Quantum Mechanics and Atomic Physics 750:361

Prof. Sean Oh, Fall 2011

HW #7

1. Reed, Prob. 6-1

Problem 6-1

Consider an electron moving in an infinite potential box of dimensions (1.0, 1.5, 1.9) Å. Tabulate all possible energy levels (in eV) for (n_x, n_y, n_z) = 1 to 3.

If a, b, and c are the x, y, and z dimensions of the box, then equation (6.1.15) tells us

$$E = \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right].$$

Substituting numerical values and converting to electron volts gives

$$E = 37.60\left[n_x^2 + \frac{n_y^2}{2.25} + \frac{n_z^2}{3.61}\right] \text{ eV}.$$

A total of 27 combinations are possible for (n_x, n_y, n_z) = 1 to 3. The energies are tabulated below, in increasing values:

n_x	n_y	n_z	E (eV)
1	1	1	64.7
1	1	2	96.0
1	2	1	114.9
1	2	2	146.1
1	1	3	148.1
2	1	1	177.6
1	2	3	198.2
1	3	1	198.5
2	1	2	208.8
2	2	1	227.7
1	3	2	229.7
2	2	2	258.9
2	1	3	260.9
1	3	3	281.8
2	2	3	311.1
2	3	1	311.3
2	3	2	342.6

3	1	1	365.6
2	3	3	394.6
3	1	2	396.9
3	2	1	415.8
3	2	2	446.9
3	1	3	449.0
3	2	3	499.1
3	3	1	499.3
3	3	2	530.6
3	3	3	582.7

2. Reed, Prob. 6-3

Problem 6-3

For which of the following three-dimensional potentials would the Schrödinger equation be separable?

(a) $V(x,y,z) = x^2 y + \sin(z)$

(b) $V(x,y,z) = x^2 + y + \mathrm{Tan}^{-1}(\sqrt{z})$

(c) $V(x,y,z) = e^x y^{7/2} z^2$

(d) $V(x,y,z) = y\sin(x) + z\cos(y) + y\tan(z)$

(e) $V(x,y,z) = y^{-4} + \mathrm{Sin}^{-1}(e^{\sqrt{x}}) + \tan(z)$

(f) $V(x,y,z) = e^{xy\sqrt{z}}$

(g) $V(x,y,z) = e^{x + y - \sqrt{z}}$

Only potentials of the form f(x) + g(y) + h(z) are separable. Hence only functions (b) and (e) will be separable.

3. Reed, Prob. 6-5

Reed 6.5.

$$\frac{\partial \hat{r}}{\partial r} = \cos\theta\cos\phi\,\hat{x} + \cos\theta\sin\phi\,\hat{y} - \sin\theta\,\hat{z}$$
$$= \hat{\theta}$$

$$\frac{\partial \hat{\theta}}{\partial \theta} = -\sin\theta\cos\varphi\,\hat{x} - \sin\theta\sin\varphi\,\hat{y} - \cos\theta\,\hat{z}$$
$$= -\hat{r}$$

$$\frac{\partial \hat{\varphi}}{\partial \theta} = \frac{\partial}{\partial \theta}\left(-\sin\varphi\,\hat{x} + \cos\varphi\,\hat{y}\right)$$
$$= 0$$

$$\frac{\partial \hat{r}}{\partial \varphi} = -\sin\theta\sin\varphi\,\hat{x} + \sin\theta\cos\varphi\,\hat{y}$$
$$= \sin\theta\left(-\sin\varphi\,\hat{x} + \cos\varphi\,\hat{y}\right)$$
$$= \sin\theta\,\hat{\varphi}$$

$$\frac{\partial \hat{\theta}}{\partial \varphi} = -\cos\theta\sin\varphi\,\hat{x} + \cos\theta\cos\varphi\,\hat{y}$$
$$= \cos\theta\left(-\sin\varphi\,\hat{x} + \cos\varphi\,\hat{y}\right)$$
$$= \cos\theta\,\hat{\varphi}$$

$$\frac{\partial \hat{\varphi}}{\partial \varphi} = -\cos\varphi\,\hat{x} - \sin\varphi\,\hat{y}$$
$$= -\cos\varphi\left(\sin\theta\cos\varphi\,\hat{r} + \cos\theta\cos\varphi\,\hat{\theta} - \sin\varphi\,\hat{\varphi}\right)$$
$$- \sin\varphi\left(\sin\theta\sin\varphi\,\hat{r} + \cos\theta\sin\varphi\,\hat{\theta} + \cos\varphi\,\hat{\varphi}\right)$$
$$= -\Big[\sin\theta\left(\cos^2\varphi + \sin^2\varphi\right)\hat{r} + \cos\theta\left(\cos^2\varphi + \sin^2\varphi\right)\hat{\theta} + \left(-\cos\varphi\sin\varphi + \sin\varphi\cos\varphi\right)\hat{\varphi}\Big]$$
$$= -\sin\theta\,\hat{r} - \cos\theta\,\hat{\theta}$$