1.2.8. Additional solutions to Schrödinger's equation

This section is devoted to some specific quantum structures that are present in semiconductor devices. These are: 1) the finite quantum well, a more realistic version of the infinite well as found in quantum well laser diodes, 2) a triangular well, as found in MOSFETs and HEMTs, 3) a quantum well in the presence of an electric field as found in electro-optic modulators based on the quantum confined stark effect and 4) the harmonic oscillator which has a quadratic confining potential.

1.2.8.1. The finite rectangular quantum well

The finite rectangular quantum well is characterized by zero potential inside the well and a potential V_0 outside the well, as shown in Figure 1.2.12. The width of the well is L_x.

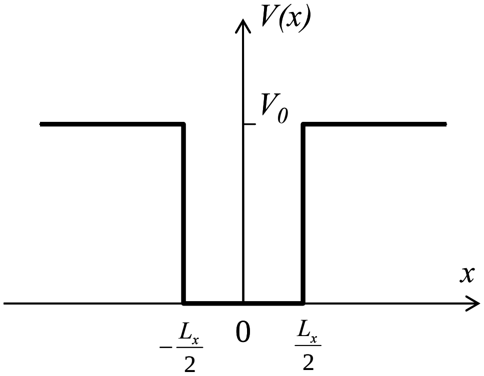

Figure 1.2.12 Potential of a finite rectangular quantum well with width L_x.

The origin is chosen in the middle of the well. Schrödinger's equation is therefore:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x) \text{ for } -L_x/2 < x < L_x/2\text{, inside the well} \tag{1.2.48}$$

and

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V_0\Psi(x) = E\Psi(x)\text{, outside the well} \tag{1.2.49}$$

Since we are looking for bound states (i.e. solutions for which electrons are confined to the well), the electron energy must be smaller than the energy in the barriers, or:

$$0 < E < V_0 \tag{1.2.50}$$

The general solution to Schrödinger's equation outside the well is:

$$\Psi(x) = Ae^{\alpha x} + Be^{-\alpha x}\text{, where } \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{1.2.51}$$

Since the electron is expected to be inside the well, the wavefunction must go to zero as x approaches infinity. The wavefunctions outside the well can then be simplified to:

$$\Psi(x) = Ae^{\alpha x}\text{, for } -\infty \le x \le -\frac{L_x}{2} \tag{1.2.52}$$

$$\Psi(x) = Be^{-\alpha x}\text{, for } \frac{L_x}{2} \le x \le \infty \tag{1.2.53}$$

The general solution to Schrödinger's equation inside the well is:

$$\Psi(x) = C\cos kx + D\sin kx\text{, for } -\frac{L_x}{2} \le x \le \frac{L_x}{2} \tag{1.2.54}$$

$$\text{where } k = \frac{\sqrt{2mE}}{\hbar} \tag{1.2.55}$$

We now use a symmetry argument to further simplify the problem and to find the electron energies. As defined above the potential energy is an even function since $V(x) = V(-x)$ for all x. The probability density $\Psi(x)\Psi^*(x)$ must therefore also be an even function, which implies that the wavefunction itself can either be an even function or an odd function. The even solution in the well is a cosine function, while the odd function in the well is a sine function. Continuity of the wavefunction and its derivative at $x = L_x/2$ implies for the even solution that:

$$C\cos\frac{kL_x}{2} = B\exp(-\frac{\alpha L_x}{2}) \tag{1.2.56}$$

and

$$-kC\sin\frac{kL_x}{2} = -\alpha\ B\exp(-\frac{\alpha L_x}{2}) \tag{1.2.57}$$

while for the odd solution it implies:

$$D\sin\frac{kL_x}{2} = B\exp(-\frac{\alpha L_x}{2}) \tag{1.2.58}$$

and

$$kD\cos\frac{kL_x}{2} = -\alpha\ B\exp(-\frac{\alpha L_x}{2}) \tag{1.2.59}$$

Taking the ratio of both sets of equations one finds:

$$k\tan\frac{kL_x}{2} = \alpha \tag{1.2.60}$$

and

$$k \cot \frac{kL_x}{2} = -\alpha \tag{1.2.61}$$

This equation can be rewritten as

$$k \tan(\frac{kL_x}{2} - \frac{\pi}{2}) = \alpha \tag{1.2.62}$$

since

$$\cot(a + \frac{\pi}{2}) = \frac{\cos(a + \pi/2)}{\sin(a + \pi/2)} = -\frac{\sin a}{\cos a} = -\tan a \tag{1.2.63}$$

The resulting relations for the even and odd solutions are:

$$\frac{kL_x}{2} = n\pi + \operatorname{atan}(\frac{\alpha}{k})\text{, for } n = 0, 1, 2, 3, \ldots \tag{1.2.64}$$

$$\frac{kL_x}{2} = \frac{\pi}{2} + n\pi + \operatorname{atan}(\frac{\alpha}{k})\text{, for } n = 0, 1, 2, 3, \ldots \tag{1.2.65}$$

and can then be combined into a single equation:

$$\frac{kL_x}{\pi} = (n-1)\pi + \frac{2}{\pi} \operatorname{atan}\sqrt{\frac{V_0}{E} - 1}\text{, for } n = 1, 2, 3, \ldots \tag{1.2.66}$$

where the odd values of n now correspond to the even solutions. After squaring and multiplying with the ground state energy, E_{10}, of an infinite well with width, L_x, (1.2.23),

$$E_{10} = \frac{\hbar^2}{2m}(\frac{\pi}{L_x})^2 \tag{1.2.67}$$

one obtains:

$$E_n = E_{10}[(n-1) + \frac{2}{\pi} \operatorname{atan}(\sqrt{\frac{V_0}{E_n} - 1})]^2 \tag{1.2.68}$$

One should note that the derivation of equation (1.2.68) assumes that the mass of the particle is the same in the well as outside the well.

To numerically solve equation (1.2.68) one starts with a reasonable guess for E_n (for instance E_{10}, provided it is smaller than V_0), and then obtains the solution through iteration. The normalized solution, E_n/E_{n0}, is shown in Figure 1.2.13 for the first four quantized states.

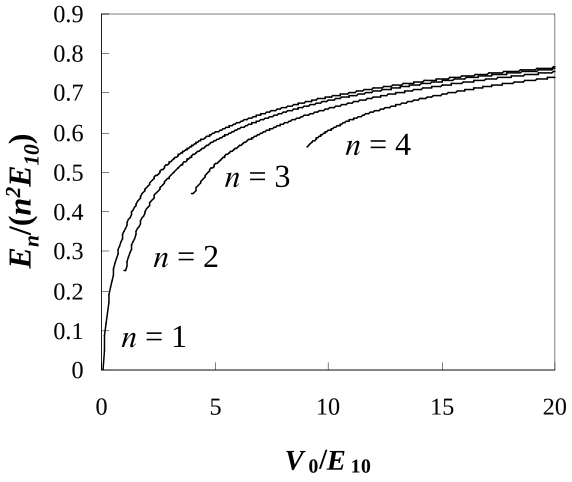

Figure 1.2.13 Normalized energies E_n/E_{n0} versus the normalized potential V_0/E_{10} for carriers in a finite well. Curves correspond to n = 1 (top curve), n = 2, n = 3 and n = 4 (bottom curve)

The lowest value, $E_{n,min}$, for a specific quantum level, n, is obtained from (1.2.68), namely:

$$E_{n,\min} = E_{10}(n-1)^2 \qquad (1.2.69)$$

A graphical solution can also be obtained by plotting E/E_{10} versus E/V_0 as shown in Figure 1.2.14.

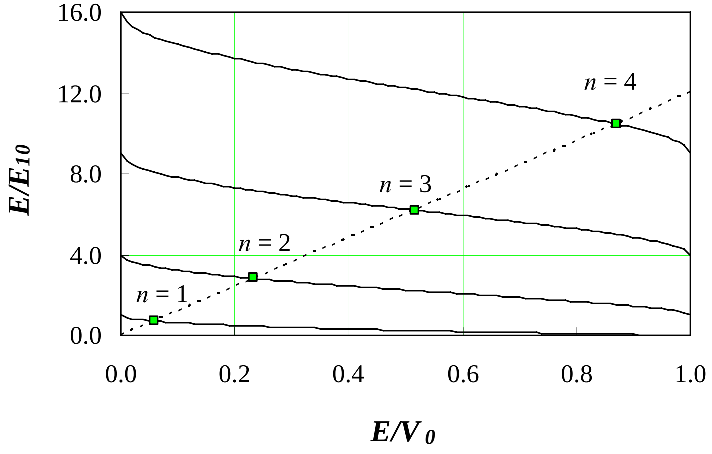

Figure 1.2.14 Graphical solution to the finite rectangular quantum well. Solutions are obtained at the intersection of the curves. Parameters are V_0 = 0.3 eV, m/m_0 = 0.67 and L_x = 15 nm.

Solutions are obtained at the intersection of the dotted line, which has a slope equal to V_0/E_{10}. Since both axes are normalized, Figure 1.2.14 can be customized by adjusting the slope of the dotted line to a specific value of V_0/E_{10} to find the solutions for any finite well depth and width.

Equation (1.2.68) implies that there is always one bound state in the well. The same conclusion can be drawn from the graphical solution in Figure 1.2.14 since there will always be one intercept with the dotted line no matter how small its slope.

We can also find the number of bound states, n_{max}, from equation (1.2.68). Since the maximum energy of a bound state equals V_0, one finds:

$$V_0 = E_{\max} = E_{10}(n_{\max} - 1)^2 \qquad (1.2.70)$$

which can be solved for $n_{\max}$ yielding:

$$n_{\max} = \mathrm{Int}\,(1 + \sqrt{\frac{V_0}{E_{10}}}) \qquad (1.2.71)$$

Also for the special case where $n_{\max} = 1$, one finds that there is only one bound state when $V_0 < E_{10}$.

1.2.8.2. The triangular quantum well

Consider a triangular well with constant electric field, $\mathcal{E}$, and an infinite barrier at $x = 0$.

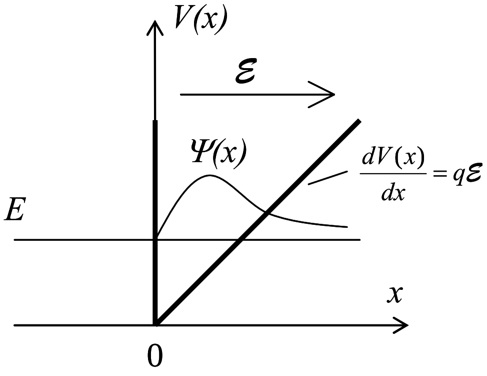

Figure 1.2.15 Potential of a triangular quantum well with electric field $\mathcal{E}$.

Schrodinger's equation (1.2.15) for this potential becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + q\mathcal{E}\,x\Psi(x) = E_n\Psi(x)\text{, for } x > 0 \qquad (1.2.72)$$

Since the Airy function is a solution to $y'' - x\,y = 0$ and approaches zero as x approaches infinity, one can write the solution to the Schrödinger equation as:

$$\Psi(x) = A\;Ai[(\frac{2m}{\hbar^2 q^2 \mathcal{E}^2})^{1/3}(q\mathcal{E}\;x - E_n)] \qquad (1.2.73)$$

where A is a proportionality constant which can be determined by normalization. Since $\Psi(x = 0)$ has to be zero at the infinite barrier the energy eigenvalues, E_n, are obtained from:

$$E_n = -(\frac{q^2 \mathcal{E}^2 \hbar^2}{2m})^{1/3} a_n \qquad (1.2.74)$$

where a_n is the n^{th} zero of the Airy function. The Airy function is shown in Figure 1.2.16.

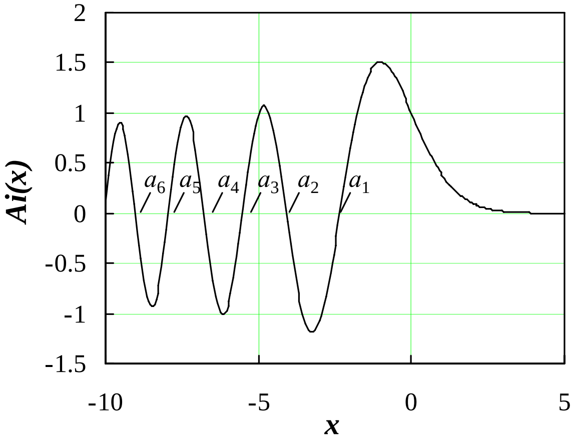

Figure 1.2.16 Plot of the Airy function normalized to $Ai(0) = 1$, with the first six zeros a_1 through a_6.

Its zeros are approximately given by:

$$a_n = -[\frac{3\pi}{2}(n - \frac{1}{4})]^{2/3}, \text{ with } n = 1, 2, \ldots \qquad (1.2.75)$$

and the corresponding energy values are:

$$E_n = (\frac{\hbar^2}{2m})^{1/3}(\frac{3\pi q\mathcal{E}}{2}(n - \frac{1}{4}))^{2/3}, \text{ with } n = 1, 2, \ldots \qquad (1.2.76)$$

Of particular interest is the first energy level, obtained for $n = 1$, resulting in:

$$E_1 = (\frac{\hbar^2}{2m})^{1/3}(\frac{9\pi q\mathcal{E}}{8})^{2/3} \qquad (1.2.77)$$

1.2.8.3. A quantum well with an applied electric field

The solution for a triangular well can also be applied to a quantum well with width L_x and infinitely high barriers, in the presence of an electric field. The potential and electron wavefunction are shown in Figure 1.2.17:

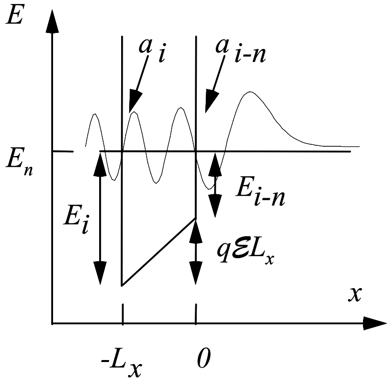

Figure 1.2.17 Potential and electron wavefunction for an infinitely deep well within an electric field.

Since the wave function must be zero at both boundaries, these boundaries must coincide with two different zeros of the Airy function. Since the zeros are discreet rather than continuous our solution will only be valid for specific electric fields. For intermediate values of the electric field we will interpolate linearly. A more sophisticated treatment would require a linear combination of the Airy function and the second independent solution of $y'' - xy = 0$.

From Figure 1.2.17 we find that the electric field is related to the energy difference on both sides of the well:

$$q\mathcal{E}(i,n)L_x = E_i - E_{i-n} \qquad (1.2.78)$$

where the subscript i refers to the ith zero of the Airy function and the subscript n to the nth quantized energy level in the well. This expression can be solved using (1.2.73) for the electric field, $\mathcal{E}$, as:

$$\mathcal{E}(i,n) = \frac{\hbar^2}{qL_x^3 2m}(a_{i-n} - a_i)^3, \; i = n + 1, n + 2, \ldots \qquad (1.2.79)$$

and the corresponding electron energy (using the left-hand corner as the zero energy reference) is:

$$E_n(i) = -a_i(a_{i-n} - a_i)^2 \frac{\hbar^2}{2mL_x^2}, \; i = n + 1, n + 2, \ldots \qquad (1.2.80)$$

It can be shown that in the limit for i going to infinity, which corresponds to a zero electric field, the energy levels correspond those of the infinite quantum well.

The energy levels as a function of the electric field are obtained by selecting a value for i and calculating the corresponding field and energy. The resulting energies, normalized to the first energy level in an infinite well, E_{10}, are shown in Figure 1.2.18:

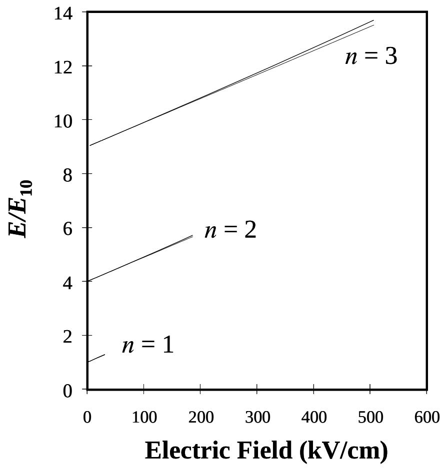

Figure 1.2.18 Energy levels in an infinite well in the presence of an applied field. Energies are shown for n = 1, 2 and 3 (solid line) and compared to $E_{n0} + q\mathcal{E}L_x/2$ (dotted line) where E_{n0} is the energy of quantum level n in absence of an applied field.

From the figure one finds that the expression $E_n = E_{n0} + q\,\mathcal{E}L_x/2$ (where E_{n0} is the energy, given by (1.2.23), of quantum level, n, in absence of an applied field) is a good approximation for the electron energy provided $E_n >> q\,\mathcal{E}\,L_x$

1.2.8.4. The harmonic oscillator

The next problem of interest is the harmonic oscillator, which is characterized by a quadratic potential, $V(x) = kx^2/2$, yielding the following Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+\frac{k\,x^2}{2}\Psi(x)=E_l\Psi(x) \tag{1.2.81}$$

where k is the spring constant which relates to the restoring force of the equivalent classical problem of a mass, m, connected to a spring for which:

$$\omega=\sqrt{\frac{k}{m}}\text{, or } k=m\omega^2 \tag{1.2.82}$$

The Schrödinger equation can be solved by assuming the solution to be of the form:

$$\Psi(x)=f(x)\exp(-\frac{\gamma\,x^2}{2}) \tag{1.2.83}$$

where $\gamma^2=\frac{mk}{\hbar^2}$, which reduces the Schrödinger equation to:

$$\frac{d^2f(x)}{dx^2}-2\gamma\,x\frac{df(x)}{dx}+f(x)(\frac{2mE}{\hbar^2}-\gamma)=0 \tag{1.2.84}$$

A polynomial of order, *n*-1, satisfies this equation if:

$$\frac{2mE_n}{\hbar^2\gamma}+1-2n=0\text{, or }E_n=\hbar\omega(n-\frac{1}{2})\text{, with }n = 1, 2, 3 \ldots \qquad (1.2.85)$$

so that the minimal energy $E_0 = \hbar\omega/2$ while all the energy levels are separated from each other by an energy $\hbar\omega$. The polynomials which satisfy equation (1.2.84) are knows as the Hermite polynomials of order *n*, H_n, so that the wavefunction $\Psi(x)$ equals:

$$\Psi_n(x)=H_{n-1}(\sqrt{\gamma}\,x)\exp(-\frac{\gamma\,x^2}{2})\text{, with }n = 1, 2, 3 \ldots \qquad (1.2.86)$$

As an example, we present the wavefunctions for the first three bound states in Figure 1.2.19.

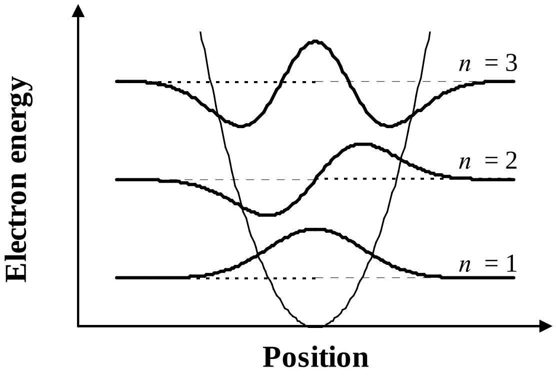

Figure 1.2.19 Electron wavefunctions of the first three bound states of a harmonic oscillator