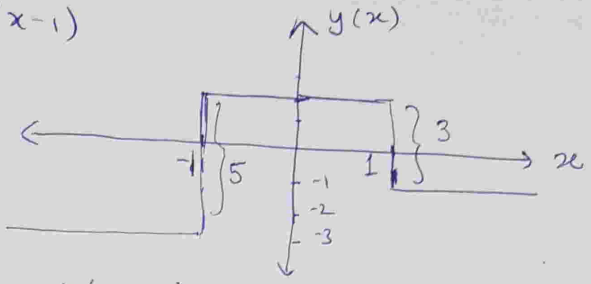
ADVANCED MATHEMATICAL METHODS FOR CHEMISTRY - QUIZ 3 - SOLUTIONS

1. $y(x) = -3 + 5\,h(x+1) - 3\,h(x-1)$



2. Function is $y(x) = +2 \neq -h(x+3) - h(x) + h(x-1)$

Derivative is $\therefore \quad -\delta(x+3) - \delta(x) + \delta(x-1)$

Answer (d) – None of above

3. $\Gamma(7/2) = \frac{5}{2}\,\Gamma\left(\frac{5}{2}\right) = \frac{5}{2} \times \frac{3}{2}\,\Gamma\left(\frac{3}{2}\right) = \frac{5}{2} \times \frac{3}{2} \times \frac{1}{2}\,\Gamma(1/2)$

$$\frac{\Gamma(7/2)}{\Gamma(1/2)} = \frac{15}{8}$$

4. $$\int_0^\infty x^3 e^{-4x^2} dx = \int_0^\infty \frac{u}{4} e^{-u} \frac{du}{8} = \frac{1}{32}$$

Answer (d) – None of the above

5. $\mathrm{erf}(0) = 0$, so (a) is wrong, (c) is wrong but (b) is correct

6. $0 \le r < \infty \quad 0 \le \theta < \pi \quad 0 \le \phi < 2\pi$

$0 \le \rho < \infty \quad 0 \le \theta < 2\pi \quad -\infty < z < \infty$

7. $$\frac{\partial}{\partial x}\left[\tan^{-1}\left(\frac{y}{x}\right)\right] = \frac{1}{1 + \frac{y^2}{x^2}} \cdot -\frac{y}{x^2} = \frac{-y}{x^2+y^2}$$

8. $$\left(\frac{\partial \phi}{\partial x}\right)_{y,z}$$

9. $$p(v_x) = \left(\frac{m}{2\pi k_B T}\right)^{1/2} \cdot e^{-\frac{m v_x^2}{2 k_B T}}$$

Probability that $|v_x| \ge \sqrt{\frac{2k_BT}{m}} = \int_{-\sqrt{\frac{2k_BT}{m}}}^{+\sqrt{\frac{2k_BT}{m}}} \left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{-\frac{m v_x^2}{2k_BT}} dv_x$

$$= 2 \int_0^1 \frac{1}{\sqrt{\pi}} e^{-x^2} dx \qquad x = \frac{v_x}{\sqrt{\frac{2k_BT}{m}}}$$

$$= \mathrm{Erf}(1)$$

10. $N \int_0^{\infty} r^2 e^{-r}\, r^2 dr \int_0^{\pi} \cos^2\theta \sin\theta\, d\theta \int_0^{2\pi} d\phi = 1$

$N \times 4! \times 2\pi \times \int_0^{\pi} \cos^2\theta \sin\theta\, d\theta = 1$

$u = \cos\theta \qquad -\sin\theta\, d\theta = du$

$48\pi N \times \int_{-1}^{1} u^2\, du = 32\pi N = 1$

$N = \frac{1}{32\pi}$