Selected Solution to Assignment # 8

19.4 a  To find a separation of variables solution to the equation \(-\frac{k^2}{2m} \nabla^2 u = i\hbar u\), assume the solution \(\psi(x, y, z, t) = X(x)Y(y)Z(z)T(t)\). This separates into

\[
\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = -\frac{2im T'}{\hbar T} = c.
\]

The temporal function \(T(t)\) solves \(T' = i\hbar T/2m\) giving \(T(t) = T_0 \exp(i\hbar ct/2m)\) where \(T_0\) is an arbitrary constant. For the spatial terms, let \(-k_x^2 - k_y^2 - k_z^2 = c\). Then \(X(x)\) is a solution to \(X'' + k_x^2 X = 0\), which is \(X(x) = X_0 \exp[ik_xx]\) and similarly for functions \(Y, Z\). This gives

\[
\psi(x, y, z, t) = X_0 Y_0 Z_0 T_0 \exp \left[ i \left( k_xx + k_yy + k_zz + \frac{\hbar c}{2m} t \right) \right] = A \exp[i(k \cdot r - \omega t)]
\]

where \(k = (k_x, k_y, k_z)\) and \(r = (x, y, z)\), and \(\omega = -\hbar c/2m\). The spatial separation constants must satisfy the relationship \(c = -k_x^2 - k_y^2 - k_z^2 = -k \cdot k\), which is \(-p \cdot p/\hbar^2\) by de Broglie’s formula. Also, \(c = -2m\omega/\hbar\), which is equal to \(-2mE/\hbar^2\) by Einstein’s equation. Since both representations of the separation constant \(c\) must be equal, \(-p \cdot p/\hbar^2 = -2mE/\hbar^2\), or

\[
p_x^2 + p_y^2 + p_z^2 = 2mE.
\]

19.4 b  This problem is essentially the same as part a, except there are Dirichlet boundary conditions at the surfaces of the box of side \(a\). Since this imposes no temporal constraints, we still have \(T(t) = T_0 \exp(i\hbar ct/2m)\). With the same notation as above, the spatial functions must each now solve an ODE BVP. For example, \(X(x)\) is a solution to \(X'' + k_x^2 X = 0\) with \(X(0) = X(a) = 0\). The general solution is \(X(x) = A \sin(k_xx) + B \cos(k_xx)\). The boundary conditions give \(B = 0\), leaving \(X\) to be nontrivial only when \(k_xx = n_x \pi\) where \(n_x\) is an integer. In other words, \(k_xx = n_x \pi/a\), so \(X(x) = A \sin(n_x \pi x/a)\). The solutions for \(Y, Z\) are similar, which gives

\[
\psi(x, y, z, t) = (\text{constant}) \sin \left( \frac{n_x \pi x}{a} \right) \sin \left( \frac{n_y \pi y}{a} \right) \sin \left( \frac{n_z \pi z}{a} \right) \exp[-i\omega t]
\]

where \(\omega = -\hbar c/2m\) and \(n_x, n_y, n_z\) are integers. The separation constant \(c\) is given by \(c = -2m\omega/\hbar = -2mE/\hbar^2\) and also by

\[
-k_x^2 - k_y^2 - k_z^2 = -\frac{n_x^2 \pi^2}{a^2} - \frac{n_y^2 \pi^2}{a^2} - \frac{n_z^2 \pi^2}{a^2} = -\frac{\pi^2}{a^2} (n_x^2 + n_y^2 + n_z^2).
\]

Equating representations for \(c\) and isolating \(E\) gives

\[
E = \frac{\hbar^2 \pi^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)
\]

where \(n_x, n_y, n_z\) are integers.