

Math 307: Problems for section 4.5

1. **If $V_1 = -5$, and all the other V_n 's are zero in the tight binding model, compute the probability that the bound state electron is located at the n th site for $n = 1, 2, 3$.**

The probabilities are

$$p_n = |\psi_n|^2 / N^2$$

where $N^2 = \sum_{n=0}^{\infty} |\psi_n|^2$. We have $\psi_0 = 0$ and $\psi_1 = 1$. To compute the rest of the ψ_n we use the fact that $a_1 = 0$ for $E = -5.2$. Thus, for this value of E , $\mathbf{x}_1 = a_2 \mathbf{v}_2$ so that

$$\begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix} = \mathbf{x}_n = A^{n-1} a_2 \mathbf{v}_2 = a_2 \lambda_2^{n-1} \mathbf{v}_2$$

Since

$$\mathbf{v}_2 = \begin{bmatrix} -1 \\ E + \lambda_2 \end{bmatrix}$$

we find that for $n \geq 1$

$$\psi_n = a_2 \lambda_2^{n-1} (E + \lambda_2).$$

Using the formula for the sum of the geometric series, we find

$$N^2 = \sum_{n=1}^{\infty} |a_2(E + \lambda_2)|^2 |\lambda_2|^{2(n-1)} = |a_2(E + \lambda_2)|^2 (1 - |\lambda_2|^2)^{-1}$$

Now we can substitute the numerical values to obtain $\lambda_1 = 5$, $\lambda_2 = 0.2$, $a_2 = -0.2$, $N^2 = 1.041666667$ and finally

$$p_1 = 0.9599999997$$

$$p_2 = 0.0383999999$$

$$p_3 = 0.0015360000$$