The main concept of Gauss-seidel relaxtion is to guess an initial solution for the eigenvalue, then compute the solution at each discrete point based on that guess. At each step, we solve the equation exactly. Of course, when we solve it at the next step, the previous one is no longer a solution.

This is clearer if we work through the problem. The discrete equation to solve is:

$$\frac{-\Psi_{i-1,j,k} - \Psi_{i+1,j,k} - \Psi_{i,j-1,k} - \Psi_{i,j+1,k} - \Psi_{i,j,k-1} - \Psi_{i,j,k+1} + 6\Psi_{i,j,k}}{h^2} + V_{i,j,k}\Psi_{i,j,k} = E\Psi_{i,j,k} \tag{1}$$

We rearrange this to solve to $\Psi_{i,j,k}$, which is the value we want to update:

$$\Psi_{i,j,k} = \frac{\Psi_{i-1,j,k} + \Psi_{i+1,j,k} + \Psi_{i,j-1,k} + \Psi_{i,j+1,k} + \Psi_{i,j,k-1} + \Psi_{i,j,k+1}}{6 + V_{i,j,k}h^2 - Eh^2} \tag{2}$$

So after making an initial guess for E and Ψ (for all values of i, j, k), we loop through each $\Psi_{i,j,k}$ and update it via eq. 2. Suppose we are looping through the k variable. The equation has been exactly satisfied at $\Psi_{i,j,k-1}$. Then we update $\Psi_{i,j,k}$. But now the value of $\Psi_{i,j,k}$ is different than when it was used to update $\Psi_{i,j,k-1}$, so now $\Psi_{i,j,k-1}$ is no longer a solution. But the idea is that at each overall loop through the variables, we get closer to the actual solution. At the end of each loop, we also update the value of E according to:

$$E = \sqrt{\frac{< H\Psi|H\Psi >}{< \Psi|\Psi >}} \tag{3}$$

where H is our Hamiltonian and Ψ is the updated approximate solution.