Phys 5870: Modern Computational Methods in Solids

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Solution to the one-dimensional Schrödinger Eq. using a Taylor expansion

We want to solve the 1-d SE. Taking $\hbar^2/2m = 1$:

$$\left[-\frac{d^2}{dx^2} + (V(x) - E)\right]\psi(x) = 0 \quad (1)$$

We are seeking a solution of the form

$$y(x) = \sum_{n=0}^{\infty} a_n x^n \quad (2)$$

Square well

Replacing (2) in (1), with $V(x) = -V_0$ for $|x| < x_0$, we obtain

$$-\sum_{n=0}^{\infty} a_{n+1}x^n(n+2)(n+1) - (E + V_0)\sum_{n=0}^{\infty} a^n x^n = 0 \quad (3)$$

Equalizing the terms with equal powers of x, we obtain the recursion relation:

$$a_{n+2}(n+2)(n+1) = -(E + V_0)a_n \quad (4)$$

Clearly, we need to know a_0 and a_1. For the even solutions we take $a_0 = 1$, $a_1 = 0$, and for the odd solutions, $a_0 = 0$, $a_1 = 1$.

Triangular well

Proceeding as before, with $V(x) = -V_0 + \frac{V_0}{x_0}|x|$ for $|x| < x_0$, we obtain, for positive x

$$-\sum_{n=0}^{\infty} a_{n+1}x^n(n+2)(n+1) - (E+V_0)\sum_{n=0}^{\infty} a_n x^n + \frac{V_0}{x_0}\sum_{n=1}^{\infty} a_{n-1}x^n = 0 \quad (5)$$

For the zeroeth power we obtain

$$-2a_2 = (E+V_0)a_0 \quad (6)$$

For the higher order terms we get

$$-a_{n+1}(n+2)(n+1) = (E+V_0)a_n - \frac{V_0}{x_0}a_{n-1} \quad (7)$$

Again, by setting the boundary conditions for even and odd solutions as before, we obtain the desired sequence.

Bound states

Bound states decay exponentially outside the well. More explicily:

$$y_>(x) = C\exp(-\kappa x) \quad (8)$$

for $x > x_0$, where $\kappa = \sqrt{|E|}$, and C is some constant. In order to satisfy the matching conditions at $x = x_0$ we can renormalize this solutions by choosing a value of the constant C as

$$C = y_<(x_0)/\exp(-\kappa x_0) \quad (9)$$

where $y_<$ is the numerical solution inside the well.

We are seeking solutions that satisfy also that $y'_<(x_0) = y'_>(x_0)$, where

$$\begin{aligned} y'_<(x) &= \sum_{n=0}^{\infty} a_{n+1}(n+1)x^n \\ y'_>(x) &= -C\kappa\exp(-\kappa x). \end{aligned} \quad (10)$$

The corresponding energy spectrum will be discrete. We obtain the bound states by using the bisection method.