Bound states of the square well

One of the simplest potentials to study the properties of is the so-called square

$$V = \begin{cases} 0 & |x| > a \\ -V_0 & |x| < a \end{cases} . \tag{2.1}$$

well potential,

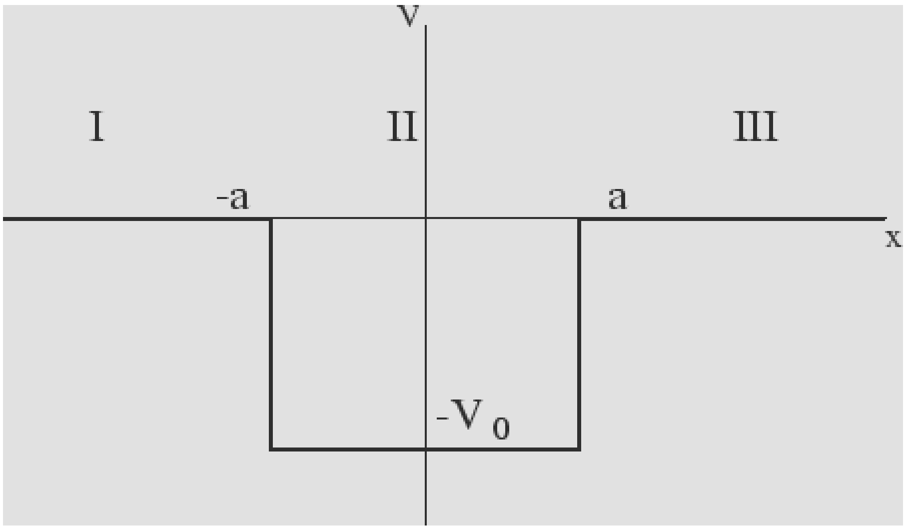

Figure 4.1: The square well potential

We define three areas, from left to right I, II and III. In areas I and III we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \tag{2.2}$$

whereas in area II we have the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E+V_0)\psi(x) \tag{2.3}$$

Solution to a few ODE's. In this class we shall quite often encounter the ordinary differential equations

$$\frac{d^2}{dx^2}f(x) = -\alpha^2 f(x) \tag{2.4}$$

which has as solution

$$f(x) = A_1\cos(\alpha x) + B_1\sin(\alpha x) = C_1 e^{i\alpha x} + D_1 e^{-i\alpha x}, \tag{2.5}$$

and

$$\frac{d^2}{dx^2}g(x) = +\alpha^2 g(x) \tag{2.6}$$

which has as solution

$$g(x) = A_2 \cosh(\alpha x) + B_2 \sinh(\alpha x) = C_2 e^{\alpha x} + D_2 e^{-\alpha x}. \tag{2.7}$$

Let us first look at $E > 0$. In that case the equation in regions I and III can be written as

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2m}{\hbar^2}E\psi(x) = -k^2\psi(x), \tag{2.8}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}E}. \tag{2.9}$$

The solution to this equation is a sum of sines and cosines of kx, which cannot be normalised: Write $\psi_{III}(x) = A\cos(kx) + B\sin(kx)$
(A, B, complex) and calculate the part of the norm originating in region III,

$$\int_a^\infty |A|^2\cos^2 kx + |B|^2\sin^2 kx + 2\Re(AB^*)\sin(kx)\cos(kx)dx$$

$$\lim_{N\to\infty} N\int_a^{2\pi/k} |A|^2\cos^2(kx) + |B|^2\sin^2(kx) \tag{2.10}$$

$$\lim_{N\to\infty} N(|A|^2/2 + |B|^2/2) = \infty.$$

We also find that the energy cannot be less than $-V_0$, since we cannot construct a solution for that value of the energy.

We thus restrict ourselves to $-V_0 < E < 0$.

We write

$$E = -\frac{\hbar^2 k^2}{2m}, \quad E + V_0 = \frac{\hbar^2\kappa^2}{2m}. \tag{2.11}$$

The solutions in the areas I and III are of the form ($i = 1,3$)

$$\psi(x) = A_i e^{kx} + B_i e^{-kx}. \tag{2.12}$$

In region II we have the oscillatory solution

$$\psi(x) = A_2 \cos(\kappa x) + B_2 \sin(\kappa x). \tag{2.13}$$

Now we have to impose the conditions on the wave functions we have discussed before, continuity of ψ and its derivatives. Actually we also have to impose normalizability, which means that $A_1 = B_3 = 0$ (exponentially growing functions can not be normalized).

As we shall see we only have solutions at certain energies.

Continuity implies that

$$\begin{aligned}
A_1 e^{-k\alpha} + B_1 e^{k\alpha} &= A_2 \cos(\kappa\alpha) - B_2 \sin(\kappa\alpha) \\
A_3 e^{-k\alpha} + B_3 e^{k\alpha} &= A_2 \cos(\kappa\alpha) + B_2 \sin(\kappa\alpha) \\
k\, A_1 e^{-k\alpha} - k\, B_1 e^{k\alpha} &= \kappa\, A_2 \cos(\kappa\alpha) + \kappa\, B_2 \sin(\kappa\alpha) \\
k\, A_3 e^{-k\alpha} - k\, B_3 e^{k\alpha} &= -\kappa\, A_2 \cos(\kappa\alpha) + \kappa\, B_2 \sin(\kappa\alpha)
\end{aligned} \tag{2.14}$$

Tactical approach: We wish to find a relation between k and κ. The trick is to first find an equation that only contains A_2 and B_2. To this end we take the ratio of the first and third and second and fourth equation:

$$\begin{aligned}
k &= \frac{\kappa[A_2 \sin(\kappa a) + B_2 \cos(\kappa a)]}{A_2 \cos(\kappa a) - B_2 \sin(\kappa a)} \\
k &= \frac{\kappa[A_2 \sin(\kappa a) - B_2 \cos(\kappa a)]}{A_2 \cos(\kappa a) + B_2 \sin(\kappa a)}
\end{aligned} \tag{2.15}$$

We can combine these two equations to a single one by equating the right-hand sides.

After deleting the common factor κ, and multiplying with the denominators we find

$$[A_2\cos(\kappa a) + B_2\sin(\kappa a)][A_2\sin(\kappa a) - B_2\cos(\kappa a)] = \\ [A_2\sin(\kappa a) + B_2\cos(\kappa a)][A_2\cos(\kappa a) - B_2\sin(\kappa a)], \tag{2.16}$$

which simplifies to

$$A_2 B_2 = 0$$

We thus have two families of solutions, those characterised by $A_2 = 0$ and those that have $B_2 = 0$.

Some consequences

There are a few good reasons why the dependence in the solution is on ka, κa and $\kappa_0 a$: These are all dimensionless numbers, and mathematical relations can *never* depend on parameters that have a dimension! For the case of the even solutions, the ones with $B_2 = 0$, we find that the number of bound states is determined by how many times we can fit 2π into $\kappa_0 a$. Since κ_0 is proportional to (the square root) of V_0, we find that increasing V_0 increases the number bound states, and the same happens when we increase the width a. Rewriting $\kappa_0 a$ slightly we find that the governing parameter is

$$\sqrt{\frac{2m}{\hbar^2} V_0 a^2} \quad ,$$

so that a factor of two change in a is the same as a factor four change in V_0.

If we put the two sets of solutions on top of one another we see that after every even solution we get an odd solution, and vice versa.

There is always at least one solution (the lowest even one), but the first odd solution only occurs when $\kappa_0 a = \pi$.

Lessons from the square well

The computer demonstration showed the following features:

1. If we drop the requirement of normalisability, we have a solution to the TISE at every energy. Only at a few discrete values of the energy do we have normalisable states.
2. The energy of the lowest state is always higher than the depth of the well (uncertainty principle).
3. Effect of depth and width of well. Making the well deeper gives more eigen functions, and decreases the extent of the tail in the classically forbidden region.
4. Wave functions are oscillatory in classically allowed, exponentially decaying in classically forbidden region.
5. The lowest state has no zeroes; the second one has one, etc. Normally we say that the n-th state has $n-1$ ``nodes".
6. Eigen states (normalisable solutions) for different eigen values (energies) are orthogonal.

A physical system (approximately) described by a square well

After all this tedious algebra, let us look at a possible physical realization of such a system. In order to do that, we shall have to talk a little bit about semi-conductors. A semiconductor is a quantum system where the so-called valence electrons completely fill a valence band, and are separated by a gap from a set of free states in a conduction band. These can both be thought of a continuous set of quantum states. The energy difference between the valence and conduction bands is different for different semi-conductors. This can be used in so-called quantum-well structures, where we sandwich a thin layer of, e.g., GaAs between very thick layers of GaAlAs.

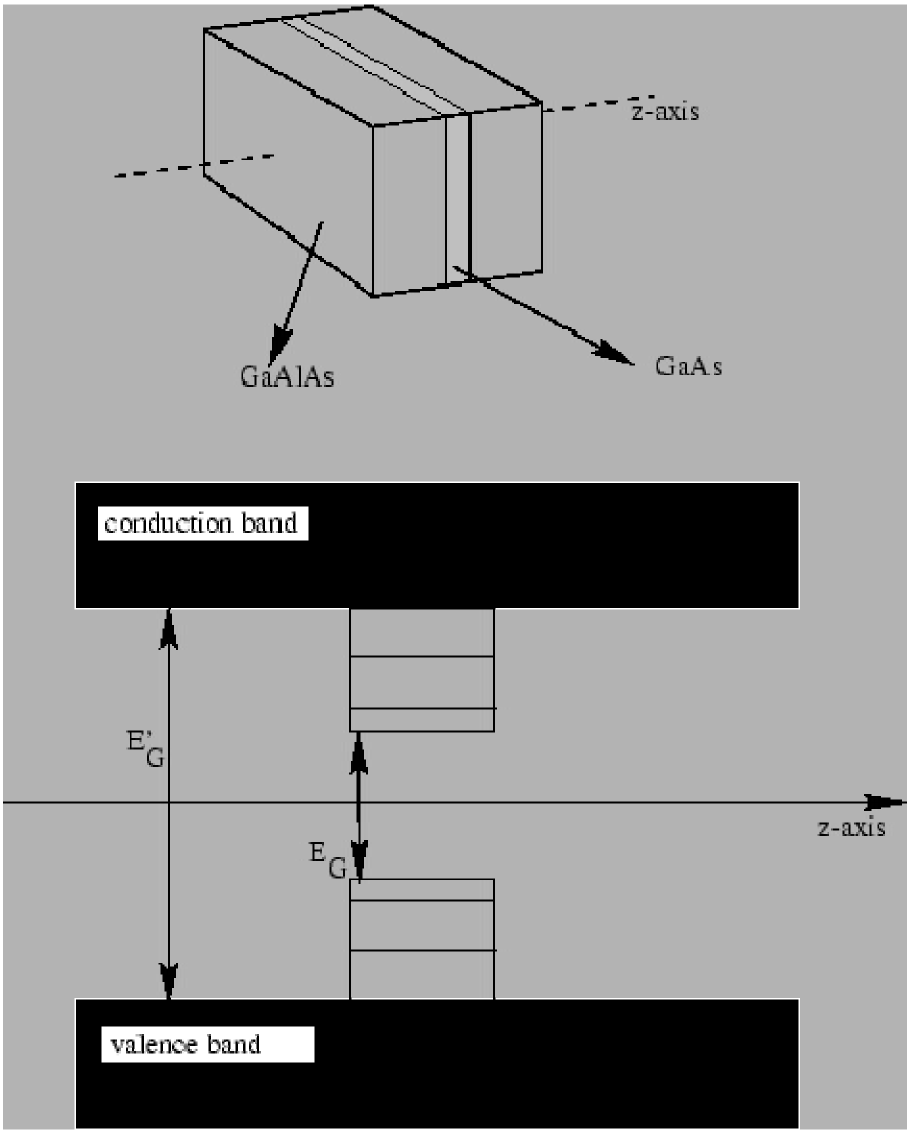

Figure 4.4: A schematic representation of a quantum well

Since the gap energy is a lot smaller for GaAs than for GaAlAs, we get the effect of a small square well (in both valence and conduction bands). The fact that we can have a few occupied additional levels in the valence, and a few empty levels in the conduction band can be measured.

The best way to do this, is to shine light on these systems, and see for which frequency we can create a transition (just like in atoms).

Glossary

1. square well potential – потенциал прямоугольной ямы,
2. Schrödinger equation – уравнение Шрёдингера,
3. whereas - тогда как
4. quite often – очень часто, довольно часто
5. encounter – сталкиваться, наталкиваться
6. the ordinary differential equations – обычные (общие) дифференциальные уравнения
7. solution – решение (уравнения)
8. restrict – ограничивать
9. to impose – налагать связь,
10. derivative – производная
11. continuity – непрерывность
12. normalized – нормализованный
13. exponential – экспоненциальный
14. trick – прием (технический), оригинальное решение
15. denominator – знаменатель
16. simplify - упрощать
17. drop the requirement – накладывать требование
18. depth – глубина
19. uncertainty principle - принцип неопределённости
20. even solution – четное решение
21. odd solution – нечетное решение
22. vice versa – наоборот, противоположно
23. consequence – результат (чего-либо), (по)следствие
24. tedious algebra – нудная (скучная) алгебра
25. semi-conductor – полупроводник
26. valence band – валентная зона
27. gap – щель, интервал, разрыв
28. band зона, лента, полоса, ремень
29. think of – представлять (себе)
30. layer – слой, прослойка
31. shine light – освещение светом