In part I, the assumption was made that the particles will stay in the middle of the slab. This assumption will now be relaxed. The two particles are at postitions (x_1, y_1) and (x_2, y_2). The potential V depends on y_1, y_2, and $|x_2 - x_1|$. The effects of the ends of the slab in the x direction are being ignored (periodicity is enforced instead of a boundary like in the y direction). Therefore, the actual x positions do not matter, but only their relative difference. We define $x \equiv |x_2 - x_1|$. Also, to minimize subscripts, let $y \equiv y_1$ and $z \equiv y_2$.

The Schrodinger equation now reads:

$$-\Delta_{x,y,z}\Psi(x, y, z) + V(x, y, z)\Psi(x, y, z) = E\Psi(x, y, z) \tag{1}$$

where

$$\Delta_{x,y,z} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{2}$$

The discretized version of the equation computes the second derivative with a second-order approximation that includes the nearest-neighbor sites in each direction, for a total of nine terms. The laplacian is now (with explicit x, y, z dependence suppressed):

$$\begin{aligned} \Delta_{i,j,k} = \quad & \frac{\Psi_{i-1,j,k} - 2\Psi_{i,j,k} + \Psi_{i+1,j,k}}{h_x^2} + \\ & \frac{\Psi_{i,j-1,k} - 2\Psi_{i,j,k} + \Psi_{i,j+1,k}}{h_y^2} + \\ & \frac{\Psi_{i,j,k-1} - 2\Psi_{i,j,k} + \Psi_{i,j,k+1}}{h_z^2} \end{aligned} \tag{3}$$

where we use i, j, k to represent x, y, z coordinate lattice sites and h_x, h_y, h_z are the step sizes in the appropriate directions. (Of course, h_y and h_z are always equal.)

The discretized Schrodinger equation is now:

$$\begin{aligned} & \frac{\Psi_{i-1,j,k} - 2\Psi_{i,j,k} + \Psi_{i+1,j,k}}{h_x^2} + \\ & \frac{\Psi_{i,j-1,k} - 2\Psi_{i,j,k} + \Psi_{i,j+1,k}}{h_y^2} + \\ & \frac{\Psi_{i,j,k-1} - 2\Psi_{i,j,k} + \Psi_{i,j,k+1}}{h_z^2} + \quad V_{i,j,k}\Psi_{i,j,k} = E\Psi_{i,j,k} \end{aligned} \tag{4}$$

Each particle has an infinite number of image particles associated with it. The potential at particle 1 is a sum of all the interactions with particle 2 and its image particles, and likewise for particle 2 with particle 1's image particles. There is also the potential on each particle due to its own images. The total potential is the addition of these four interactions.

Let the image particles for particle 1 be at locations $(x_1, y_{1,i})$ where $i = ..., -3, -2, -1, 0, 1, 2, 3, ...,$ and $(x_1, y_{1,0})$ is the location of the particle itself. Similarly, let $(x_2, y_{2,j})$ be the location of the second particles images and $(x_2, y_{2,0})$ be the location of the second particle.

The potential for two particles depends only on the distance between them. Let z be the distance and $U(z)$ be the potential between two particles. Then we have

$$U(z) = K_0(\frac{z}{\lambda}) - K_0(\frac{z}{\xi}) \tag{5}$$

where K_0 is the 0th order bessel function, λ is the penetration depth and ξ is the coherence length. The distance z is

$$z = \sqrt{(x_2 - x_1)^2 + (y_{2,i} - y_{1,0})^2} = \sqrt{x^2 + (y_{2,i} - y_{1,0})^2} \tag{6}$$

or, for the other particle

$$z = \sqrt{x^2 + (y_{1,i} - y_{2,0})^2} \tag{7}$$

Therefore, the total potential is

$$\begin{aligned} V(y_1, y_2, x) = \quad & \sum_{i=-\infty}^{\infty} U(\sqrt{x^2 + (y_{2,i} - y_{1,0})^2}) + \sum_{i=-\infty}^{\infty} U(\sqrt{x^2 + (y_{1,i} - y_{2,0})^2}) \\ & + \sum_{i=-\infty, i\neq 0}^{\infty} U(|y_{1,i} - y_{1,0}|) + \sum_{i=-\infty, i\neq 0}^{\infty} U(|y_{2,i} - y_{2,0}|) \end{aligned} \tag{8}$$

Boundary conditions:

$$\Psi(y_1, y_2, x) = \Psi(y_1, y_2, -x) \tag{9}$$

$$\frac{\partial \Psi}{\partial x}(y_1, y_2, x = 0) = 0 \tag{10}$$

Let the middle of the slab be coordinate $y = 0$, and w be the width of the slab. Then the boundaries are at $y = \pm\frac{w}{2}$. The boundary conditions are

$$\Psi(y_1 = \pm\frac{w}{2}, y_2, x) = \Psi(y_1, y_2 = \pm\frac{w}{2}, x) = 0 \tag{11}$$