Ex2060: Particle in a 3D box

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The problem:

Consider a particle of mass m in a three dimensional box of height a, length and width L and with periodical boundary conditions (torus geometry) on the length and width.

1. Write the eigenvalues and the eigenstates of the energy.

Assuming $L >> a$. We will find a condition such that the system can be treated as a two dimensional system.

2. Find an energy range, $E_{min} < E < E_{max}$, where we can neglect the third dimension.

3. Solve again for $V(z) = -u\delta(z)$.

The solution:

1. Solving schrödinger equation with the following boundary conditions:

(a) $\psi(0, y, z) = \psi(L, y, z)$
(b) $\psi(x, 0, z) = \psi(x, L, z)$
(c) $\psi(x, y, 0) = 0$
(d) $\psi(x, y, a) = 0$

yields:
$\psi(x, y, z) = A \sin(k_z z) e^{i(k_x x + k_y y)}$

with:
$k_x = \frac{2\pi}{L} n_x$; $k_y = \frac{2\pi}{L} n_y$; $k_z = \frac{\pi}{a} n_z$

from the normalization condition $\langle\psi|\psi\rangle = 1$, one can get: $|A| = \frac{1}{L}\sqrt{\frac{2}{a}}$

the energy is: $E = \frac{k_x^2}{2m} + \frac{k_y^2}{2m} + \frac{k_z^2}{2m} = \frac{2\pi^2}{mL^2}\left[n_x^2 + n_y^2 + \frac{L^2}{4a^2}n_z^2\right]$

2. From the condition $L >> a$ we conclude that the main term in the energy is $\frac{\pi^2}{2ma^2}n_z^2$
The first mode that is not the trivial solution of the schrödinger equation, i.e. $\psi = 0$, is $(n_x, n_y, n_z) = (0, 0, 1)$. In this region, small changes in n_x and n_y would not result in significant changes of the energy, so we can treat the box as a two dimensional square. (In other words, the energy in the z axis is constant and can be treated as a shift in the Hamiltonian).
Thus, $E_{min} = E(n_x = 0, n_y = 0, n_z = 1) = \frac{\pi^2}{2ma^2}$

E_{max} will simply be the next mode. In this case, the term $\frac{\pi^2}{2ma^2}n_z^2$ is no longer constant and cannot be neglected.
$E_{max} = E(n_x = 0, n_y = 0, n_z = 2) = \frac{2\pi^2}{ma^2}$

$$\frac{\pi^2}{2ma^2} < E < \frac{2\pi^2}{ma^2}$$

(Notice that after we set n_z to be 1, we can change n_x and n_y as we wish. Actually, it would not change the answer since E_{max} will stay the same.)

3. Generally speaking, delta potential creates two different states- bound state and unbound state. In our case, we consider only the bound state, that is, $E < 0$.
Solving schrödinger equation with the following boundary conditions:

(a) $\psi\left(0, y, z\right) = \psi\left(L, y, z\right)$
(b) $\psi\left(x, 0, z\right) = \psi\left(x, L, z\right)$
(c) $\psi\left(x, y, 0^-\right) = \psi\left(x, y, 0^+\right)$
(d) $[\frac{\partial \psi}{\partial z}]_{z=0^+} - [\frac{\partial \psi}{\partial z}]_{z=0^-} = -2mu\psi(0)$

yields:
$\psi(x, y, z) = Ae^{i(k_x x + k_y y)} \begin{cases} e^{-k_z z}; z > 0 \\ e^{k_z z}; z < 0 \end{cases}$
with:
$k_x = \frac{2\pi}{L} n_x$; $k_y = \frac{2\pi}{L} n_y$; $k_z = mu$

from the normalization condition $\langle \psi | \psi \rangle = 1$, one can get: $|A| = \frac{1}{L}\sqrt{mu}$

the energy is: $E = \frac{k_x^2}{2m} + \frac{k_y^2}{2m} - \frac{k_z^2}{2m} = \frac{2\pi^2}{mL^2}(n_x^2 + n_y^2) - \frac{mu^2}{2}$

E_{min} will be, again, the first mode that is not the trivial solution of the schrödinger equation:
$E_{min} = E(n_x = 0, n_y = 0) = -\frac{mu^2}{2}$
In order to ensure ψ is a bound state, E_{max} will be zero.
We are interested in a bound state because otherwise we will get a free wave in the z axis (the scatterer will affect the system via boundary conditions, but the there will be no bound states), which means that the third dimension cannot be neglected.

$$-\frac{mu^2}{2} < E < 0$$