Homework 1

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1. What are the results of operating on the following functions with the operator d/dx and d^2/dx^2: (a) $\exp(-ax^2)$, (b) $\cos(bx)$, (c) $\exp(ikx)$? Which functions are eigen functions of these operators? What are the corresponding eigen values?

   Solution: (a) (i) $\frac{\mathrm{d}\exp(-ax^2)}{\mathrm{d}x} = -2ax\exp(-ax^2)$; (ii) $\frac{\mathrm{d}^2\exp(-ax^2)}{\mathrm{d}x^2} = -2a\exp(-ax^2)\,(-2ax^2+1)$
   (b) (i) $\frac{\mathrm{d}\cos bx}{\mathrm{d}x} = -b\sin bx$; (ii) $\frac{\mathrm{d}^2\cos bx}{\mathrm{d}x^2} = -b^2\sin bx$; $\cos bx$ is an eigenfunction of $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with an eigenvalue of $-b^2$
   (c) (i) $\frac{\mathrm{d}e^{ikx}}{\mathrm{d}x} = ike^{ikx}$; (ii) $\frac{\mathrm{d}^2e^{ikx}}{\mathrm{d}x^2} = -k^2e^{ikx}$; e^{ikx} is an eigen function of $\frac{\mathrm{d}}{\mathrm{d}x}$ and $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with eigenvalue of ik and $-k^2$ respectively.

2. Which of the following operators are linear? (a) d/dx; (b) $\surd$; (c) exponentiation; (d) integration.

   Solution: An operator, $\hat{Op}$, is linear if it satisfies the relation $\hat{Op}(af(x) + bg(x) = a\hat{Op}f(x) + b\hat{Op}g(x)$. Of the operators given, $\frac{\mathrm{d}}{\mathrm{d}x}$ and integration satisfy the relation given above and are linear. You can verify that $\surd$ and exponentiation are not linear. For example, we know that $\sqrt{3+2} \neq \sqrt{3} + \sqrt{2}$, and similarly for exponentiation.

3. In algebra it can be easily shown that $(P+Q)(P-Q) = P^2 - Q^2$. What is the value of $(P+Q)(P-Q)$ if P and Q are operators? Under what conditions will this result be equal to $P^2 - Q^2$.

   Solution: For operators P and Q, $(P+Q)(P-Q) = P^2 - PQ + QP - Q^2$. If $PQ = QP$, that is, $[P,Q] = 0$, then $(P+Q)(Q-P) = P^2 - Q^2$

4. Find $[z^3, d/dz]$ and $[d^2/dx^2, ax^2 + bx + c]$.

   Solution: $[z^3, \frac{\mathrm{d}}{\mathrm{d}z}] = z^3\frac{\mathrm{d}}{\mathrm{d}z} - \frac{\mathrm{d}}{\mathrm{d}z}z^3 = 3z^2$ and, similarly, $[\frac{\mathrm{d}^2}{\mathrm{d}x^2}, ax^2 + bx + c] = 2a$

5. Prove by induction that $[\hat{x}^n, \hat{p}_x] = i\hbar n\hat{x}^{n-1}$ and that $[\hat{x}, \hat{p}_x^n] = i\hbar n\hat{p}_x^{n-1}$ where n is a positive integer.

   Solution: Given the result from the previous problem, this result is easily proved.

6. Which of the following functions cannot be solutions of the Schrödinger equation for all values of x? Why not? (a) $A\sec(x)$; (b) $A\tan(x)$; (c) $A\exp(x^2)$; (d) $A\exp(-x^2)$.

   Solution: (a) No; diverges at $x = (2n+1)\pi/2$; (b) No; diverges at $x = (2n+1)\pi/2$; (c) No; diverges at $x = \infty$; (d) Yes.

7. Normalize the following wave functions to unity: (a) $\sin(n\pi x/L)$ for the range $0\ x\ L$, (b) c, a constant in the range $-L\ x\ L$, (c) $\exp(-r/a_0)$ in three dimensions, (d) $x\exp(-r/2a_0)$ in three dimensions.

   Solution: (a) $A^2\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)\mathrm{d}x = A^2\frac{L}{2}$
   (b) $A^2\int_{-L}^{L} c^2\,\mathrm{d}x = A^2c^2 2L$

(c) $A^2 \int_0^\infty \exp\left(-\frac{2r}{a_0}\right) r^2 dr \int_0^\pi \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi$; Note the volume elements

(d) Substituting $x = r\sin\theta\cos\phi$, we get $A^2 \int_0^\infty \exp\left(-\frac{2r}{a_0}\right) r^4 dr \int_0^\pi \sin^3\theta \, \mathrm{d}\theta \int_0^{2\pi} \cos^2\phi \, \mathrm{d}\phi$

8. Construct the squares of the following operators: (a) $\hat{D}\phi(x) = \partial\phi(x)/\partial x$, (b) $\hat{\triangle}\phi(x) = -\partial^2\phi(x)/\partial x^2$, (c) $\hat{Q}\phi(x) = \int_0^1 dx'\phi(x')$, (d) $\hat{F}\phi(x) = F(x)\phi(x)$, (e) $\hat{B}\phi(x) = \frac{1}{3}\phi(x)$, (f) $\hat{P}\phi = \phi^3 - 3\phi^2 - 4$, (g) $\hat{G}\phi(x) = (d/dx + x)\phi(x)$. Which of these operators are linear?

   Solution: (a) $\frac{\partial^2\phi}{\partial x^2}$; (b) $\frac{\partial^4\phi}{\partial x^4}$; (c) $\int_0^1 dx'' \int_0^1 dx'$; (d) $F^2(x)\phi(x)$; (e) $\frac{1}{9}\phi(x)$; (f) $(\phi^3 - 3\phi^2 - 4)^3 - 3(\phi^3 - 3\phi^2 - 4) - 4$; (g) $\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2x\frac{\mathrm{d}}{\mathrm{d}x} + x^2 + 1)\phi(x)$. Operators a, b, c, e, and g are linear.

9. Write down the Schrödinger for the following systems: (a) a particle of mass m in a cubical box of side a; (b) a particle of mass m in a spherical box of radius a; (c) a particle of mass m moving on the x-axis subjected to a force directed towards the origin, of magnitude proportional to the distance from the origin; (d) an electron moving in the presence of a nuclear charge $+Ze$; (e) two electrons moving in the presence of a fixed nucleus of charge $+Ze$.

   Solution: (a) $-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\psi(x,y,z)$
   (b) $-\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$
   (c) You are given that $F = -kx$, where x is the displacement from equilibrium. Given that $F = -\frac{\mathrm{d}V}{\mathrm{d}x}$, we find that the potential $V = -\int F\,\mathrm{d}x = \frac{1}{2}kx^2$. So the Schrödinger equation is $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$.
   (d) $\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}\right)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$
   (e) $\left(-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} - -\frac{Ze^2}{4\pi\epsilon_0 r_2}\right)\psi(r_1,\theta_1,\phi_1,r_2,\theta_2,\phi_2) = E\psi(r_1,\theta_1,\phi_1,r_2,\theta_2,\phi_2)$

10. Let s be the number of spots shown by a die thrown at random. (a) Calculate $\langle s\rangle$. (b) Calculate Δs.

    Solution: $\langle s\rangle = \sum_i p_i i$, where p_i is the probability of the die face showing i. The result is $\langle s\rangle = \frac{1}{6}(1+2+3+4+5+6) = \frac{21}{6} = 3.5$. Similarly $\langle s^2\rangle = \frac{1}{6}(1+4+9+16+25+36) = 15.166$ and $\Delta s = \sqrt{\langle s^2\rangle - \langle s\rangle^2} = \sqrt{15.166 - 3.5^2}$.

11. A particle is known to be in the state

$$\psi(x,t) = A\exp\left[-\frac{(x-x_0)^2}{4a^2}\right]\exp\left(\frac{ip_0 x}{\hbar}\right)\exp\left(i\omega_0 t\right)$$

    (a) Determine A (You might find the following integral useful: $\int_{-\infty}^\infty e^{-\beta^2/2}d\beta = \sqrt{2\pi}$).
    (b) Determine the expectation value of position of the particle.
    (c) What is the uncertainty in the position?
    (d) What is the expectation value of the momentum? And its uncertainty?

    Solution:

    (a) $A^2 a\int_{-\infty}^\infty \mathrm{e}^{-\eta^2/2}\mathrm{d}\eta$, where $\eta = \frac{x-x_0}{a}$. Or, $A^2 = \frac{1}{a\sqrt{2\pi}}$.
    (b) $\langle x\rangle = \int_{-\infty}^\infty \psi^* x\psi\,\mathrm{d}x = A^2a^2\int_{-\infty}^\infty \mathrm{e}^{-\eta^2}2(\eta+\eta_0)\,\mathrm{d}\eta$, where $\eta_0 = \frac{x_0}{a}$. Notice that by symmetry $\int_{-\infty}^\infty \mathrm{e}^{-\eta^2}2\eta\,\mathrm{d}\eta = 0$ because it is an integral of an odd function. So the result is $a\eta_0 A^2 a\int_{-\infty}^\infty \mathrm{e}^{-\eta^2/2}\mathrm{d}\eta = a\eta_0 = x_0$
    (c) $(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2 + x_0^2 - x_0^2 = a^2$

(d) $\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p_x} \psi \, \mathrm{d}x$. Using $\hat{p_x} = -i\hbar \frac{\partial}{\partial x}$, we get $\int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, \mathrm{d}x = A^2 a^2 \int_{-\infty}^{\infty} \mathrm{e}^{-\eta^2} 2 \left(p_0 + \frac{i\hbar}{2a}\right) \eta \right) \mathrm{d}$
p_0

12. A particle is in a state described by the wave function $\psi = (\cos\chi)\exp(ikx) + (\sin\chi)\exp(-ikx)$ where χ is a parameter. What is the probability that the particle will be found with a linear momentum (a) $+k\hbar$, (b) $-k\hbar$? What form would the waveunction have if it were 90% certain that the particle had linear momentum $+k\hbar$?

    Solution: (a) $\cos^2\chi$; (b) $\sin^2\chi$; (c) $\psi = \sqrt{0.9}\exp(ikx) + \sqrt{0.1}\exp(-ikx)$.