Selected Solution to Assignment # 8

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

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

The temporal function $T(t)$ solves $T' = i\hbar cT/2m$ 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 $X(x) = X_0 \exp[ik_x x]$ and similarly for functions Y and Z. This gives

$$\psi(x,y,z,t) = X_0Y_0Z_0T_0 \exp\left[i\left(k_x x + k_y y + k_z z + \frac{\hbar c}{2m}t\right)\right] = A\exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)]$$

where $\mathbf{k} = \langle k_x, k_y, k_z\rangle$ and $\mathbf{r} = \langle x, y, z\rangle$, and $\omega = -\hbar c/2m$. The spatial separation constants must satisfy the relationship $c = -k_x^2 - k_y^2 - k_z^2 = -\mathbf{k}\cdot\mathbf{k}$, which is $-\mathbf{p}\cdot\mathbf{p}/\hbar^2$ 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, $-\mathbf{p}\cdot\mathbf{p}/\hbar^2 = -2mE/\hbar^2$, 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 $X(x) = A\sin(k_x x) + B\cos(k_x x)$. The boundary conditions give $B = 0$, leaving X to be nontrivial only when $k_x a = n_x\pi$ where n_x is an integer. In other words, $k_x = n_x\pi/a$, so $X(x) = A\sin(n_x\pi x/a)$. The solutions for Y and Z are similar, which gives

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

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

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

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.