NORMALIZATION FOR BOUND STATES

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In this document, I will use the following notation:

$$\psi_(x) = \text{unnormalized wave function (what we have now)} \tag{1}$$

$$\psi_n(x) = \text{normalized wave function} \tag{2}$$

$$\psi_n(x) = A\psi(x) \tag{3}$$

The definition of a normalized wave function is:

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = 1 \tag{4}$$

In other words, the area under the probability density is 1.

In terms of our discrete grid, we can write this as:

$$\sum_i |\psi_n(x_i)|^2 \Delta x = 1 \tag{5}$$

where x_i is the position of the i^{th} grid point and Δx is the spacing between the grid points in nm. As long as the wave function goes to zero at the edges of the active region, we only have to sum over the grid points in the active region.

To find A in terms of $\psi(x)$, substitute equation 3 into equation 5:

$$A^2 \sum_i |\psi(x_i)|^2 \Delta x = 1 \tag{6}$$

This reduces to:

$$A = 1/\sqrt{\sum_i |\psi(x_i)|^2 \Delta x} \tag{7}$$

Equation 7 should be used to find A for all wells except for 1D and 3D Coulomb.

For 1D Coulomb, use:

$$A = 1/A_n \tag{8}$$

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where A_n are the scaling factors given in the Coulomb potential document:

$$\begin{aligned} A_1 &= 1.10851 \\ A_2 &= -1.86636 \\ A_3 &= 2.55958 \\ A_4 &= -3.21387 \\ A_5 &= 3.84064 \\ A_6 &= -4.44633 \\ A_7 &= 5.03504 \\ A_8 &= -5.6096 \\ A_9 &= 6.17208 \\ A_{10} &= -6.72406 \end{aligned}$$

For 3D Coulomb, use:

$$A = 1/\left(\sqrt{\pi}(na)^{3/2}\right)$$