QM stastes of a particle in a 1-D well are essentially standing waves:

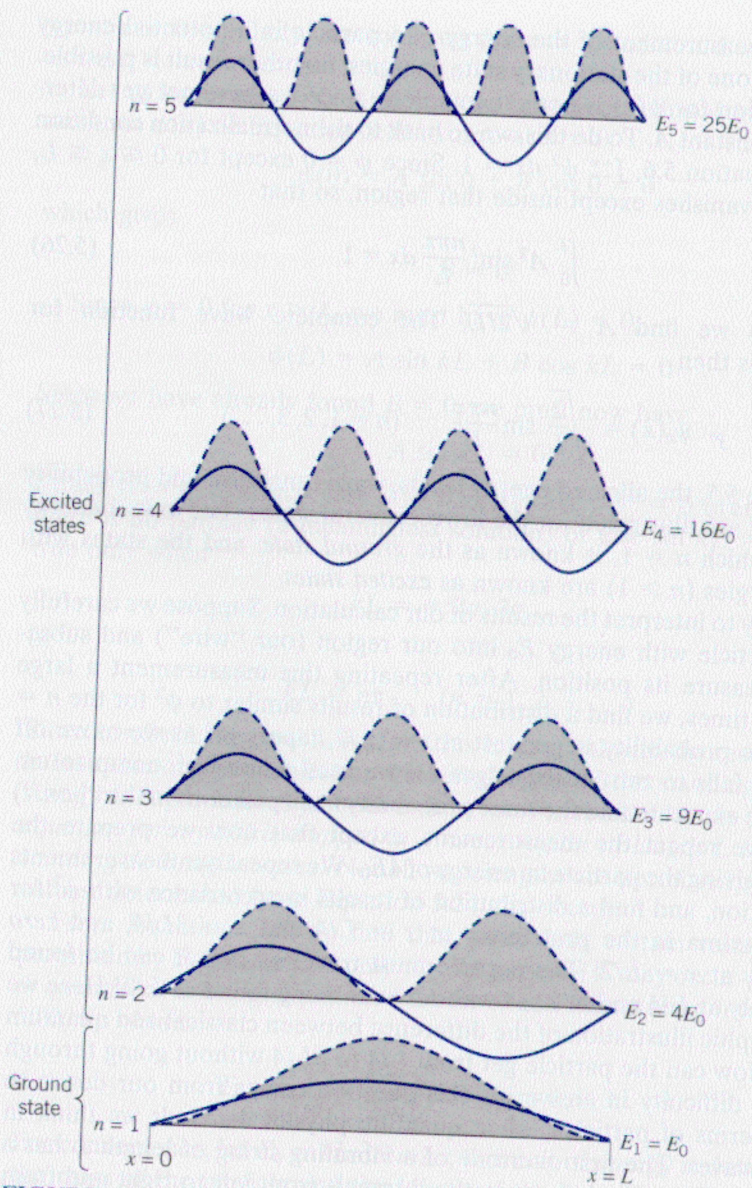
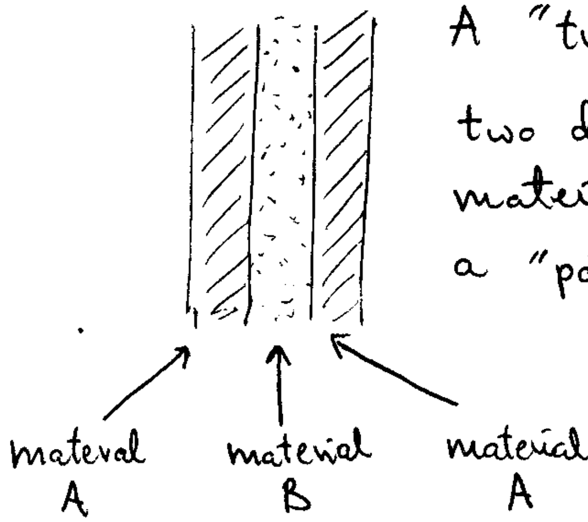


FIGURE 5.5 The permitted energy levels of a particle in a one-dimensional infinite well. The wave function for each level is shown by the solid curve, and the shaded region gives the probability density for each level.

"Particle in a One-Dimensional Box" is not only a "book problem".

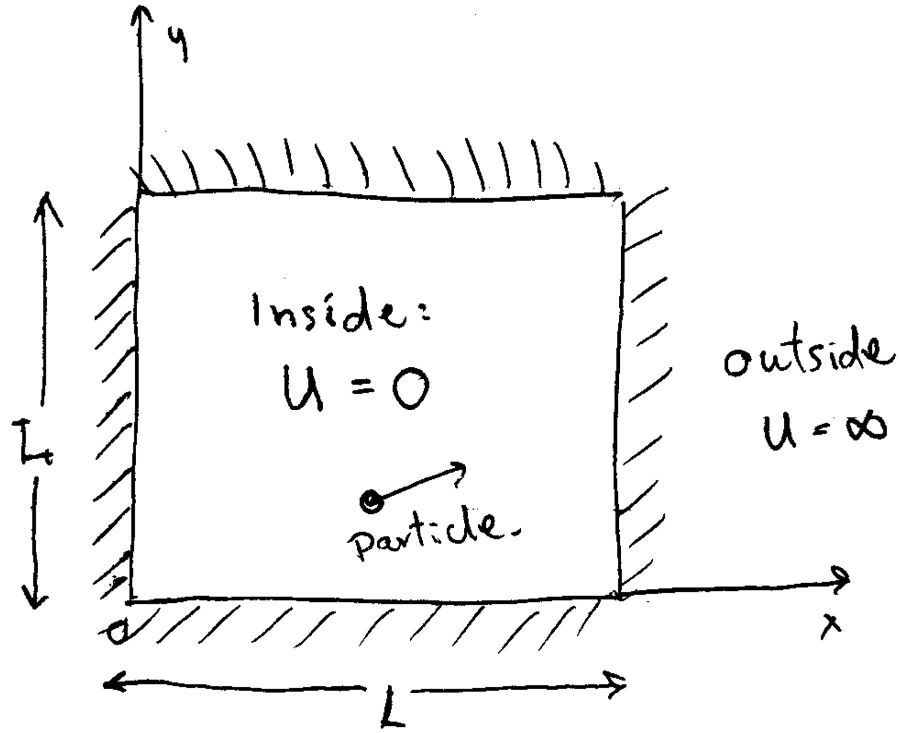


A "trilayer" made of two different semiconductor material may be such a "potential well" for the electrons in material B.

Such structures are used in modern OPTO-ELECTRONIC devices, e.g. in <u>diode lasers.</u>

"PARTICLE IN A <u>THREE-DIMENSIONAL BOX</u>" is a very important model in modern thermal physics (e.g., the theory of gases is based on it) and solid-state physics.

But we will not discuss a 3-D box, only a 2D box.



Outside the box, $U = \infty$

The Schrödinger Equation for 3-D is:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y,z)}{\partial x^2} + \frac{\partial^2\psi(x,y,z)}{\partial y^2} + \frac{\partial^2\psi(x,y,z)}{\partial z^2}\right] + U(x,y,z)\,\psi(x,y,z) = E\,\psi(x,y,z)$$

For <u>two</u> dimensions, it of course reduces to:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right] + U(x,y)\,\psi(x,y) = E\,\psi(x,y)$$

Outside, the only possible solution is $\psi(x,y) = 0$

Inside, $U(x,y) = 0$

We seek a <u>separable</u> solution $\psi(x,y) = f(x)\cdot g(x)$

~~Use~~ A convenient way is to use complex exponential function $\psi(x,y) = A e^{i(k_x \cdot x + k_y \cdot y)}$

But it also can be checked that

$$f(x) = A \sin(k_x x) + B \cos(k_x x)$$

$$g(y) = C \sin(k_y y) + D \cos(k_y y)$$

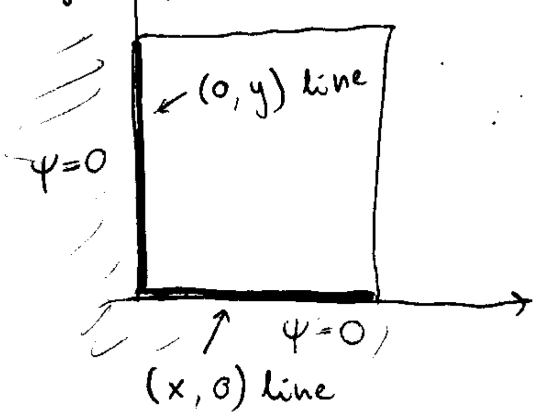
where k_x, k_y are two separate wavenumbers.

Now, we have to work with the boundary conditions and continuity requirements

It must be:

$$\psi(0, y) = 0$$

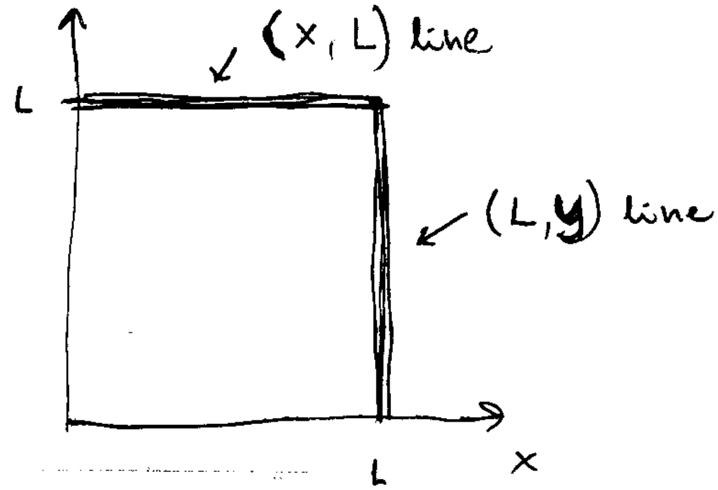
$$\psi(x, 0) = 0$$



Which automatically sets the factors B and D at the cosine terms to zero

So, we have: $\psi(x,y) = AC \cdot \sin(k_x x) \cdot \sin(k_y y)$

Now, the function also must be zero at the other two walls:



So: $\psi(L, y) = AC \sin(k_x L) \sin(k_y y) = 0$

and $\psi(x, L) = AC \sin(k_x x) \sin(k_y L) = 0$

Which is assured when these two sine function arguments are $0, \pi, 2\pi, 3\pi \ldots n\pi$

Zero is a non-physical solution, right? (same reasons as for 1-D well).

It means that k_x, k_y may only take values: $k_x = \frac{n_x \pi}{L}$, $k_y = \frac{n_y \pi}{L}$ where $n_x, n_y = 1, 2, 3 \ldots$

Next, replacing the constants product AC by $A' \equiv AC$, we obtain:

$$\psi = A' \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right)$$

with n_x, n_y being <u>integers</u>, and they need not to be equal, but may be equal:

$$n_x = 0, 1, 2, 3 \ldots \quad ; \quad n_y = 0, 1, 2, 3 \ldots$$

with $n_x \neq n_y$ or $n_x = n_y$.

Still, we need to determine the A' constant – here we use the normalization condition

$$\int_0^L \int_0^L \psi(x,y)\, dx\, dy = \int_0^L \int_0^L A' \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) dx\, dy = 1$$

which leads to: $A' = \dfrac{2}{L}$

Finally, by plugging the solution we found into the original Schrödinger Equation, we readily obtain the expression for E (total energy):

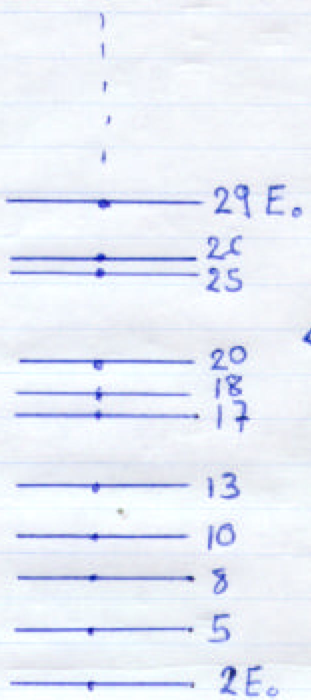
$$E = \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^2 + n_y^2\right)$$

Denoting: $E_0 \equiv \frac{\hbar^2 \pi^2}{2mL^2}$

we obtain: $E = E_0\left(n_x^2 + n_y^2\right)$

Let's examine possible values of $n_x^2 + n_y^2$:

$n_x^2 + n_y^2 =$	
1	no such option (NSO)
2	$n_x = 1,\ n_y = 1$
3	NSO
4	NSO
5	$n_x = 1,\ n_y = 2$ or $n_x = 2,\ n_y = 1$
6, 7,	NSO
8	$n_x = 2,\ n_y = 2$
9	NSO
10	$n_x = 1$ and $n_y = 3$, or $n_x = 3$ or $n_y = 1$
11, 12	NSO
13	$n_x = 2,\ n_y = 3$ or $n_x = 3,\ n_y = 2$
14, 15, 16	NSO
17	$n_x = 1,\ n_y = 4$ or $n_x = 4,\ n_y = 1$



Applying the commonly used plotting sheme, we can display the possible energy values using horizontal "bars":

Now, for different pairs of n_x, n_y values we can plot the probability density function profiles in the $L \times L$ area:

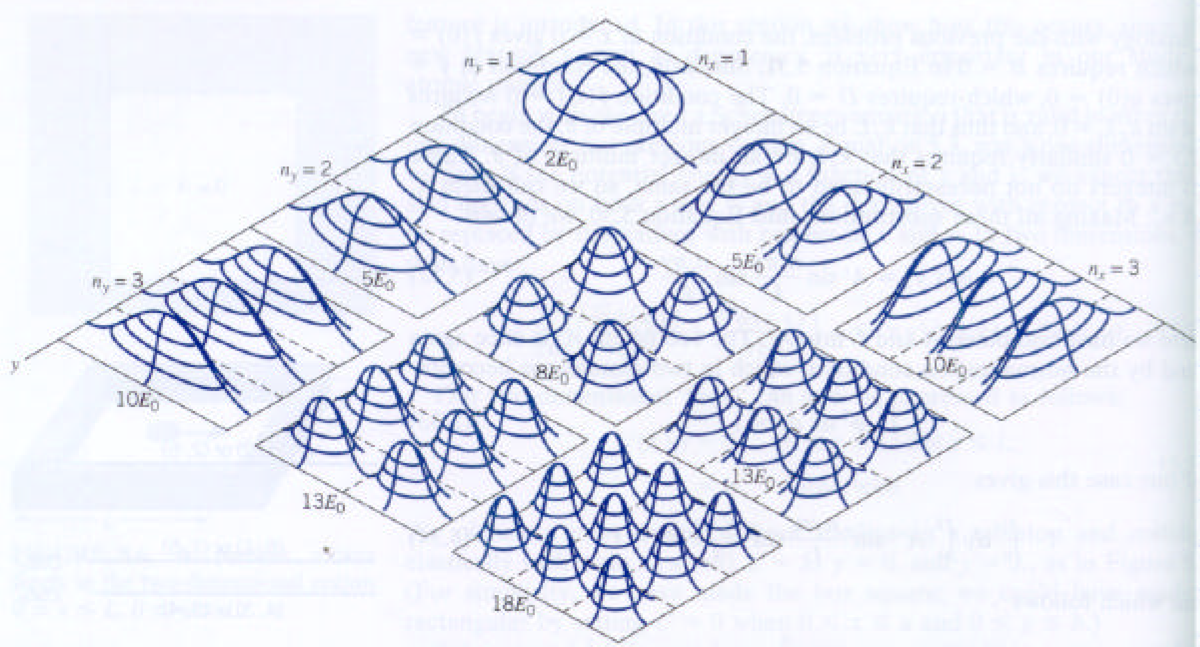


FIGURE 5.8 The probability density ψ^2 for some of the lower energy levels of the particle confined to the tw dimensional box.