The Chemistry Maths Book

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Solutions

Chapter 10. Functions in 3 dimensions

Section 10.2

Find the cartesian coordinates (x, y, z) of the points whose spherical polar coordinates are:

1. $(r,\ \theta,\ \phi) = (1,\ 0,\ 0)$

$$x = 1\times\sin 0\times\cos 0 = 0, \quad y = 1\times\sin 0\times\sin 0 = 0, \quad z = 1\times\cos 0 = 1$$

Therefore $(x, y, z) = (0, 0, 1)$

2. $(r,\theta,\phi) = (2, \pi/2, \pi/2)$

$$x = 2\times\sin\pi/2\times\cos\pi/2 = 0, \quad y = 2\times\sin\pi/2\times\sin\pi/2 = 2, \quad z = 1\times\cos\pi/2 = 0$$

Therefore $(x, y, z) = (0, 2, 0)$

3. $(r,\theta,\phi) = (2, 2\pi/3, 3\pi/4)$

We have $\cos 2\pi/3 = -\cos\pi/3 = -1/2, \quad \sin 2\pi/3 = \sin\pi/3 = \sqrt{3}/2$

$\cos 3\pi/4 = -\cos\pi/4 = -1/\sqrt{2}, \quad \sin 3\pi/4 = \sin\pi/4 = 1/\sqrt{2}$

Therefore $x = 2\times\frac{\sqrt{3}}{2}\times\left(-\frac{1}{\sqrt{2}}\right) = -\sqrt{\frac{3}{2}}, \quad y = 2\times\frac{\sqrt{3}}{2}\times\frac{1}{\sqrt{2}} = \sqrt{\frac{3}{2}}, \quad z = 2\times\left(-\frac{1}{2}\right) = -1$

and $(x, y, z) = \left(-\sqrt{3/2},\ \sqrt{3/2}\ , -1\right)$

Find the spherical polar coordinates (r,θ,ϕ) of the points:

4. $(x, y, z) = (1,\ 0,\ 0)$

We have

$$r = \sqrt{x^2+y^2+z^2} = 1, \quad \theta = \cos^{-1}(z/r) = \cos^{-1}(0) = \pi/2, \quad \phi = \tan^{-1}(y/x) = \tan^{-1}(0) = 0$$

Therefore $(r,\ \theta,\ \phi) = (1,\ \pi/2, 0)$

5. $(x,\ y,\ z) = (0,\ 1,\ 0)$

We have $r = 1, \quad \theta = \cos^{-1}(0) = \pi/2, \quad \phi = \tan^{-1}(\infty) = \pi/2$

Therefore $(r,\ \theta,\ \phi) = (1,\ \pi/2, \pi/2)$

6. $(x,\ y,\ z) = (1,\ 2,\ 2)$

We have $r = \sqrt{1+4+4} = 3, \quad \theta = \cos^{-1}(2/3) \approx 0.27\pi \approx 48°, \quad \phi = \tan^{-1}(2) \approx 0.35\pi \approx 63°$

Therefore $(r,\ \theta,\ \phi) = \left(3,\ \cos^{-1}(2/3), \tan^{-1}(2)\right)$

7. $(x, y, z) = (1, -4, -8)$

We have

$$r = 9, \quad \theta = \cos^{-1}(-8/9) \approx 0.85\pi \approx 153°, \quad \phi = \tan^{-1}(-4) \approx -0.42\pi \approx -76°$$

But angle ϕ is defined to lie in the range $0 \to 2\pi$ with $\tan(2\pi + \phi) = \tan\phi$. Therefore when the principal value of the inverse tangent is negative, $\phi = \tan^{-1}\left(y/x\right) + 2\pi$. In the present case,

$$\phi = \tan^{-1}\left(-4\right) + 2\pi \approx 1.58\,\pi \approx 284°$$

Then $$(r,\ \theta,\ \phi) = \left(9,\ \cos^{-1}\left(-8/9\right), \tan^{-1}(-4) + 2\pi\right)$$

8. $(x, y, z) = (-2, -3,\ 6)$

We have $r = 7, \quad \theta = \cos^{-1}\left(6/7\right) \approx 0.17\pi \approx 31°$

and, because $x < 0$,

$$\phi = \tan^{-1}(3/2) + \pi \approx 1.31\pi \approx 236°$$

Therefore $$(r,\ \theta,\ \phi) = \left(7,\ \cos^{-1}\left(6/7\right), \tan^{-1}(3/2) + \pi\right)$$

9. $(x, y, z) = (-3,\ 4, -12)$

We have $r = 13, \quad \theta = \cos^{-1}\left(-12/13\right) \approx 0.87\pi \approx 157°, \quad \phi = \tan^{-1}(-4/3) + \pi \approx 0.70\pi \approx 127°$

Therefore $$(r,\ \theta,\ \phi) = \left(13,\ \cos^{-1}\left(-12/13\right), \tan^{-1}(-4/3) + \pi\right)$$

Section 10.3

Express in spherical polar coordinates:

10. $x^2 - y^2 = r^2\sin^2\theta\cos^2\phi - r^2\sin^2\theta\sin^2\phi = r^2\sin^2\theta(\cos^2\phi - \sin^2\phi)$

$$= r^2\sin^2\theta\cos 2\phi$$

11. $\dfrac{x^2 + y^2}{z^2} = \dfrac{r^2\sin^2\theta\ (\cos^2\phi + \sin^2\phi)}{r^2\cos^2\theta} = \tan^2\theta$

12. $2z^2 - x^2 - y^2 = 2r^2\cos^2\theta - r^2\sin^2\theta(\cos^2\phi + \sin^2\phi) = r^2(2\cos^2\theta - \sin^2\theta)$

$$= r^2(3\cos^2\theta - 1)$$

13. Express in spherical polar coordinates:

(i) $(x^2+y^2+z^2)^{-1/2} = (r^2)^{-1/2} = \dfrac{1}{r}$,

(ii) $\dfrac{\partial}{\partial x}(x^2+y^2+z^2)^{-1/2} = \dfrac{d}{dr}\left(\dfrac{1}{r}\right)\times\dfrac{\partial r}{\partial x} = -\dfrac{1}{r^2}\times\dfrac{x}{r} = -\dfrac{x}{r^3}$

Section 10.4

Find the total mass of a mass distribution of density ρ in region V of space:

14. $\rho = x^2+y^2+z^2$; V: the cube $0\le x\le 1,\ 0\le y\le 1,\ 0\le z\le 1$

$$\int_V \rho(x,y,z)\,dv = \int_0^1\int_0^1\left[\int_0^1 (x^2+y^2+z^2)\,dx\right]dy\,dz$$

$$= \int_0^1\int_0^1\left[\frac{x^3}{3}+xy^2+xz^2\right]_0^1 dy\,dz = \int_0^1\left[\int_0^1\left(\frac{1}{3}+y^2+z^2\right)dy\right]dz$$

$$= \int_0^1\left[\frac{y}{3}+\frac{y^3}{3}+yz^2\right]_0^1 = \int_0^1\left(\frac{2}{3}+z^2\right)dz = \left[\frac{2z}{3}+\frac{z^3}{3}\right]_0^1$$

$$= \frac{2}{3}+\frac{1}{3} = 1$$

15. $\rho = xy^2z^3$; V: the box $0\le x\le a,\ 0\le y\le b,\ 0\le z\le c$

$$\int_V \rho(x,y,z)\,dv = \int_0^c\int_0^b\int_0^a xy^2z^3\,dx\,dy\,dz = \int_0^a x\,dx\times\int_0^b y^2\,dy\times\int_0^z z^3\,dz$$

$$= \frac{a^2}{2}\times\frac{b^3}{3}\times\frac{c^4}{4} = \frac{a^2b^3c^4}{24}$$

16. $\rho = x^2$; V: the region $1-y\le x\le 1,\ 0\le y\le 1,\ 0\le z\le 2$

$$\int_V \rho(x,y,z)\,dv = \int_{z=0}^2\int_{y=0}^1\int_{1-y}^1 x^2\,dx\,dy\,dz = \int_{z=0}^2 dz\times\int_{y=0}^1\left[\int_{1-y}^1 x^2\,dx\right]dy$$

$$= 2\int_{y=0}^1\left[\frac{x^3}{3}\right]_{1-y}^1 dy = \frac{2}{3}\int_{y=0}^1\left[1-(1-y)^3\right]dy = \frac{2}{3}\left[y+\frac{(1-y)^4}{4}\right]_0^1$$

$$= \frac{2}{3}\left[1-\frac{1}{4}\right] = \frac{1}{2}$$

17. $\rho = e^{-(x+y+z)}$; V: the infinite region $x \ge 0,\ y \ge 0,\ z \ge 0$

$$\int_V \rho(x,y,z)\,dv = \int_0^\infty\int_0^\infty\int_0^\infty e^{-(x+y+z)}\,dx\,dy\,dz$$

$$= \int_0^\infty e^{-x}\,dx \times \int_0^\infty e^{-y}\,dy \times \int_0^\infty e^{-z}\,dz = 1\times1\times1 = 1$$

18. $\rho = x^2 + y^2 + z^2$ **;** V: the sphere of radius *a*, centre at the origin

$$\int_V \rho(r,\theta,\phi)\,dv = \int_0^{2\pi}\int_0^{\pi}\int_0^{a}\left(r^2\right) r^2 \sin\theta\,dr\,d\theta\,d\phi = \int_0^{2\pi} d\phi \times \int_0^{\pi}\sin\theta\,d\theta \times \int_0^a r^4\,dr$$

$$= 2\pi \times 2 \times \frac{a^5}{5} = \frac{4\pi a^5}{5}$$

19. $\rho = \dfrac{\sin^2\theta\cos^2\phi}{r}$; V: the sphere of radius *a*, centre at the origin

$$\int_V \rho(r,\theta,\phi)\,dv = \int_0^{2\pi}\int_0^{\pi}\int_0^{a}\left(\frac{\sin^2\theta\cos^2\phi}{r}\right) r^2 \sin\theta\,dr\,d\theta\,d\phi$$

$$= \int_0^{2\pi}\cos^2\phi\,d\phi \times \int_0^{\pi}\sin^3\theta\,d\theta \times \int_0^a r\,dr$$

We have $\displaystyle\int_0^{2\pi}\cos^2\phi\,d\phi = \frac{1}{2}\int_0^{2\pi}(1+\cos 2\phi)\,d\phi = \frac{1}{2}\left[\phi + \frac{1}{2}\sin 2\phi\right]_0^{2\pi} = \pi$

$$\int_0^{\pi}\sin^3\theta\,d\theta = \int_0^{\pi}(1-\cos^2\theta)\sin\theta\,d\theta = \left[-\cos\theta + \frac{\cos^3\theta}{3}\right]_0^{\pi} = \frac{4}{3}$$

Therefore $\displaystyle\int_V \rho(r,\theta,\phi)\,dv = \int_0^{2\pi}\cos^2\phi\,d\phi \times \int_0^{\pi}\sin^3\theta\,d\theta \times \int_0^a r\,dr$

$$= \pi \times \frac{4}{3} \times \frac{a^2}{2} = \frac{2\pi a^2}{3}$$

20. $\rho = r^3 e^{-r}$; V: all space

$$\int_V \rho(r,\theta,\phi)\,dv = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\left(r^3 e^{-r}\right) r^2 \sin\theta\,dr\,d\theta\,d\phi = 4\pi\int_0^\infty r^5 e^{-r}\,dr$$

$$= 4\pi \times 5! = 480\pi$$

21. The 2*s* orbital of the hydrogen atom is

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi a_0^3}}(2 - r/a_0)e^{-r/2a_0}.$$

Show that the integral of ψ_{2s}^2 over all space is unity.

$$\int \psi_{2s}{}^2\, dv = \frac{1}{32\pi a_0^3}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}(2 - r/a_0)^2 e^{-r/a_0}\ r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{1}{32\pi a_0^3}\times 4\pi \times \int_0^{\infty}\left(4r^2 - \frac{4r^3}{a_0} + \frac{r^4}{a_0{}^2}\right)e^{-r/a_0}\, dr$$

Then, using the standard integral, $\int_0^{\infty} e^{-ar}\, r^n\, dr = n!/a^{n+1}$ with $a = (1/a_0)$,

$$\int \psi_{2s}{}^2\, dv = \frac{1}{8a_0^3}\left[\frac{4\times 2!}{(1/a_0)^3} - \frac{4\times 3!}{a_0(1/a_0)^4} + \frac{4!}{a_0{}^2(1/a_0)^5}\right]$$

$$= \frac{1}{8}\left[8 - 24 + 24\right] = 1$$

22. The $3p_z$ orbital of the hydrogen atom is

$$\psi_{3p_z} = C(6-r)re^{-r/3}\cos\theta$$

(in atomic units) where *C* is a constant. Find the value of *C* that normalizes the $3p_z$ orbital.

$$\int \psi_{3p_z}{}^2\, dv = C^2\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\left((6-r)re^{-r/3}\cos\theta\right)^2 r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$= C^2\int_0^{2\pi} d\phi \times \int_0^{\pi}\cos^2\theta\sin\theta\, d\theta \times \int_0^{\infty} e^{-2r/3}(36r^4 - 12r^5 + r^6)\, dr$$

$$= C^2 \times 2\pi \times \frac{2}{3}\times\left[\frac{36\times 4!}{(2/3)^5} - \frac{12\times 5!}{(2/3)^6} + \frac{6!}{(2/3)^7}\right] = \frac{3^8\pi C^2}{2}$$

Therefore $\int \psi_{3p_z}{}^2\, dv = 1$ when $C = \frac{1}{81}\sqrt{\frac{2}{\pi}}$

and the normalized $3p_z$ orbital is

$$\psi_{3p_z} = \frac{1}{81}\sqrt{\frac{2}{\pi}}(6-r)re^{-r/3}\cos\theta$$

23. Calculate the average distance from the nucleus of an electron in the 2*s* orbital (see Exercise 21).

$$\overline{r} = \int \psi_{2s}{}^2 r\,dv \quad = \frac{1}{8a_0^3}\int_0^\infty \left(4r^3 - \frac{4r^4}{a_0} + \frac{r^5}{a_0{}^2}\right)e^{-r/a_0}\,dr$$

$$= \frac{1}{8a_0^3}\left[\frac{4\times 3!}{(1/a_0)^4} - \frac{4\times 4!}{a_0(1/a_0)^5} + \frac{5!}{a_0{}^2(1/a_0)^5}\right] = 6a_0$$

24. Calculate the average value of r^2 for the $3p_z$ orbital (see Exercise 22).

$$\overline{r^2} = \int \psi_{3p_z}{}^2 r^2\,dv = \frac{8}{3^9}\int_0^\infty e^{-2r/3}(36r^6 - 12r^7 + r^8)\,dr$$

$$= \frac{8}{3^9}\left[\frac{36\times 6!}{(2/3)^7} - \frac{12\times 7!}{(2/3)^8} + \frac{8!}{(2/3)^9}\right] = 180$$

Section 10.5

Find $\nabla^2 f$:

25. $f(x,y,z) = x^2y^3z^4$

$$\nabla^2\left(x^2y^3z^4\right) = \left(\frac{\partial^2}{\partial x^2}x^2\right)y^3z^4 + x^2\left(\frac{\partial^2}{\partial y^2}y^3\right)z^4 + x^2y^3\left(\frac{\partial^2}{\partial z^2}z^4\right)$$

$$= 2y^3z^4 + 6x^2yz^4 + 12x^2y^3z^2$$

26. $f(r) = r^n e^{-ar}$: $f(r)$ is a function of *r* only. Therefore

$$\nabla^2 r^n e^{-ar} = \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)r^n e^{-ar}$$

We have

$$\frac{d}{dr}(r^n e^{-ar}) = (nr^{n-1} - ar^n)e^{-ar} = \left[\frac{n}{r} - a\right]r^n e^{-ar}$$

$$\frac{d^2}{dr^2}(r^n e^{-ar}) = \frac{d}{dr}(n - ar)r^{n-1}e^{-ar} = \left[-ar^{n-1} + (n-1)(n-ar)r^{n-2} - a(n-ar)r^{n-1}\right]e^{-ar}$$

$$= \left[\frac{n(n-1)}{r^2} - \frac{2an}{r} + a^2\right]r^n e^{-ar}$$

Therefore $\quad \nabla^2 r^n e^{-ar} = \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)r^n e^{-ar} = \left[\frac{n(n+1)}{r^2} - \frac{2a(n+1)}{r} + a^2\right]r^n e^{-ar}$

27. $f(r) = \dfrac{e^{-r}}{r}$

We have $\dfrac{d}{dr}\left(\dfrac{e^{-r}}{r}\right) = -\left[\dfrac{1}{r} + \dfrac{1}{r^2}\right]e^{-r}, \quad \dfrac{d^2}{dr^2}\left(\dfrac{e^{-r}}{r}\right) = \left[\dfrac{1}{r} + \dfrac{2}{r^2} + \dfrac{2}{r^3}\right]e^{-ar}$

Therefore $\nabla^2\left(\dfrac{e^{-r}}{r}\right) = \left(\dfrac{d^2}{dr^2} + \dfrac{2}{r}\dfrac{d}{dr}\right)\dfrac{e^{-r}}{r} = \dfrac{e^{-r}}{r}$

28. $f(r, \theta, \phi) = e^{-r/3}\sin\theta\sin\phi$

Let $f(r, \theta, \phi) = e^{-r/3}\sin\theta\sin\phi = R(r)\times\Theta(\theta)\times\Phi(\phi)$

Then $\nabla^2 f = \left[\dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right)\right]\Theta\Phi + \left[\dfrac{1}{\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d\Theta}{d\theta}\right)\right]\dfrac{R\Phi}{r^2} + \left[\dfrac{d^2\Phi}{d\phi^2}\right]\dfrac{R\Theta}{r^2\sin^2\theta}$

We have $R = e^{-r/3}: \quad \dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right) = \left[\dfrac{1}{9} - \dfrac{2}{3r}\right]R$

$\Theta = \sin\theta: \quad \dfrac{1}{\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d\Theta}{d\theta}\right) = \dfrac{\cos^2\theta - \sin^2\theta}{\sin^2\theta}\Theta$ (as in Example 10.11)

$\Phi = \sin\phi: \quad \dfrac{d^2\Phi}{d\phi^2} = -\sin\phi = -\Phi(\phi)$

Therefore $\nabla^2 f = \left(\dfrac{1}{9} - \dfrac{2}{3r} + \dfrac{\cos^2\theta - \sin^2\theta}{r^2\sin^2\theta} - \dfrac{1}{r^2\sin^2\theta}\right)R\Theta\Phi = \left(\dfrac{1}{9} - \dfrac{2}{3r} - \dfrac{2}{r^2}\right)f$

29. $f = xze^{-r/2}$

We have $\dfrac{\partial f}{\partial x} = ze^{-r/2} + xz\left(\dfrac{\partial}{\partial x}e^{-r/2}\right)$, $\dfrac{\partial^2 f}{\partial x^2} = 2z\left(\dfrac{\partial}{\partial x}e^{-r/2}\right) + xz\left(\dfrac{\partial^2}{\partial x^2}e^{-r/2}\right)$

and, similarly,

$$\frac{\partial^2 f}{\partial y^2} = xz\left(\frac{\partial^2}{\partial y^2}e^{-r/2}\right), \quad \frac{\partial^2 f}{\partial z^2} = 2x\left(\frac{\partial}{\partial z}e^{-r/2}\right) + xz\left(\frac{\partial^2}{\partial z^2}e^{-r/2}\right)$$

Therefore $\nabla^2 f = \dfrac{\partial^2 f}{\partial x^2} + \dfrac{\partial^2 f}{\partial y^2} + \dfrac{\partial^2 f}{\partial z^2} = 2z\left(\dfrac{\partial}{\partial x}e^{-r/2}\right) + 2x\left(\dfrac{\partial}{\partial z}e^{-r/2}\right) + xz\left(\nabla^2 e^{-r/2}\right)$

Now $r = (x^2 + y^2 + z^2)^{1/2}$ and $\dfrac{dr}{dx} = x/r$, $\dfrac{dr}{dz} = z/r$.

Then $\dfrac{\partial}{\partial x}e^{-r/2} = -\dfrac{1}{2}e^{-r/2} \times \dfrac{x}{r} = -\dfrac{x}{2r}e^{-r/2}$

$$\frac{\partial}{\partial z}e^{-r/2} = -\frac{z}{2r}e^{-r/2}$$

Also $\nabla^2 e^{-r/2} = \left(\dfrac{d^2}{dr^2} + \dfrac{2}{r}\dfrac{d}{dr}\right)e^{-r/2} = \left(\dfrac{1}{4} - \dfrac{1}{r}\right)e^{-r/2}$

Therefore $\nabla^2 f = \left[-\dfrac{xz}{r}\right]e^{-r/2} + \left[-\dfrac{xz}{r}\right]e^{-r/2} + xz\left(\dfrac{1}{4} - \dfrac{1}{r}\right)e^{-r/2} = \left(\dfrac{1}{4} - \dfrac{3}{r}\right)xze^{-r/2}$

$$= \left(\frac{1}{4} - \frac{3}{r}\right)f$$

30. If $f = (2-r)e^{-r/2}$ show that $\nabla^2 f + \dfrac{2f}{r} = \dfrac{f}{4}$.

We have $f(r) = (2-r)e^{-r/2} \;\to\; \dfrac{df}{dr} = \left[\dfrac{r}{2} - 2\right]e^{-r/2}$, $\dfrac{d^2 f}{dr^2} = \left[\dfrac{3}{2} - \dfrac{r}{4}\right]e^{-r/2}$

Therefore $\nabla^2 f(r) = \left(\dfrac{d^2}{dr^2} + \dfrac{2}{r}\dfrac{d}{dr}\right)f(r) = \left[\dfrac{5}{2} - \dfrac{r}{4} - \dfrac{4}{r}\right]e^{-r/2}$

and $\nabla^2 f + \dfrac{2f}{r} = \left[\dfrac{5}{2} - \dfrac{r}{4} - \dfrac{4}{r}\right]e^{-r/2} + \left[\dfrac{4}{r} - 2\right]e^{-r/2}$

$$= \frac{1}{4}(2-r)e^{-r/2} = \frac{1}{4}f$$

31. If $f = ze^{-3r/2}$ show that $\nabla^2 f + \dfrac{6f}{r} = \dfrac{9f}{4}$.

We have $\dfrac{\partial^2 f}{\partial x^2} = z\left(\dfrac{\partial^2}{\partial x^2}e^{-3r/2}\right), \quad \dfrac{\partial^2 f}{\partial y^2} = z\left(\dfrac{\partial^2}{\partial y^2}e^{-3r/2}\right)$

and $\dfrac{\partial f}{\partial z} = e^{-3r/2} + z\left(\dfrac{\partial}{\partial z}e^{-3r/2}\right), \quad \dfrac{\partial^2 f}{\partial z^2} = 2\left(\dfrac{\partial}{\partial z}e^{-3r/2}\right) + z\left(\dfrac{\partial^2}{\partial z^2}e^{-3r/2}\right)$

Therefore $\nabla^2 f = \dfrac{\partial^2 f}{\partial x^2} + \dfrac{\partial^2 f}{\partial y^2} + \dfrac{\partial^2 f}{\partial z^2} = 2\left(\dfrac{\partial}{\partial z}e^{-3r/2}\right) + z\left(\nabla^2 e^{-3r/2}\right)$

Now $\dfrac{\partial}{\partial z}e^{-3r/2} = -\dfrac{3}{2}e^{-3r/2} \times \dfrac{z}{r} = -\dfrac{3z}{2r}e^{-3r/2}$

and $\nabla^2 e^{-3r/2} = \left(\dfrac{d^2}{dr^2} + \dfrac{2}{r}\dfrac{d}{dr}\right)e^{-3r/2} = \left(\dfrac{9}{4} - \dfrac{3}{r}\right)e^{-3r/2}$

Therefore $\nabla^2 f = -\dfrac{3z}{r}e^{-3r/2} + z\left(\dfrac{9}{4} - \dfrac{3}{r}\right)e^{-3r/2} = \dfrac{9}{4}f - \dfrac{6}{r}f$

$$\nabla^2 f + \frac{6}{r}f = \frac{9}{4}f$$

32. If $f = xye^{-r}$ show that $\nabla^2 f + \dfrac{6f}{r} = f$.

We have $\dfrac{\partial f}{\partial x} = ye^{-r} + xy\left(\dfrac{\partial}{\partial x}e^{-r}\right), \quad \dfrac{\partial^2 f}{\partial x^2} = 2y\left(\dfrac{\partial}{\partial x}e^{-r}\right) + xy\left(\dfrac{\partial^2}{\partial x^2}e^{-r}\right)$

$$\frac{\partial f}{\partial y} = xe^{-r} + xy\left(\frac{\partial}{\partial y}e^{-r}\right), \quad \frac{\partial^2 f}{\partial y^2} = 2x\left(\frac{\partial}{\partial y}e^{-r}\right) + xy\left(\frac{\partial^2}{\partial y^2}e^{-r}\right)$$

$$\frac{\partial^2 f}{\partial z^2} = xy\frac{\partial^2}{\partial z^2}e^{-r}$$

Now $\dfrac{\partial}{\partial x}e^{-r} = -\dfrac{x}{r}e^{-r}, \ \dfrac{\partial}{\partial y}e^{-r} = -\dfrac{y}{r}e^{-r}$, and $\nabla^2 e^{-r} = \left(\dfrac{2}{r}\dfrac{\partial}{\partial r} + \dfrac{d^2}{dr^2}\right)e^{-r} = \left(1 - \dfrac{2}{r}\right)e^{-r}$

Therefore $\nabla^2 f = \dfrac{\partial^2 f}{\partial x^2} + \dfrac{\partial^2 f}{\partial y^2} + \dfrac{\partial^2 f}{\partial z^2} = -\dfrac{4}{r}xye^{-r} + xy\nabla^2 e^{-r}$

$$= \left(1 - \frac{6}{r}\right)xye^{-r} = \left(1 - \frac{6}{r}\right)f$$

and $\nabla^2 f + \dfrac{6}{r}f = f$

33. Show that $f(r) = \dfrac{e^{ar}}{r}$, where a is an arbitrary number, satisfies $\nabla^2 f = a^2 f$.

We have $\quad \dfrac{d}{dr}\left(\dfrac{e^{ar}}{r}\right) = \left[\dfrac{a}{r} - \dfrac{1}{r^2}\right]e^{ar}, \quad \dfrac{d^2}{dr^2}\left(\dfrac{e^{ar}}{r}\right) = \left[\dfrac{a^2}{r} - \dfrac{2a}{r^2} + \dfrac{2}{r^3}\right]e^{ar}$

Therefore $\quad \nabla^2\left(\dfrac{e^{ar}}{r}\right) = \left(\dfrac{d^2}{dr^2} + \dfrac{2}{r}\dfrac{d}{dr}\right)\dfrac{e^{ar}}{r} = a^2\,\dfrac{e^{-r}}{r}$

or $\quad \nabla^2 f = a^2 f$

Show that the following functions satisfy the Laplace equation:

34. $f(x, y, z) = 2x^3 - 3x(y^2 + z^2)$

We have $\quad \dfrac{\partial^2 f}{\partial x^2} = 12x, \quad \dfrac{\partial^2 f}{\partial y^2} = -6x = \dfrac{\partial^2 f}{\partial x^2}$

Therefore $\quad \nabla^2 f = 0$

35. $f(r, \theta, \phi) = \dfrac{\cos 2\phi}{r^2 \sin^2\theta}$

Let $\quad f(r, \theta, \phi) = \dfrac{1}{r^2} \times \dfrac{1}{\sin^2\theta} \times \cos 2\phi = R(r) \times \Theta(\theta) \times \Phi(\phi)$

We have $\quad R = \dfrac{1}{r^2}: \quad \dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2 \dfrac{dR}{dr}\right) = \dfrac{2}{r^2}R$

$$\Theta = \frac{1}{\sin^2\theta}: \quad \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) = \frac{2(1+\cos^2\theta)}{\sin^2\theta}\Theta$$

$$\Phi = \cos 2\phi: \quad \frac{d^2\Phi}{d\phi^2} = -4\cos 2\phi = -4\Phi$$

Therefore $\quad \nabla^2 f = \left[\dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right)\right]\Theta\Phi + \dfrac{1}{r^2}R\left[\dfrac{1}{\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d\Theta}{d\theta}\right)\right]\Phi + \dfrac{R\Theta}{r^2\sin^2\theta}\left[\dfrac{d^2\Phi}{d\phi^2}\right]$

$$= \left[\frac{2}{r^2} + \frac{2(1+\cos^2\theta)}{r^2\sin^2\theta} - \frac{4}{r^2\sin^2\theta}\right]R(r)\Theta(\theta)\Phi(\phi)$$

$$= \frac{4}{r^2\sin^2\theta}\left[2\sin^2\theta + 2 + 2\cos^2\theta - 4\right]f = \frac{4}{r^2\sin^2\theta}\left[2+2-4\right]f = 0$$

36. $f(r,\theta,\phi) = r^n \sin^n\theta \cos n\phi,\ n = 1,2,3,\ldots$

Let $f(r,\theta,\phi) = r^n \times \sin^n\theta \times \cos n\phi = R(r)\times\Theta(\theta)\times\Phi(\phi)$

We have $R = r^n$: $\dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right) = n(n+1)r^{n-2} = \dfrac{n(n+1)}{r^2}R$

$$\Theta = \sin^n\theta:\quad \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = \left[\frac{n^2\cos^2\theta}{\sin^2\theta} - n\right]\Theta$$

$$\Phi = \cos n\phi:\quad \frac{d^2\Phi}{d\phi^2} = -n^2\Phi(\phi)$$

Therefore $\nabla^2 f = \left[\dfrac{1}{r^2}\dfrac{d}{dr}\left(r^2\dfrac{dR}{dr}\right)\right]\Theta\Phi + \dfrac{1}{r^2}R\left[\dfrac{1}{\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d\Theta}{d\theta}\right)\right]\Phi + \dfrac{R\Theta}{r^2\sin^2\theta}\left[\dfrac{d^2\Phi}{d\phi^2}\right]$

$$= \frac{1}{r^2}\left[n(n+1) + \frac{n^2\cos^2\theta}{\sin^2\theta} - n - \frac{n^2}{\sin^2\theta}\right]R\Theta\Phi$$

$$= \frac{1}{r^2}\left[n^2 + n + \frac{n^2\cos^2\theta}{\sin^2\theta} - n - \frac{n^2(\sin^2\theta + \cos^2\theta)}{\sin^2\theta}\right]f = 0$$

37. The d'Alembertian operator is

$$\Box^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$$

where *x, y, z* are coordinates, *t* is the time, and *c* is the speed of light. Show that if the function $f(x,y,z)$ satisfies Laplace's equation then the function $g(x,y,z,t) = f(x,y,z)e^{ikct}$ satisfies the equation $\Box^2 g = k^2 g$.

We have $\Box^2 g(x,y,z,t) = \left[\nabla^2 - \dfrac{1}{c^2}\dfrac{\partial^2}{\partial t^2}\right]f(x,y,z)e^{ikct}$

$$= \left[\nabla^2 f\right]e^{ikct} - f\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2}e^{ikct}\right]$$

$$= 0 - f\frac{1}{c^2}(ikc)^2 e^{ikct} = k^2 f\, e^{ikct}$$

Therefore $\Box^2 g = k^2 g$.

Section 10.6

38. What are the parametric equations of a left-handed helix in
(i) cartesian coordinates, **(ii)** cylindrical polar coordinates?

(i) As in Example 10.13 but with $y \to -y$:

$$x = a\cos t,\ \ y = -a\sin t,\ \ z = bt$$

(ii) $\rho = a,\ \ \phi = -t,\ \ z = bt$

39. Integrate the function $f = y^2 z^3$ over the cylindrical region of radius *a*, between $z = 0$ and $z = 1$, and symmetric about the *z*-axis.

In cylindrical coordinates, $f(\rho, \phi, z) = \rho^2 \sin^2\theta\, z^3$. Then

$$\int_V f(\rho,\phi,z)\,dv = \int_{z=0}^{1}\int_{\phi=0}^{2\pi}\int_{\rho=0}^{a} (\rho^2 \sin^2\phi\, z^3)\,\rho\, d\rho\, d\phi\, dz$$

$$= \int_{z=0}^{1} z^3\, dz \times \int_{\phi=0}^{2\pi} \sin^2\phi\, d\phi \times \int_{\rho=0}^{a} \rho^3 d\rho \ = \frac{1}{4} \times \pi \times \frac{a^4}{4}$$

$$= \frac{\pi a^4}{16}$$

Use confocal elliptic coordinates, $\xi = \dfrac{r_A + r_B}{R},\ \ \eta = \dfrac{r_A - r_B}{R},\ \ \phi,$ to integrate over all space:

40. $\dfrac{e^{-(r_A + r_B)}}{r_A}$

We have $\quad r_A + r_B = R\xi,\ \ r_A = \dfrac{R}{2}(\xi + \eta),$

Then $$\int \frac{e^{-(r_A + r_B)}}{r_A}\, dv = \frac{R^3}{8}\int_{\phi=0}^{2\pi}\int_{\eta=-1}^{+1}\int_{\xi=1}^{\infty}\left(\frac{e^{-R\xi}}{R(\xi+\eta)/2}\right)(\xi^2 - \eta^2)\, d\xi\, d\eta\, d\phi$$

$$= \frac{R^2}{4}\int_0^{2\pi} d\phi \int_{\eta=-1}^{+1}\int_{\xi=1}^{\infty} e^{-R\xi}(\xi - \eta)\, d\xi\, d\eta$$

$$= \frac{\pi R^2}{2}\left\{\int_{-1}^{+1} d\eta \int_1^{\infty} e^{-R\xi}\xi\, d\xi - \int_{-1}^{+1}\eta\, d\eta \int_1^{\infty} e^{-R\xi}\, d\xi\right\}$$

Now $$\int_{-1}^{+1} d\eta = 2,\quad \int_{-1}^{+1}\eta\, d\eta = 0$$

Therefore, by parts,

$$\int \frac{e^{-(r_A + r_B)}}{r_A} dv = \pi R^2 \int_1^\infty e^{-R\xi} \xi d\xi$$

$$= \pi R^2 \left\{ \left[-\frac{1}{R} e^{-R\xi} \xi \right]_1^\infty + \frac{1}{R} \int_1^\infty e^{-R\xi} d\xi \right\}$$

$$= \pi R^2 \left\{ \left[-\frac{1}{R} e^{-R\xi} \xi \right]_1^\infty + \frac{1}{R} \left[-\frac{1}{R} e^{-R\xi} \right]_1^\infty \right\}$$

$$= \pi R^2 \left\{ \frac{1}{R} e^{-R} + \frac{1}{R^2} e^{-R} \right\}$$

$$= \pi (R+1) e^{-R}$$

41. $\dfrac{e^{-(r_A + r_B)}}{r_B} \cos^2 \phi$

We have $\quad r_A + r_B = R\xi, \quad r_B = \dfrac{R}{2}(\xi - \eta),$

Then

$$\int \frac{e^{-(r_A + r_B)}}{r_B} \cos^2 \phi \, dv = \frac{R^3}{8} \int_{\phi=0}^{2\pi} \int_{\eta=-1}^{+1} \int_{\xi=1}^{\infty} \left(\frac{e^{-R\xi}}{R(\xi-\eta)/2} \right) (\xi^2 - \eta^2) \cos^2 \phi \, d\xi \, d\eta \, d\phi$$

$$= \frac{R^2}{4} \int_0^{2\pi} \cos^2 \phi \, d\phi \int_{\eta=-1}^{+1} \int_{\xi=1}^{\infty} e^{-R\xi} (\xi + \eta) \, d\xi \, d\eta$$

$$= \frac{R^2}{4} \int_0^{2\pi} \cos^2 \phi \, d\phi \left\{ \int_{-1}^{+1} d\eta \int_1^\infty e^{-R\xi} \xi \, d\xi + \int_{-1}^{+1} \eta \, d\eta \int_1^\infty e^{-R\xi} d\xi \right\}$$

Now $\quad \displaystyle\int_0^{2\pi} \cos^2 \phi \, d\phi = \pi, \quad \int_{-1}^{+1} d\eta = 2, \quad \int_{-1}^{+1} \eta \, d\eta = 0$

Therefore, as in Exercise 40,

$$\int \frac{e^{-(r_A + r_B)}}{r_B} \cos^2 \phi \, dv = \frac{\pi R^2}{2} \int_1^\infty e^{-R\xi} \xi d\xi$$

$$= \frac{\pi}{2} (R+1) e^{-R}$$