The Simple Theoretical Shell Model and the Empirical Equation for Hydrogen's Line Spectrum

From classical Newtonian mechanics, the centripetal force of an electron in a circular orbit around an atom is $\frac{mv^2}{r}$, where *m* is the electron's mass, *v* is the electron's velocity, and *r* is the orbit's radius. The force of attraction between the electron and the nucleus is $\frac{Ze^2}{r^2}$, where *Z* is the atom's atomic number and *e* is the elementary charge. To maintain a stable circular orbit, the electron's centripetal force and its force of attraction to the nucleus must be identical; thus $\frac{mv^2}{r} = \frac{Ze^2}{r^2}$ or $mv^2 = \frac{Ze^2}{r}$. Next, we note that the electron's total energy, *E*, is the sum of its kinetic energy $\frac{1}{2}mv^2$ and its potential energy, $-\frac{Ze^2}{r}$, or $E = \frac{1}{2}mv^2 - \frac{Ze^2}{r}$. Substituting $\frac{Ze^2}{r}$ for mv^2gives $E = -\frac{Ze^2}{2r}$.

This classical treatment shows us that an electron's energy is a function of the distance, *r*, between the electron and the nucleus; however, there is nothing in this treatment that limits the radius of an electron's orbit or its energy. To quantize the atom we assume that an electron's angular momentum, *L* = *mvr*, is limited to integer multiples of $\frac{h}{2\pi}$ where *h* is Planck's constant; thus $L = mvr = \frac{nh}{2\pi}$, where *n* is a positive integer. Solving $\frac{mv^2}{r} = \frac{Ze^2}{r^2}$ for velocity, *v*, and substituting into the equation for angular momentum gives $\sqrt{Zmre^2} = \frac{nh}{2\pi}$. Rearranging and solving for *r* gives $r = \frac{n^2h^2}{4\pi^2 mZe^2}$. The smallest possible radius is for *n* = 1, for which $r_1 = \frac{h^2}{4\pi^2 mZe^2}$; all other radii are integer multiples of r_1 where $r_n = n^2 r_1$; thus, the allowed orbits and allowed energies for an electron are quantized.

To see that the empirical equation for hydrogen's line spectrum emerges from this theoretial shell model, we substitute $r = \frac{n^2h^2}{4\pi^2 mZe^2}$ into the equation for the electron's energy, which gives $E = -\frac{Ze^2}{2r} = -\frac{2\pi^2 mZ^2e^4}{n^2h^2}$, or, after substituting in values for the constants, $E = -(2.18 \times 10^{-18} J)\frac{1}{n^2}$. The change in energy when an electron moves between two orbits, $\Delta E = E_{final} - E_{initial}$, becomes $\Delta E = -(2.18 \times 10^{-18} J)\left\{\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right\}$, or, in terms of wavelength, $\frac{1}{\lambda} = (1.09737 \times 10^7\ \mathrm{m}^{-1}) \times \left\{\frac{1}{n_1^2} - \frac{1}{n_2^2}\right\}$, which is the empirical equation where n_2 is greater than n_1.