{n\pi x}{a}\right)$, for different values of n are orthogonal.

6. In the lecture notes, we saw that a wavefunction ψ can be expressed in terms of a set of eigenfunctions as $\psi=\sum_n c_n\,\phi_n$, and that the probability of measuring the eigenvalue corresponding to ϕ_m is $\left|c_m\right|^2$. If ψ and the ϕ_n are normalised, confirm that $\sum_n \left|c_n\right|^2=1$.

7. An operator $\hat{A}$ has two normalised eigenfunctions, ϕ_1 and ϕ_2, with corresponding eigenvalues α_1 and α_2. A second operator $\hat{B}$ has two normalised eigenfunctions, χ_1 and χ_2, with corresponding eigenvalues β_1 and β_2. The eigenfunctions are related by

$$\phi_1 = \sqrt{\frac{1}{13}}(2\chi_1 + 3\chi_2)$$
$$\phi_2 = \sqrt{\frac{1}{13}}(3\chi_1 - 2\chi_2)$$

a) Given that χ_1 and χ_2 are normalised and orthogonal to each other, confirm that these expressions show that ϕ_1 and ϕ_2 are also normalised and orthogonal to each other.

b) Express χ_1 and χ_2 in terms of ϕ_1 and ϕ_2.

c) The observable corresponding to $\hat{A}$ is measured and the value α_1 is obtained. The observable corresponding to $\hat{B}$ is then measured, and then the first observable is measured again. What is the probability of obtaining the value α_1 again?

Note: Part c) is quite tricky, but it's a good test of how well you understand some of the principles of quantum mechanics.

8. In the lecture notes, we saw that the two expressions for the expectation value of an operator are equivalent, i.e.,

$$\langle \hat{A} \rangle = \sum_n |c_n|^2 \alpha_n = \int \psi^* \hat{A} \psi$$

where $\psi = \sum_n c_n \phi_n$ and α_n and ϕ_n are the eigenvalues and eigenfunctions of $\hat{A}$.

a) Calculate $\langle \hat{H} \rangle$ for the 1D infinite square well example we looked at in the lectures (i.e., when $\psi(x) = \sqrt{\frac{1}{a}}$) using both of the above expressions.

b) Can you understand what has gone wrong here?

9. Consider an observable with corresponding operator $\hat{Q}$. Show that the observables associated with $\hat{Q}$, $\hat{Q}^2$, $\hat{Q}^3$, etc. are all compatible. Hence show that the momentum and kinetic energy of a particle in 1D can be measured simultaneously.

10. Show that the momentum and total energy of a particle in 1D can be measured simultaneously only if the potential energy is constant everywhere.

11. Calculate the expectation values $\langle \hat{x} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p}_x \rangle$ and $\langle \hat{p}_x^2 \rangle$ for the ground state energy eigenfunction of a 1D infinite square well between $x = 0$ and $x = a$, i.e., for $\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$. Hence calculate Δx and Δp_x and show the results are consistent with the uncertainty principle.

12. At time $t = 0$, the wavefunction of a particle in a 1D infinite square well between $x = 0$ and $x = a$ is

$$\psi(x,0) = \frac{1}{\sqrt{2}}\phi_1(x) + \frac{1}{\sqrt{2}}\phi_2(x)$$

where ϕ_1 and ϕ_2 are the lowest two energy eigenfunctions:

$$\phi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \quad \text{and} \quad \phi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right).$$

a) At $t = 0$, what is the probability of measuring the energy to be E_1 or E_2, the eigenvalues corresponding to ϕ_1 and ϕ_2?

b) What is the wavefunction at a later time t?

c) What is the expectation value of the energy, $\langle \hat{H} \rangle$, at a later time t?

d) What is the expectation value of the position, $\langle \hat{x} \rangle$, at a later time t?

13. In the analysis of the spreading of a wavepacket in the lecture notes, it was shown that a wavefunction in 1D can be expressed in terms of momentum eigenfunctions:

$$\psi(x) = \int_{-\infty}^{\infty} dk\, c(k) \exp(ikx)$$

where

$$c(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\, \psi(x) \exp(-ikx).$$

We also saw that the probability of measuring the momentum $p = \hbar k$ is proportional to $|c(k)|^2$.

a) Calculate $c(k)$ for the ground state energy eigenfunction of an infinite square well in 1D (i.e., $\psi(x)$ as given in question 11). Note that $\psi(x) = 0$ outside the well.

b) Sketch $|c(k)|^2$ and comment on this function in relation to the results of question 11.

14. An electron, which is initially confined to a region on the x axis of size 1 Å, is released to be free to move anywhere along the x axis. Assume that the initial wavefunction of the electron is Gaussian.

a) How long will it take for the size of the wavepacket to double?

b) How big will the wavepacket be after 1 s?