Problem 4.2

Use separation of variables in cartesian coordinates to solve the infinite *cubical* well (or "particle in a box"):

$$V(x,y,z) = \begin{cases} 0, & x,\ y,\ z \text{ all between 0 and } a; \\ \infty, & \text{otherwise.} \end{cases}$$

(a) Find the stationary states, and the corresponding energies.

(b) Call the distinct energies E_1, E_2, E_3, $\ldots$, in order of increasing energy. Find E_1, E_2, E_3, E_4, E_5, and E_6. Determine their degeneracies (that is, the number of different states that share the same energy). *Comment*: In *one* dimension degenerate bound states do not occur (see Problem 2.44), but in three dimensions they are very common.

(c) What is the degeneracy of E_{14}, and why is this case interesting?

Solution

Part (a)

The aim is to find how a prescribed initial wave function $\Psi_0(x,y,z)$ evolves in all of space

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + V\Psi, \quad -\infty < x,y,z < \infty,\ t > 0$$

$$\Psi(x,y,z,0) = \Psi_0(x,y,z)$$

subject to the potential energy function,

$$V(x,y,z) = \begin{cases} 0 & \text{if } 0 < x,y,z < a \\ \infty & \text{elsewhere} \end{cases}.$$

Outside of the cube in the first octant with side a,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + (\infty)\Psi, \quad x,y,z \notin (0,a),$$

and the only way for both sides to be equal is if $\Psi(x,y,z,t) = 0$. The wave function is required to be continuous, so $\Psi = 0$ on the sides of this cube, that is, the $x = 0$, $x = a$, $y = 0$, $y = a$, $z = 0$, and $z = a$ planes.

Inside the cube, then, the initial boundary value problem to solve is

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right), \quad 0 < x, y, z < a,\ t > 0$$

$$\Psi(0, y, z, t) = 0, \qquad \Psi(x, 0, z, t) = 0, \qquad \Psi(x, y, 0, t) = 0,$$

$$\Psi(a, y, z, t) = 0, \qquad \Psi(x, a, z, t) = 0, \qquad \Psi(x, y, a, t) = 0,$$

$$\Psi(x, y, z, 0) = \Psi_0(x, y, z).$$

Because Schrödinger's equation and its associated boundary conditions are linear and homogeneous, the method of separation of variables can be applied: Assume a product solution of the form $\Psi(x, y, z, t) = X(x)Y(y)Z(z)T(t)$ and plug it into the PDE

$$i\hbar\frac{\partial}{\partial t}[X(x)Y(y)Z(z)T(t)] = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}[X(x)Y(y)Z(z)T(t)] + \frac{\partial^2}{\partial y^2}[X(x)Y(y)Z(z)T(t)] + \frac{\partial^2}{\partial z^2}[X(x)Y(y)Z(z)T(t)]\right]$$

$$i\hbar X(x)Y(y)Z(z)T'(t) = -\frac{\hbar^2}{2m}\left[X''(x)Y(y)Z(z)T(t) + X(x)Y''(y)Z(z)T(t) + X(x)Y(y)Z''(z)T(t)\right]$$

and the boundary conditions.

$$\Psi(0, y, z, t) = 0 \quad \rightarrow \quad X(0)Y(y)Z(z)T(t) = 0 \quad \rightarrow \quad X(0) = 0$$

$$\Psi(a, y, z, t) = 0 \quad \rightarrow \quad X(a)Y(y)Z(z)T(t) = 0 \quad \rightarrow \quad X(a) = 0$$

$$\Psi(x, 0, z, t) = 0 \quad \rightarrow \quad X(x)Y(0)Z(z)T(t) = 0 \quad \rightarrow \quad Y(0) = 0$$

$$\Psi(x, a, z, t) = 0 \quad \rightarrow \quad X(x)Y(a)Z(z)T(t) = 0 \quad \rightarrow \quad Y(a) = 0$$

$$\Psi(x, y, 0, t) = 0 \quad \rightarrow \quad X(x)Y(y)Z(0)T(t) = 0 \quad \rightarrow \quad Z(0) = 0$$

$$\Psi(x, y, a, t) = 0 \quad \rightarrow \quad X(x)Y(y)Z(a)T(t) = 0 \quad \rightarrow \quad Z(a) = 0$$

Divide both sides of the PDE by $X(x)Y(y)Z(z)T(t)$ to separate variables.

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m}\left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)}\right]$$

The only way a function of t can be equal to a function of x, y, and z is if both are equal to a constant.

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m}\left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)}\right] = E$$

Solve this second equation for $X''(x)/X(x)$.

$$\frac{X''(x)}{X(x)} = -\frac{2mE}{\hbar^2} - \frac{Y''(y)}{Y(y)} - \frac{Z''(z)}{Z(z)}$$

The only way a function of x can be equal to a function of y and z is if both are equal to another constant.

$$\frac{X''(x)}{X(x)} = -\frac{2mE}{\hbar^2} - \frac{Y''(y)}{Y(y)} - \frac{Z''(z)}{Z(z)} = F$$

Solve this second equation for $Y''(y)/Y(y)$.

$$\frac{Y''(y)}{Y(y)} = -\frac{2mE}{\hbar^2} - F - \frac{Z''(z)}{Z(z)}$$

The only way a function of y can be equal to a function of z is if both are equal to another constant.

$$\frac{Y''(y)}{Y(y)} = -\frac{2mE}{\hbar^2} - F - \frac{Z''(z)}{Z(z)} = G$$

As a result of applying the method of separation of variables, Schrödinger's equation has reduced to four ODEs—one in x, one in y, one in z, and one in t.

$$\left.\begin{aligned} i\hbar\frac{T'(t)}{T(t)} &= E \\ \frac{X''(x)}{X(x)} &= F \\ \frac{Y''(y)}{Y(y)} &= G \\ -\frac{2mE}{\hbar^2} - F - \frac{Z''(z)}{Z(z)} &= G \end{aligned}\right\}$$

The strategy is to solve the second and third eigenvalue problems first to get F and G. Once those are known, the fourth eigenvalue problem can be solved to get E. Finally, the first eigenvalue problem can be solved to get $T(t)$.

$$X''(x) = FX(x), \quad X(0) = 0,\ X(a) = 0$$

Check to see if there are positive eigenvalues: $F = \mu^2$.

$$X'' = \mu^2 X$$

The general solution can be written in terms of hyperbolic sine and hyperbolic cosine.

$$X(x) = C_1 \cosh \mu x + C_2 \sinh \mu x$$

Apply the boundary conditions to determine C_1 and C_2.

$$X(0) = C_1 = 0$$

$$X(a) = C_1 \cosh \mu a + C_2 \sinh \mu a = 0$$

Since $C_1 = 0$, the second equation reduces to $C_2 \sinh \mu a = 0$. No nonzero value of μ can satisfy this equation, so $C_2 = 0$. This leads to $X(x) = 0$, the trivial solution, which means there are no positive eigenvalues. Check to see if zero is an eigenvalue: $F = 0$.

$$X'' = 0$$

The general solution is obtained by integrating both sides with respect to x twice.

$$X(x) = C_3 x + C_4$$

Apply the boundary conditions to determine C_3 and C_4.

$$X(0) = C_4 = 0$$

$$X(a) = C_3 a + C_4 = 0$$

Since $C_4 = 0$, the second equation reduces to $C_3 a = 0$, so $C_3 = 0$. This leads to $X(x) = 0$, the trivial solution, which means zero is not an eigenvalue. Check to see if there are negative eigenvalues: $F = -\gamma^2$.

$$X'' = -\gamma^2 X$$

The general solution can be written in terms of sine and cosine.

$$X(x) = C_5 \cos \gamma x + C_6 \sin \gamma x$$

Apply the boundary conditions to determine C_5 and C_6.

$$X(0) = C_5 = 0$$

$$X(a) = C_5 \cos \gamma a + C_6 \sin \gamma a = 0$$

Since $C_5 = 0$, this second equation reduces to $C_6 \sin \gamma a = 0$.

$$\sin \gamma a = 0$$

$$\gamma a = j\pi, \quad j = 0, \pm 1, \pm 2, \ldots$$

$$\gamma = \frac{j\pi}{a}$$

There are in fact negative eigenvalues,

$$F = -\gamma^2 = -\frac{j^2\pi^2}{a^2}, \quad j = 1, 2, \ldots,$$

and the eigenfunctions associated with them are

$$X(x) = C_6 \sin \frac{j\pi x}{a},$$

where C_6 remains arbitrary. j is a positive integer because $j = 0$ leads to the zero eigenvalue, and negative values of j lead to redundant eigenvalues. The same argument can be used to solve the eigenvalue problem involving $Y(y)$.

$$Y''(y) = GY(y), \quad Y(0) = 0, \ Y(a) = 0$$

Its solution is

$$G = -\frac{k^2\pi^2}{a^2}, \quad k = 1, 2, \ldots,$$

with

$$Y(y) = C_7 \sin \frac{k\pi y}{a},$$

where C_7 is an arbitrary constant. With these values of F and G, the eigenvalue problem involving $Z(z)$ becomes

$$-\frac{2mE}{\hbar^2} - \left(-\frac{j^2\pi^2}{a^2}\right) - \frac{Z''(z)}{Z(z)} = -\frac{k^2\pi^2}{a^2}, \quad Z(0) = 0, \ Z(a) = 0.$$

Solve for $Z''(z)$.

$$Z'' = -\left(\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}\right) Z$$

This ODE for $Z(z)$ and its boundary conditions are the same as those for $X(x)$ and $Y(y)$. The general solution for which eigenvalues exist is then

$$Z(z) = C_8 \cos\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}z + C_9 \sin\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}z.$$

Apply the boundary conditions to determine C_8 and C_9.

$$Z(0) = C_8 = 0$$

$$Z(a) = C_8 \cos\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}a + C_9 \sin\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}a = 0$$

Since $C_8 = 0$, this second equation reduces to

$$C_9 \sin\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}a = 0$$

$$\sin\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}a = 0$$

$$\sqrt{\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2}}a = l\pi, \quad l = 0, \pm1, \pm2, \ldots$$

$$\frac{2mE}{\hbar^2} - \frac{j^2\pi^2}{a^2} - \frac{k^2\pi^2}{a^2} = \frac{l^2\pi^2}{a^2}.$$

Solve for E.

$$\boxed{E_{jkl} = \frac{\pi^2\hbar^2}{2ma^2}(j^2 + k^2 + l^2), \quad \begin{cases} j = 1, 2, \ldots \\ k = 1, 2, \ldots \\ l = 1, 2, \ldots \end{cases}}$$

Only positive values of l are used because $l = 0$ leads to the zero eigenvalue, and negative values lead to redundant values of E. The eigenfunctions associated with these values of E are

$$Z(z) = C_9 \sin\frac{l\pi z}{a},$$

where C_9 is an arbitrary constant. With this value of E, the eigenvalue problem involving $T(t)$ becomes

$$i\hbar\frac{T'(t)}{T(t)} = \frac{\pi^2\hbar^2}{2ma^2}(j^2 + k^2 + l^2),$$

which has the general solution,

$$T(t) = C_{10} \exp\left[-\frac{i\pi^2\hbar}{2ma^2}(j^2 + k^2 + l^2)t\right].$$

Consequently, the stationary states are

$$\begin{aligned} \Psi_{jkl}(x, y, z, t) &= X_j(x)Y_k(y)Z_l(z)T_{jkl}(t) \\ &= A \sin\frac{j\pi x}{a} \sin\frac{k\pi y}{a} \sin\frac{l\pi z}{a} \exp\left[-\frac{i\pi^2\hbar}{2ma^2}(j^2 + k^2 + l^2)t\right], \end{aligned}$$

where A is a combination of the arbitrary constants. For the solutions to be physically relevant, the normalization constant A is chosen so that

$$\begin{aligned}
1 = \iiint_{\text{the cube}} |\Psi_{jkl}(x,y,z,t)|^2\, d\mathcal{V} &= \int_0^a \int_0^a \int_0^a \Psi^*_{jkl}(x,y,z,t)\Psi_{jkl}(x,y,z,t)\, dx\, dy\, dz \\
&= A^2 \int_0^a \int_0^a \int_0^a \sin^2 \frac{j\pi x}{a} \sin^2 \frac{k\pi y}{a} \sin^2 \frac{l\pi z}{a}\, dx\, dy\, dz \\
&= A^2 \left(\int_0^a \sin^2 \frac{j\pi x}{a}\, dx\right)\left(\int_0^a \sin^2 \frac{k\pi y}{a}\, dy\right)\left(\int_0^a \sin^2 \frac{l\pi z}{a}\, dz\right) \\
&= A^2 \left(\frac{a}{2}\right)\left(\frac{a}{2}\right)\left(\frac{a}{2}\right).
\end{aligned}$$

Solve for A.

$$A = \pm \left(\frac{2}{a}\right)^{3/2}$$

Therefore, the stationary states are

$$\boxed{\Psi_{jkl}(x,y,z,t) = \left(\frac{2}{a}\right)^{3/2} \sin \frac{j\pi x}{a} \sin \frac{k\pi y}{a} \sin \frac{l\pi z}{a} \exp\left[-\frac{i\pi^2\hbar}{2ma^2}(j^2+k^2+l^2)t\right], \quad \begin{cases} j = 1, 2, \ldots \\ k = 1, 2, \ldots . \\ l = 1, 2, \ldots \end{cases}}$$

According to the principle of superposition, the general solution to the Schrödinger equation is a linear combination of the stationary states over all the eigenvalues.

$$\begin{aligned}
\Psi(x,y,z,t) &= \sum_{j=1}^\infty \sum_{k=1}^\infty \sum_{l=1}^\infty c_{jkl} \Psi_{jkl}(x,y,z,t) \\
&= \sum_{j=1}^\infty \sum_{k=1}^\infty \sum_{l=1}^\infty c_{jkl} \left(\frac{2}{a}\right)^{3/2} \sin \frac{j\pi x}{a} \sin \frac{k\pi y}{a} \sin \frac{l\pi z}{a} \exp\left[-\frac{i\pi^2\hbar}{2ma^2}(j^2+k^2+l^2)t\right] \\
&= \left(\frac{2}{a}\right)^{3/2} \sum_{j=1}^\infty \sum_{k=1}^\infty \sum_{l=1}^\infty c_{jkl} \sin \frac{j\pi x}{a} \sin \frac{k\pi y}{a} \sin \frac{l\pi z}{a} \exp\left[-\frac{i\pi^2\hbar}{2ma^2}(j^2+k^2+l^2)t\right]
\end{aligned}$$

Now apply the initial condition to determine c_{jkl}.

$$\Psi(x,y,z,0) = \left(\frac{2}{a}\right)^{3/2} \sum_{j=1}^\infty \sum_{k=1}^\infty \sum_{l=1}^\infty c_{jkl} \sin \frac{j\pi x}{a} \sin \frac{k\pi y}{a} \sin \frac{l\pi z}{a} = \Psi_0(x,y,z)$$

Multiply both sides by $(a/2)^{3/2}$.

$$\sum_{k=1}^\infty \sum_{l=1}^\infty \sin \frac{k\pi y}{a} \sin \frac{l\pi z}{a} \left(\sum_{j=1}^\infty c_{jkl} \sin \frac{j\pi x}{a}\right) = \left(\frac{a}{2}\right)^{3/2} \Psi_0(x,y,z)$$

Multiply both sides by $\sin(n\pi x/a)$, where n is a positive integer,

$$\sum_{k=1}^\infty \sum_{l=1}^\infty \sin \frac{k\pi y}{a} \sin \frac{l\pi z}{a} \left(\sum_{j=1}^\infty c_{jkl} \sin \frac{j\pi x}{a} \sin \frac{n\pi x}{a}\right) = \left(\frac{a}{2}\right)^{3/2} \Psi_0(x,y,z) \sin \frac{n\pi x}{a}$$

and then integrate both sides with respect to x from 0 to a.

$$\int_0^a \sum_{k=1}^\infty \sum_{l=1}^\infty \sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\left(\sum_{j=1}^\infty c_{jkl}\sin\frac{j\pi x}{a}\sin\frac{n\pi x}{a}\right)dx = \int_0^a \left(\frac{a}{2}\right)^{3/2}\Psi_0(x,y,z)\sin\frac{n\pi x}{a}\,dx$$

Bring the constants in front.

$$\sum_{k=1}^\infty \sum_{l=1}^\infty \sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\left(\sum_{j=1}^\infty c_{jkl}\int_0^a \sin\frac{j\pi x}{a}\sin\frac{n\pi x}{a}\,dx\right) = \left(\frac{a}{2}\right)^{3/2}\int_0^a \Psi_0(x,y,z)\sin\frac{n\pi x}{a}\,dx$$

Because the sine functions are orthogonal, the integral on the left is zero if $j \neq n$. As a result, every term in the infinite series vanishes except for the one in which $j = n$.

$$\sum_{k=1}^\infty \sum_{l=1}^\infty \sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\left(c_{jkl}\int_0^a \sin^2\frac{j\pi x}{a}\,dx\right) = \left(\frac{a}{2}\right)^{3/2}\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\,dx$$

Evaluate the integral on the left.

$$\sum_{k=1}^\infty \sum_{l=1}^\infty \sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\left(c_{jkl}\cdot\frac{a}{2}\right) = \left(\frac{a}{2}\right)^{3/2}\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\,dx$$

Multiply both sides by $2/a$.

$$\sum_{l=1}^\infty \sin\frac{l\pi z}{a}\left(\sum_{k=1}^\infty c_{jkl}\sin\frac{k\pi y}{a}\right) = \left(\frac{a}{2}\right)^{1/2}\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\,dx$$

Multiply both sides by $\sin(q\pi y/a)$, where q is a positive integer,

$$\sum_{l=1}^\infty \sin\frac{l\pi z}{a}\left(\sum_{k=1}^\infty c_{jkl}\sin\frac{k\pi y}{a}\sin\frac{q\pi y}{a}\right) = \left(\frac{a}{2}\right)^{1/2}\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{q\pi y}{a}\,dx$$

and then integrate both sides with respect to y from 0 to a.

$$\int_0^a \sum_{l=1}^\infty \sin\frac{l\pi z}{a}\left(\sum_{k=1}^\infty c_{jkl}\sin\frac{k\pi y}{a}\sin\frac{q\pi y}{a}\right)dy = \int_0^a \left(\frac{a}{2}\right)^{1/2}\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{q\pi y}{a}\,dx\,dy$$

Bring the constants in front.

$$\sum_{l=1}^\infty \sin\frac{l\pi z}{a}\left(\sum_{k=1}^\infty c_{jkl}\int_0^a \sin\frac{k\pi y}{a}\sin\frac{q\pi y}{a}\,dy\right) = \left(\frac{a}{2}\right)^{1/2}\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{q\pi y}{a}\,dx\,dy$$

Because the sine functions are orthogonal, the integral on the left is zero if $k \neq q$. As a result, every term in the infinite series vanishes except for the one in which $k = q$.

$$\sum_{l=1}^\infty \sin\frac{l\pi z}{a}\left(c_{jkl}\int_0^a \sin^2\frac{k\pi y}{a}\,dy\right) = \left(\frac{a}{2}\right)^{1/2}\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\,dx\,dy$$

Evaluate the integral on the left.

$$\sum_{l=1}^{\infty} \sin\frac{l\pi z}{a}\left(c_{jkl}\cdot\frac{a}{2}\right) = \left(\frac{a}{2}\right)^{1/2}\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\,dx\,dy$$

Multiply both sides by $2/a$.

$$\sum_{l=1}^{\infty} c_{jkl}\sin\frac{l\pi z}{a} = \left(\frac{2}{a}\right)^{1/2}\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\,dx\,dy$$

Multiply both sides by $\sin(s\pi z/a)$, where s is a positive integer,

$$\sum_{l=1}^{\infty} c_{jkl}\sin\frac{l\pi z}{a}\sin\frac{s\pi z}{a} = \left(\frac{2}{a}\right)^{1/2}\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\sin\frac{s\pi z}{a}\,dx\,dy$$

and then integrate both sides with respect to z from 0 to a.

$$\int_0^a\sum_{l=1}^{\infty} c_{jkl}\sin\frac{l\pi z}{a}\sin\frac{s\pi z}{a}\,dz = \int_0^a\left(\frac{2}{a}\right)^{1/2}\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\sin\frac{s\pi z}{a}\,dx\,dy\,dz$$

Bring the constants in front.

$$\sum_{l=1}^{\infty} c_{jkl}\int_0^a\sin\frac{l\pi z}{a}\sin\frac{s\pi z}{a}\,dz = \left(\frac{2}{a}\right)^{1/2}\int_0^a\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\sin\frac{s\pi z}{a}\,dx\,dy\,dz$$

Because the sine functions are orthogonal, the integral on the left is zero if $l \neq s$. As a result, every term in the infinite series vanishes except for the one in which $l = s$.

$$c_{jkl}\int_0^a\sin^2\frac{l\pi z}{a}\,dz = \left(\frac{2}{a}\right)^{1/2}\int_0^a\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\,dx\,dy\,dz$$

Evaluate the integral on the left.

$$c_{jkl}\cdot\frac{a}{2} = \left(\frac{2}{a}\right)^{1/2}\int_0^a\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\,dx\,dy\,dz$$

Therefore,

$$c_{jkl} = \left(\frac{2}{a}\right)^{3/2}\int_0^a\int_0^a\int_0^a \Psi_0(x,y,z)\sin\frac{j\pi x}{a}\sin\frac{k\pi y}{a}\sin\frac{l\pi z}{a}\,dx\,dy\,dz.$$

Part (b)

Evaluate the energy for many values of j, k, and l.

$$E_{111} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+1^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(3) = E_1$$
$$E_{211} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+1^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(6) = E_2$$
$$E_{121} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+2^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(6)$$
$$E_{112} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+1^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(6)$$
$$E_{221} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+2^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(9) = E_3$$
$$E_{212} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+1^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(9)$$
$$E_{122} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+2^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(9)$$
$$E_{311} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+1^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(11) = E_4$$
$$E_{131} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+3^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(11)$$
$$E_{113} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+1^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(11)$$
$$E_{222} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+2^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(12) = E_5$$
$$E_{312} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+1^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(14) = E_6$$
$$E_{321} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+2^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(14)$$
$$E_{132} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+3^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(14)$$
$$E_{231} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+3^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(14)$$
$$E_{123} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+2^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(14)$$
$$E_{213} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+1^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(14)$$

The degeneracy is the number of states that have the same energy. Therefore, $d_1 = 1$, $d_2 = 3$, $d_3 = 3$, $d_4 = 3$, $d_5 = 1$, and $d_6 = 6$.

Part (c)

Evaluate the energy for more values of j, k, and l.

$$E_{322} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+2^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(17) = E_7$$

$$E_{232} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+3^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(17)$$

$$E_{223} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+2^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(17)$$

$$E_{411} = \frac{\pi^2\hbar^2}{2ma^2}(4^2+1^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(18) = E_8$$

$$E_{141} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+4^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(18)$$

$$E_{114} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+1^2+4^2) = \frac{\pi^2\hbar^2}{2ma^2}(18)$$

$$E_{331} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+3^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(19) = E_9$$

$$E_{313} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+1^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(19)$$

$$E_{133} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+3^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(19)$$

$$E_{412} = \frac{\pi^2\hbar^2}{2ma^2}(4^2+1^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(21) = E_{10}$$

$$E_{421} = \frac{\pi^2\hbar^2}{2ma^2}(4^2+2^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(21)$$

$$E_{142} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+4^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(21)$$

$$E_{241} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+4^2+1^2) = \frac{\pi^2\hbar^2}{2ma^2}(21)$$

$$E_{124} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+2^2+4^2) = \frac{\pi^2\hbar^2}{2ma^2}(21)$$

$$E_{214} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+1^2+4^2) = \frac{\pi^2\hbar^2}{2ma^2}(21)$$

$$E_{332} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+3^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(22) = E_{11}$$

$$E_{323} = \frac{\pi^2\hbar^2}{2ma^2}(3^2+2^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(22)$$

$$E_{233} = \frac{\pi^2\hbar^2}{2ma^2}(2^2+3^2+3^2) = \frac{\pi^2\hbar^2}{2ma^2}(22)$$

Evaluate the energy for even more values of j, k, and l.

$$E_{422} = \frac{\pi^2\hbar^2}{2ma^2}(4^2 + 2^2 + 2^2) = \frac{\pi^2\hbar^2}{2ma^2}(24) = E_{12}$$

$$E_{242} = \frac{\pi^2\hbar^2}{2ma^2}(2^2 + 4^2 + 2^2) = \frac{\pi^2\hbar^2}{2ma^2}(24)$$

$$E_{224} = \frac{\pi^2\hbar^2}{2ma^2}(2^2 + 2^2 + 4^2) = \frac{\pi^2\hbar^2}{2ma^2}(24)$$

$$E_{413} = \frac{\pi^2\hbar^2}{2ma^2}(4^2 + 1^2 + 3^2) = \frac{\pi^2\hbar^2}{2ma^2}(26) = E_{13}$$

$$E_{431} = \frac{\pi^2\hbar^2}{2ma^2}(4^2 + 3^2 + 1^2) = \frac{\pi^2\hbar^2}{2ma^2}(26)$$

$$E_{143} = \frac{\pi^2\hbar^2}{2ma^2}(1^2 + 4^2 + 3^2) = \frac{\pi^2\hbar^2}{2ma^2}(26)$$

$$E_{341} = \frac{\pi^2\hbar^2}{2ma^2}(3^2 + 4^2 + 1^2) = \frac{\pi^2\hbar^2}{2ma^2}(26)$$

$$E_{134} = \frac{\pi^2\hbar^2}{2ma^2}(1^2 + 3^2 + 4^2) = \frac{\pi^2\hbar^2}{2ma^2}(26)$$

$$E_{314} = \frac{\pi^2\hbar^2}{2ma^2}(3^2 + 1^2 + 4^2) = \frac{\pi^2\hbar^2}{2ma^2}(26)$$

$$E_{333} = \frac{\pi^2\hbar^2}{2ma^2}(3^2 + 3^2 + 3^2) = \frac{\pi^2\hbar^2}{2ma^2}(27) = E_{14}$$

$$E_{511} = \frac{\pi^2\hbar^2}{2ma^2}(5^2 + 1^2 + 1^2) = \frac{\pi^2\hbar^2}{2ma^2}(27)$$

$$E_{151} = \frac{\pi^2\hbar^2}{2ma^2}(1^2 + 5^2 + 1^2) = \frac{\pi^2\hbar^2}{2ma^2}(27)$$

$$E_{115} = \frac{\pi^2\hbar^2}{2ma^2}(1^2 + 1^2 + 5^2) = \frac{\pi^2\hbar^2}{2ma^2}(27)$$

The degeneracies are $d_7 = 3$, $d_8 = 3$, $d_9 = 3$, $d_{10} = 6$, $d_{11} = 3$, $d_{12} = 3$, $d_{13} = 6$, and $d_{14} = 4$. Unlike the previous energies, E_{14} is obtained not only from the permutations of three numbers (5, 1, and 1), but also from another set of numbers (3, 3, and 3).