To solve this equation for $\psi(x,y,z)$ we must specify six boundary conditions.[5] These conditions result from the reasoning that as x approaches 0 or L_x (or as y and z approach 0 or L_y and L_z) the position probability must vanish since the particle cannot leave the box. Noticing that whenever the position probability is zero so also is the wave function (eqn. IIIA-1), the boundary conditions for our example are

$$\begin{array}{lll} \psi(0,y,z) = 0 & \psi(x,0,z) = 0 & \psi(x,y,0) = 0 \\ \psi(L_x,y,z) = 0 & \psi(x,L_y,z) = 0 & \psi(x,y,L_z) = 0 \end{array} \qquad \text{(IIIA-2b)}$$

A solution of eqns. IIIA-2 is presented in Ref. 5, pgs. 127-130. It yields a family of solutions

$$\psi_{\ell,m,n}(x,y,z) = A \sin\left(\frac{\ell\pi x}{L_x}\right) \sin\left(\frac{m\pi y}{L_y}\right) \sin\left(\frac{n\pi z}{L_z}\right) \qquad \text{(IIIA-3)}$$

corresponding to all nonzero positive integer values of the *quantum numbers*, $\ell,m,n = 1,2,3,\ldots$, and all combinations.[6,7] The following problems verify the validity of this solution by assuring that it satisfies both the boundary conditions (Exer. 2) and the equation (Exmp. 2).

Exercise 2. Show that the wave functions, $\psi_{\ell,m,n}(x,y,z)$, (eqn. IIIA-3), satisfy the boundary conditions, (eqns. IIIA-2b), provided ℓ, m, and n are integers.

Example 2. Determine if the proposed solution, eqn. IIIA-3, satisfies the Schroedinger equation as specialized for the example of a point particle in a field-free box. Determine the restrictions imposed on the energy by the form of the solution.

To establish the conditions for which $\psi_{\ell,m,n}(x,y,z)$ satisfies the Schroedinger equation we need only substitute the proposed wave functions into the equation and perform the indicated partial differentiations. Thus for the first term

$$\frac{\partial}{\partial x}\left[\frac{\partial\psi_{\ell,m,n}(x,y,z)}{\partial x}\right] = \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} A \sin\left(\frac{\ell\pi x}{L_x}\right) \sin\left(\frac{m\pi y}{L_y}\right) \sin\left(\frac{n\pi z}{L_z}\right)\right]$$

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[5]Two boundary conditions are required for each of the second-order derivatives.

[6]The quantity A is an integration constant. Its values are determined through the requirement that the integral of the squared wave function over the dimensions of the box must equal one, i.e., the probability of the particle being in the box is one. The result is $A = (8/L_xL_yL_z)^{\frac{1}{2}}$.

[7]Note that negative values of ℓ,m,n are not included. No new solutions are obtained with negatives since $\sin(-\ell\pi x/L_x) = -\sin(\ell\pi x/L_x)$ and the minus is taken by A. Also neither ℓ,m, nor n are zero since this makes the probability zero for all x,y,z, which implies that the particle is not in the box.

Ans. 1. In determining electrical resistivity one must consider both the charge carriers and the scattering centers which interfere with their motion through the media. In this case, the analysis includes the *free electrons* and the vibrating lattice points or *molecules* of the solid.