

## Approximate solutions of the Schrödinger equation

### 9.1 The WKB method

The Schrödinger equation has analytic solutions only for very few selected potential energies  $U(x)$ . For example, the infinite square well has an analytic solution. If the one-dimensional potential energy does not have a very simple form, the solution of the one-dimensional time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + U(x) \psi(x) = E \psi(x) \quad (9.1)$$

is generally a complicated problem. Some approximate methods to solve the Schrödinger equation are the perturbation method (see Chaps. 10 and 11) or the variational method (see Chap. 9). An approximate method of great versatility has been developed by Wentzel, Kramers and Brillouin (1926) and is called the WKB method or WKB approximation. This method provides approximate wave functions in one-dimensional problems. The WKB method

can also be applied to three-dimensional problems, where the potential is spherically symmetric and a radial differential equation can be separated from the three-dimensional problem (see, for example, Bohm, 1951).

The WKB approximation can be used, if the potential energy  $U(x)$  varies *slowly*. Specifically, changes in  $U(x)$  should be small on the length scale of the de Broglie wavelength. In a constant potential, the Schrödinger equation has the solutions  $\exp(\pm i k x)$ , with  $k = 2\pi/\lambda = \text{const}$ . If  $U(x)$  varies slowly with  $x$ , we write the solution in the form

$$\psi(x) = e^{i\phi(x)} \quad (9.2)$$

where the function  $\phi(x)$  represents the *phase* of the wave. In a constant potential  $\phi(x) = \pm k x$ , that is, the phase changes linearly with  $x$ . In a slowly varying potential, it is expected that  $\phi(x)$  deviates slightly from the linear dependence on  $x$ . To further investigate the function  $\phi(x)$  it is convenient to use the abbreviations

$$k(x) = \frac{1}{\hbar} \sqrt{2m[E - U(x)]} \quad \text{for } E \geq U(x) \quad (9.3)$$

$$k(x) = \frac{-i}{\hbar} \sqrt{2m [U(x) - E]} = -i \kappa(x) \quad \text{for } E \leq U(x). \quad (9.4)$$

Insertion of Eq. (9.2) into the time-independent Schrödinger equation and using Eqs. (9.3) and (9.4) yields

$$i \frac{d^2 \phi}{dx^2} - \left( \frac{d\phi}{dx} \right)^2 + k(x)^2 = 0 \quad (9.5)$$

which is just a different representation of the Schrödinger equation, which has, however, the same physical content. The WKB approximation is intended for potentials that do not vary rapidly. Therefore, as a zero-order approximation, we assume that the second derivative of  $\phi(x)$  with respect to  $x$  is very small

$$\frac{d^2 \phi}{dx^2} \approx 0. \quad (9.6)$$

One obtains

$$\left( \frac{d\phi_0}{dx} \right)^2 = k(x)^2 . \quad (9.7)$$

The subscript zero in  $\phi_0$  is used to emphasize that this is a zero-order approximation. Integration yields

$$\phi_0(x) = \pm \int k(x) dx + C_0 \quad (9.8)$$

where  $C_0$  is an integration constant. This equation is the simplest form of the WKB approximation.

A successive approximation method can be obtained by taking into account a *finite* second derivative, instead of the more crude approximation made in Eq. (9.6). Equation (9.5) can then be rewritten as

$$\left( \frac{d\phi}{dx} \right)^2 = k(x)^2 + i \frac{d^2\phi}{dx^2} . \quad (9.9)$$

Integration of  $\phi' = d\phi/dx$  without neglecting the second derivative on the right-hand side of this equation (in contrast to the previous omission of

$\phi'' = d^2\phi / dx^2$ , see Eq. 9.6) yields

$$\phi(x) = \pm \int_x \sqrt{k(x)^2 + i \phi_0''(x)} dx + C_1 . \quad (9.10)$$

Using Eq. (9.7) to determine  $\phi''(x)$ , one obtains

$$\phi_1(x) = \pm \int_x \sqrt{k(x)^2 + i \phi_0''(x)} dx + C_1 = \pm \int_x \sqrt{k(x)^2 \pm i k'(x)} dx + C_1 \quad (9.11)$$

where  $k'(x) = dk(x)/dx$ . The subscript one in  $\phi_1$  is used to emphasize that this is a first-order approximation. Since we have required that the wave function does not vary too violently, one can state that

$$|k'(x)| \ll |k(x)^2| . \quad (9.12)$$

Thus, the first-order approximation is only slightly different from the zero-order approximation of Eq. (9.8). With the condition of Eq. (9.12), one can further simplify Eq. (9.11) and expand the square-root as follows

$$\phi_1(x) \approx \int_x \left( \pm k(x) + \frac{i}{2} \frac{k'(x)}{k(x)} \right) dx + C_1 \approx \pm \int_x k(x) dx + \frac{i}{2} \ln k(x) + C_1 . \quad (9.13)$$

We have thus derived the zero-order (Eq. 9.8) and the first-order approximation (Eqs. 9.11 and 9.13) for  $\phi(x)$ . Both approximations are known as the WKB method. Insertion of Eqs. (9.8) and (9.13) into Eq. (9.2) yields the wave function for the zero order and first order WKB approximation

$$\psi(x) \approx \exp \left( \pm i \int_x k(x) dx \right) \quad (\text{zero-order WKB}) \quad (9.14)$$

$$\psi(x) \approx \frac{1}{\sqrt{k(x)}} \exp \left( \pm i \int_x k(x) dx \right) \quad (\text{first-order WKB}) \quad (9.15)$$

This wave function can be used in the classically allowed and forbidden regions, as illustrated by region II and III in **Fig. 9.1**, respectively.

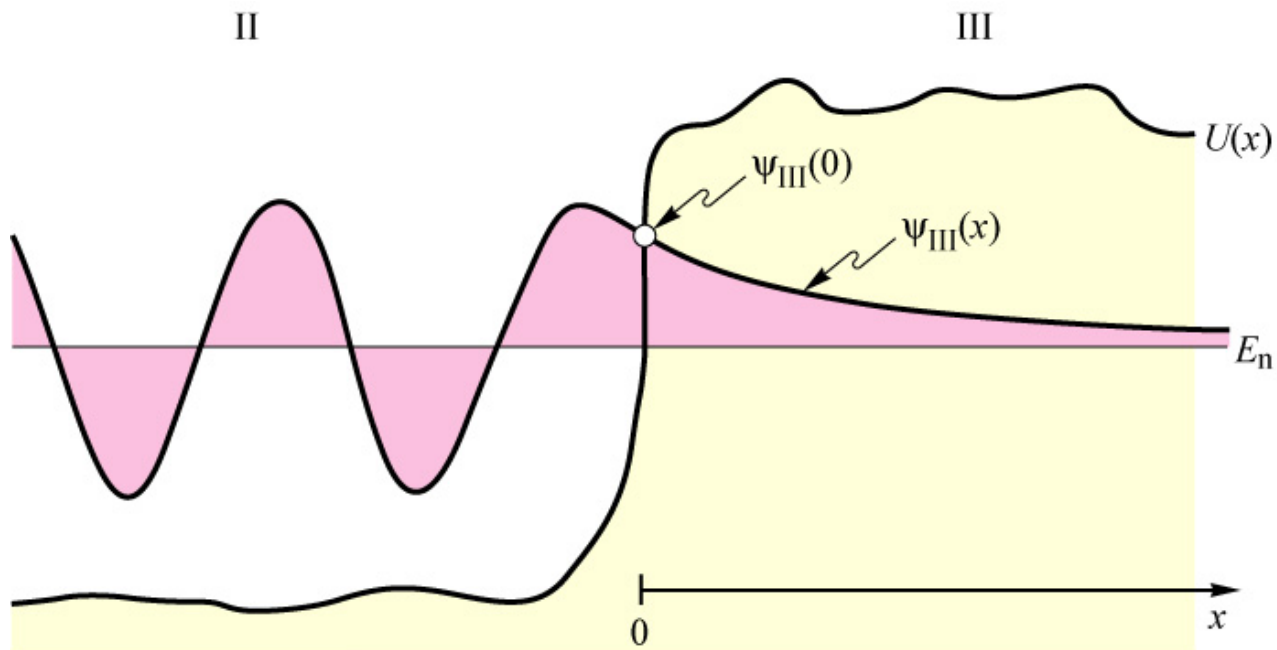


Fig. 9.1 Oscillating and exponentially decaying wavefunction in the classically allowed region II and disallowed region III, respectively. The decaying wavefunction in region III can be calculated by the WKB approximation.

As an example, we use the WKB approximation to calculate the amplitude of a wave function in the classically forbidden region of a potential energy  $U(x)$ . Such a classically forbidden region is shown in **Fig. 9.1**. A particle with total energy  $E$  has a kinetic energy  $E - U(x)$ . In the classically forbidden region, the kinetic energy is negative which cannot occur for classical particles. Therefore, regions where the condition  $E - U(x) < 0$  is satisfied, are forbidden for classical particles. In contrast, the Schrödinger equation has solutions even in classically forbidden regions. As will be seen below, the

amplitude of the wave function rapidly decreases in these regions. The particle or the wave function **tunnels** into the barrier. The amplitude of the wave function in the barrier will be denoted as  $\psi_{\text{III}}(x)$ , as shown in **Fig. 9.1**. To calculate  $\psi_{\text{III}}(x)$ , we assume that the wave function has an amplitude  $\psi_{\text{III}}(0)$  at the boundary between the classically allowed region II and the classically forbidden region III. Calculating the amplitude of the wave function according to the zero-order WKB approximation Eq. (9.14) yields

$$\psi_{\text{III}}(x) = \psi_{\text{III}}(0) \exp\left[-\int_0^x \kappa(x) dx\right] = \psi_{\text{III}}(0) \exp\left\{-\int_0^x \frac{1}{\hbar} \sqrt{2m [U(x) - E]} dx\right\} \quad (9.16)$$

Equations (9.14), (9.15), and (9.16) are valid for an arbitrary potential  $U(x)$ .

Applying the WKB approximation to the classically allowed region II, provides further insight. In region II, it is  $E > U(x)$  and  $k(x)$  is a real quantity. We define the **effective wavelength** as

$$\lambda(x) = \frac{2\pi}{k(x)} . \quad (9.17)$$

If  $U(x)$  is constant, then  $k(x)$  is a constant as well, and, according to Eq. (9.17),  $\lambda$  is a constant. In the classical picture, a particle in a constant potential has a constant momentum. In the quantum-mechanical picture, the wave in a constant potential has a constant wavelength. Now consider a varying potential energy  $U(x)$ . In this case, the momentum of a classical particle varies according to the variations of the potential energy. The wavelength of the quantum wave depends on the potential energy  $U(x)$ . This dependence is given by Eqs. (9.17) and (9.4). Hence, the WKB method can be understood as going from a *constant* wavelength  $\lambda$  in a *constant* potential to a *slowly varying* wavelength in a *slowly varying* potential. Recall that the WKB approximation was derived for a slowly varying potential (see Eq. 9.12). Using Eq. (9.17), this condition can be rewritten as

$$\frac{dU(x)}{dx} \ll \frac{U(x)}{\lambda} . \quad (9.18)$$

That is, the changes of  $U(x)$  must be slow on the scale of  $\lambda$ .

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**Exercise: Tunneling probability through a barrier.** Consider the quantum barrier shown in **Fig. 9.2**. Electrons in Region I do not have sufficient energy

to overcome the barrier by thermal emission over the barrier. However, carriers have a non-zero probability to tunnel through the barrier. The probability of “finding” the electron at the left-hand side of the barrier is given by  $\psi_{II}^*(0)\psi_{II}(0)$ . Similarly, the probability of “finding” the electron at the right-hand side of the barrier is given by  $\psi_{II}^*(L_B)\psi_{II}(L_B)$ . Thus the tunneling probability is given by

$$T = \frac{\psi_{II}^*(L_B)\psi_{II}(L_B)}{\psi_{II}^*(0)\psi_{II}(0)} \quad (9.19)$$

Using the zero-order WKB approximation to calculate the wave function in the barrier yields

$$\psi_{II}(x) = \psi_{II}(0) e^{-\int_0^x \kappa(x) dx} = \psi_{II}(0) e^{-\int_0^x \hbar^{-1} \sqrt{2m^* [U(x)-E]} dx} \quad (9.20)$$

Thus the tunneling probability is given by

$$T = e^{-\int_{x=0}^{L_B} 2\hbar^{-1} \sqrt{2m^* [U(x)-E]} dx} \quad (9.21)$$

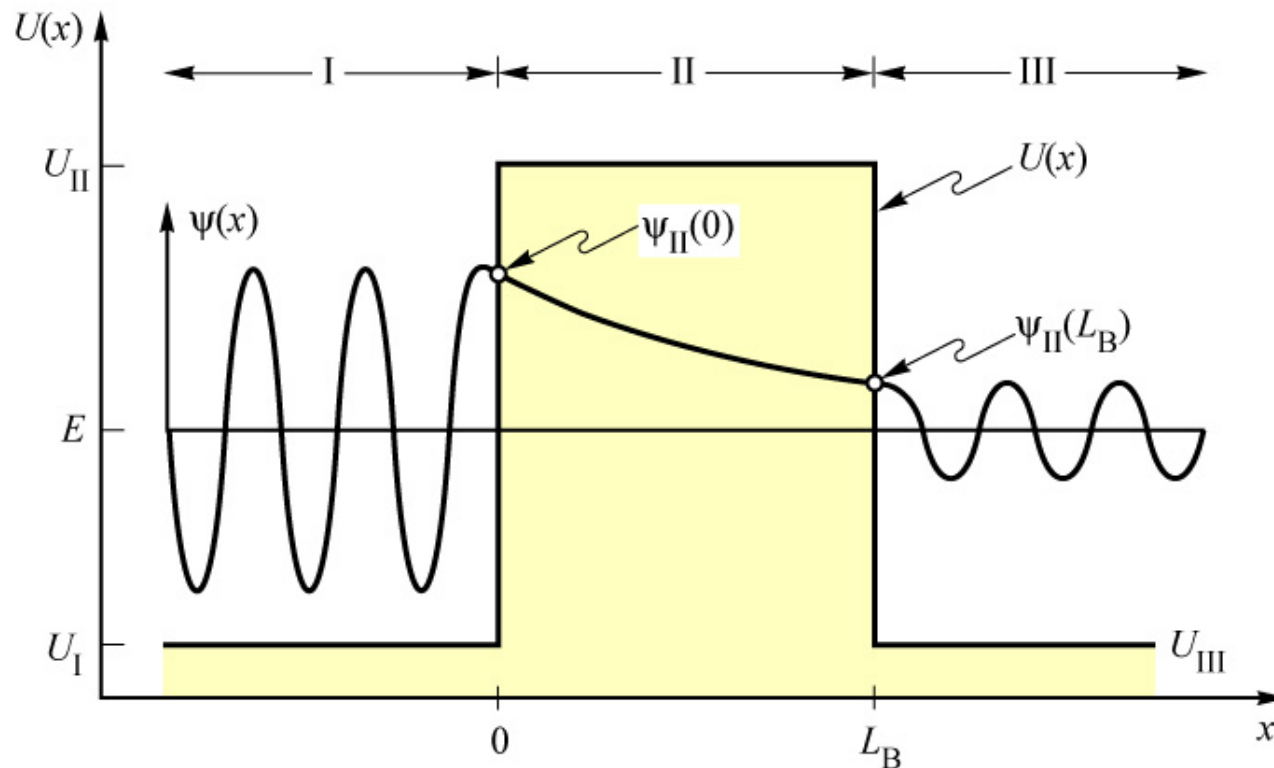


Fig. 9.2. Wave function of a particle with energy  $E$  tunneling through a quantum barrier.

Calculate the tunneling probability of an electron with mass  $m^* = 0.067m_0$  and energy  $E = 100 \text{ meV}$  through a rectangular barrier with height  $U_{II} = 200 \text{ meV}$  and barrier thickness  $L_B = 100 \text{ \AA}$ . Assume that  $U_I = U_{III} = 0$ . What is the dependence of the tunneling probability through a rectangular barrier on (i) the barrier thickness, (ii) the barrier height? What is the tunneling probability for  $L_B = 1000 \text{ \AA}$ ?

Answer: The tunneling probability is  $T = 2.2 \times 10^{-4}$  and  $T = 2.8 \times 10^{-37}$  for  $L_B = 100 \text{ \AA}$  and  $1000 \text{ \AA}$ , respectively. The tunneling probability decreases exponentially with the barrier thickness. It decreases exponentially with the square root of the barrier height. This exercise shows that tunneling effects are significant for barrier thicknesses on the order of  $100 \text{ \AA}$  and smaller. It also shows that the tunneling probability through thick barriers (e. g.  $1000 \text{ \AA}$ ) is extremely small.

**What are the implications for the gate leakage current in devices such as Si MOSFETs with an oxide thickness of  $100 \text{ \AA}$ ?**

Answer: In Si MOSFETs, the tunneling barrier height is  $\gg 100 \text{ meV}$  since  $\text{SiO}_2$  has a large bandgap ( $E_g \approx 5 \text{ eV}$ ). Therefore, the gate leakage current is negligibly small for an oxide thickness of  $100 \text{ \AA}$ .

**What are the implications for the doping concentration in ohmic metal-semiconductor contacts?**

Answer: Ohmic contacts are made by heavily doping the semiconductor of

a metal-semiconductor contact. The depletion region thickness in the semiconductor is so small that tunneling is the dominant transport mechanism between the metal and the semiconductor. Thus, the doping concentration in the semiconductor must be so high that the depletion region thickness is  $\ll 100 \text{ \AA}$ .

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## 9.2 The connection formulas in the WKB method

The WKB approximation provides a quasi-oscillatory solution and a quasi-exponentially damped solution in the classically allowed and forbidden regions of a potential respectively. Special care must be taken to use the WKB method in the vicinity of a so-called classical turning point. As shown in **Fig. 9.3**, a classical particle would be allowed only in region II where  $E > U(x)$ . A classical particle with total energy  $E$  would *turn around* at  $x = a$ , since its kinetic energy at this point is zero, *i. e.*  $E - U(a) = 0$ . In contrast, a quantum-mechanical particle can tunnel beyond the classical turning point.

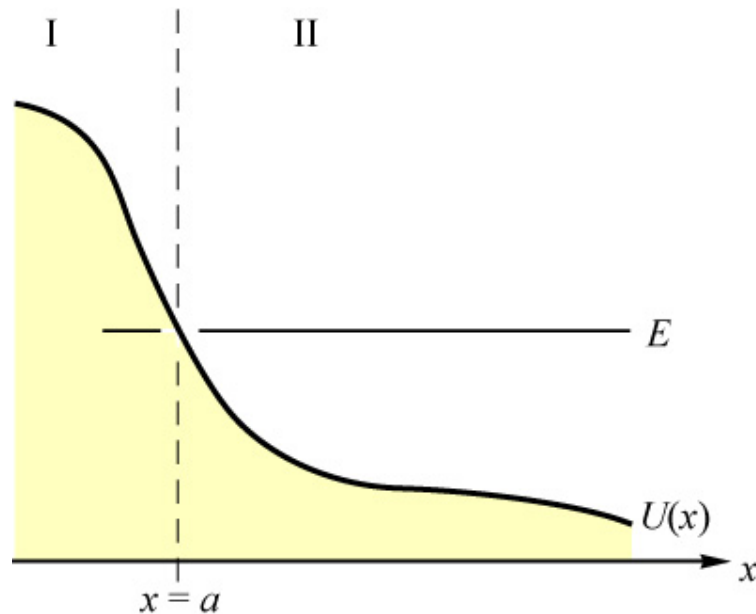


Fig. 9.3. The classical turning point at  $x = a$  is to the left of the classically allowed region II.

In the vicinity of the classical turning point, the wavevector approaches zero, *i. e.*  $k(x) \rightarrow 0$ . However, the derivative remains finite, that is

$$\frac{dk(x)}{dx} = \frac{d}{dx} \frac{-i}{\hbar} \sqrt{2m[E - U(x)]} \neq 0. \quad (9.22)$$

The application of the WKB method requires that  $k(x)$  does not vary violently, as stated in Eqs. (9.12) and (9.18). This condition can be also expressed as

$$\Delta k(x) = \frac{dk(x)}{dx} \Delta x \ll k(x) . \quad (9.23)$$

This condition is obviously not fulfilled in the vicinity of a classical turning point where  $k(x) \rightarrow 0$ . Hence, the WKB approximation cannot be applied in the vicinity of classical turning points. However, because the WKB method is problematic *only* in the vicinity of a turning point, it is desirable to find some *connection formulas* that would make possible the utilization of the WKB approximation even in the vicinity of turning points.

An excellent derivation of the connection formulas was given by Merzbacher (1970). In this derivation, it was assumed that the potential energy  $U(x)$  depends linearly on  $x$  in the vicinity of the classical turning point. The derivation of the connection formulas shall be omitted here and only the results will be summarized. The connection formulas *connect* the wave functions obtained by the WKB-method in regions I, II, and III (see **Fig. 9.3** and **Fig. 9.4**). The classical turning point may be to the left or to the right of the allowed region II as shown in **Fig. 9.3** and **Fig. 9.4**, respectively. The connection formulas are given by:

(1) Turning point is to the left of the classically allowed region (see **Fig. 9.3**)

$$\frac{1}{\sqrt{\kappa}} \exp\left(-\int_x^a \kappa \, dx\right) \quad \text{connects with} \quad \frac{2}{\sqrt{k}} \cos\left(\int_a^x k \, dx - \frac{\pi}{4}\right) \quad (9.24)$$

$$\frac{-1}{\sqrt{\kappa}} \exp\left(\int_x^a \kappa \, dx\right) \quad \text{connects with} \quad \frac{1}{\sqrt{k}} \sin\left(\int_a^x k \, dx - \frac{\pi}{4}\right) \quad (9.25)$$

(2) Turning point is to the right of the classically allowed region (see **Fig. 9.3**)

$$\frac{2}{\sqrt{k}} \cos\left(\int_x^b k \, dx - \frac{\pi}{4}\right) \quad \text{connects with} \quad \frac{1}{\sqrt{\kappa}} \exp\left(-\int_b^x \kappa \, dx\right) \quad (9.26)$$

$$\frac{1}{\sqrt{k}} \sin\left(\int_x^b k \, dx - \frac{\pi}{4}\right) \quad \text{connects with} \quad \frac{-1}{\sqrt{\kappa}} \exp\left(\int_b^x \kappa \, dx\right) \quad (9.27)$$

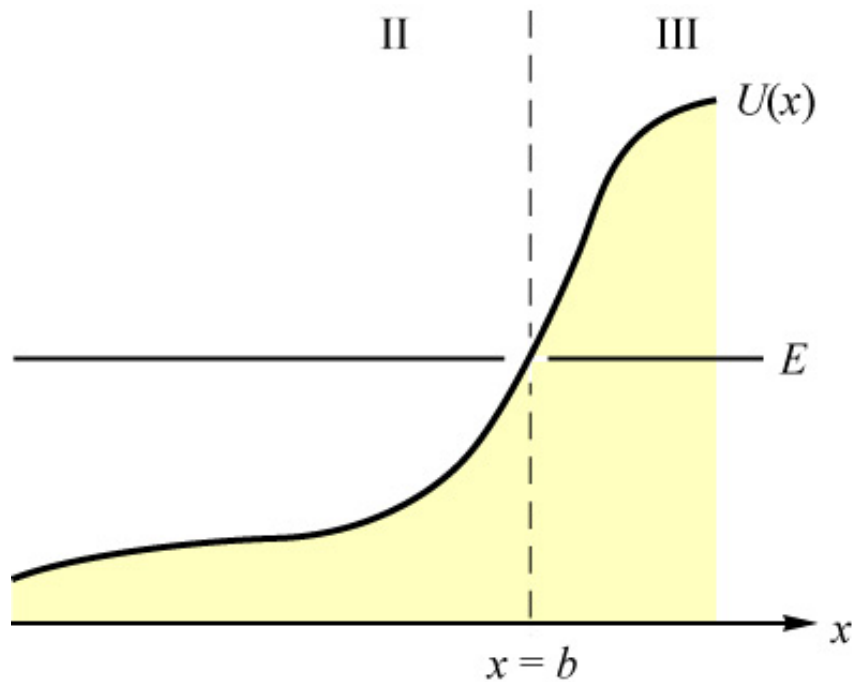


Fig. 9.4. The classical turning point at  $x = b$  is to the right of the classically allowed region II.

Caution has to be exercised, if the connection formulas are applied. Consider Case (1), in which the classical turning point is to the left of the classically allowed region. According to Eqs. (9.24) and (9.25), the wave function on the left side of the turning point may either *decrease* exponentially (Eq. 9.25) or *increase* exponentially (Eq. 9.24) with  $x$ . Even though a wave function may be adequately described by a single exponential function at some position  $x_0$ , the connecting wave function may become important at another position  $x_1$ , due to the exponential nature of the two functions. Therefore, caution must be

exercised, if one of the two wave functions is neglected.

### 9.3 The WKB method for bound states

The WKB method can be used to obtain the eigenstate energies of a potential well. An example of such a potential well is shown in **Fig. 9.5**. The WKB approximation can be used in the three regions I, II, and III. In the vicinity of the classical turning points, the connection formulas will be used. In region I, the wave function must vanish for sufficiently small  $x$ . Therefore, the unnormalized wave function in region I is given by

$$\psi_{\text{I}} \approx \frac{1}{\sqrt{\kappa}} \exp\left(-\int_x^a \kappa \, dx\right) \quad (x < a). \quad (9.28)$$

According to the connection formula Eq. (9.24) the wave function in the classically allowed region II is given by

$$\psi_{\text{II}} \approx \frac{2}{\sqrt{k}} \cos\left(\int_a^x k \, dx - \frac{\pi}{4}\right) \quad (a \leq x \leq b). \quad (9.29)$$

Rewriting this equation by employing a trigonometric conversion yields

$$\psi_{\text{II}} \approx \frac{2}{\sqrt{k}} \cos \left( \int_a^b k \, dx - \int_x^b k \, dx - \frac{\pi}{4} \right) \quad (9.30)$$

$$= \frac{-2}{\sqrt{k}} \cos \left( \int_a^b k \, dx \right) \sin \left( \int_x^b k \, dx - \frac{\pi}{4} \right) + \frac{2}{\sqrt{k}} \sin \left( \int_a^b k \, dx \right) \cos \left( \int_x^b k \, dx - \frac{\pi}{4} \right)$$

Comparing the two terms of this equation with the connection formulas, Eqs. (9.26) and (9.27), yields that only the last cosine term yields an exponentially decreasing wave function in region III. Hence, the first term must vanish; this yields the condition

$$\int_a^b k(x) \, dx = \left( n + \frac{1}{2} \right) \pi \quad \text{for } n = 0, 1, 2 \dots \quad (9.31)$$

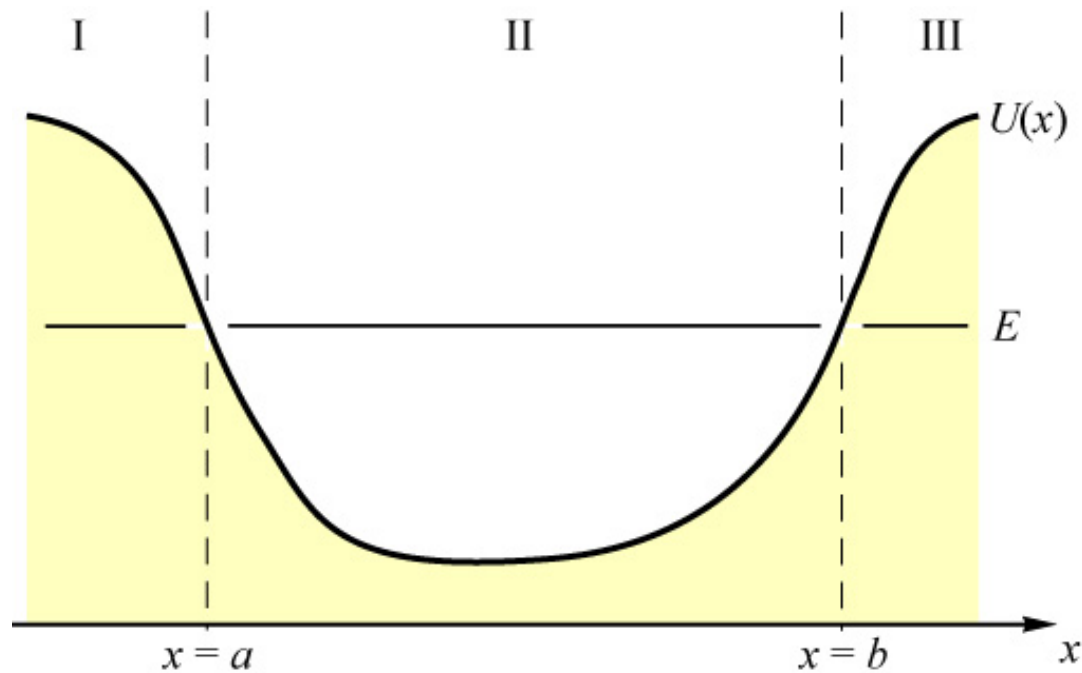


Fig. 9.5. Schematic potential well with potential energy  $U(x)$  and two classical turning points  $x = a$  and  $x = b$ . A classical particle of energy  $E$  would be confined to the region  $a \leq x \leq b$ .

This equation enables us to obtain the discrete (approximate) eigenstate energies of an arbitrary shaped quantum well. Note that the validity of the connection formulas is limited to potential energies  $U(x)$  which depend linearly on  $x$  in the vicinity of the classical turning point. With the de Broglie relation  $p = \hbar k$  one obtains

$$\int_a^b p(x) dx = \left( n + \frac{1}{2} \right) \pi \hbar \quad \text{for } n = 0, 1, 2 \dots \quad (9.32)$$

Integration of  $p(x)$  in terms of a closed curve (*i. e.* one round trip of the quantum wave in the potential well) yields

$$\oint p(x) dx = 2 \int_a^b p(x) dx = \left( n + \frac{1}{2} \right) 2\pi \hbar \quad \text{for } n = 0, 1, 2 \dots \quad (9.33)$$

The physical interpretation of this equation is facilitated by rewriting the equation as

$$\frac{2}{\hbar} \int_a^b p(x) dx = 2\pi n + 2\pi c_a + 2\pi c_b \quad \text{for } n = 0, 1, 2 \dots \quad (9.34)$$

The term  $2\pi n$  represents the integral number of wavelengths of the quantum mechanical wave in the quantum well between the classical turning points. In the example shown in **Fig. 9.6**, three full wavelengths fit into the round-trip distance of the quantum well and hence  $n = 3$ . The terms  $2\pi c_a$  and  $2\pi c_b$  in Eq. (9.34) can be interpreted as the change of the phase of the quantum mechanical wave incurred at the classical turning points  $x = a$  and  $x = b$ . Comparison of Eq. (9.34) with Eq. (9.33) reveals that  $c_a = c_b = (1/4)$ , *i. e.*, the change of phase of the wave function at the classical turning points is a

quarter wave. Note that this change of phase of  $\pi/2$  deduced here is the result of the connection formulas discussed in the previous section. The connection formulas were derived for potential energies  $U(x)$  that are, in the vicinity of the turning points, linear functions of  $x$ . This situation is shown in **Fig. 9.6(a)**. Consequently, a phase change of  $\pi/2$  applies only to potentials  $U(x)$  that depend linearly on  $x$  in the vicinity of the turning point.

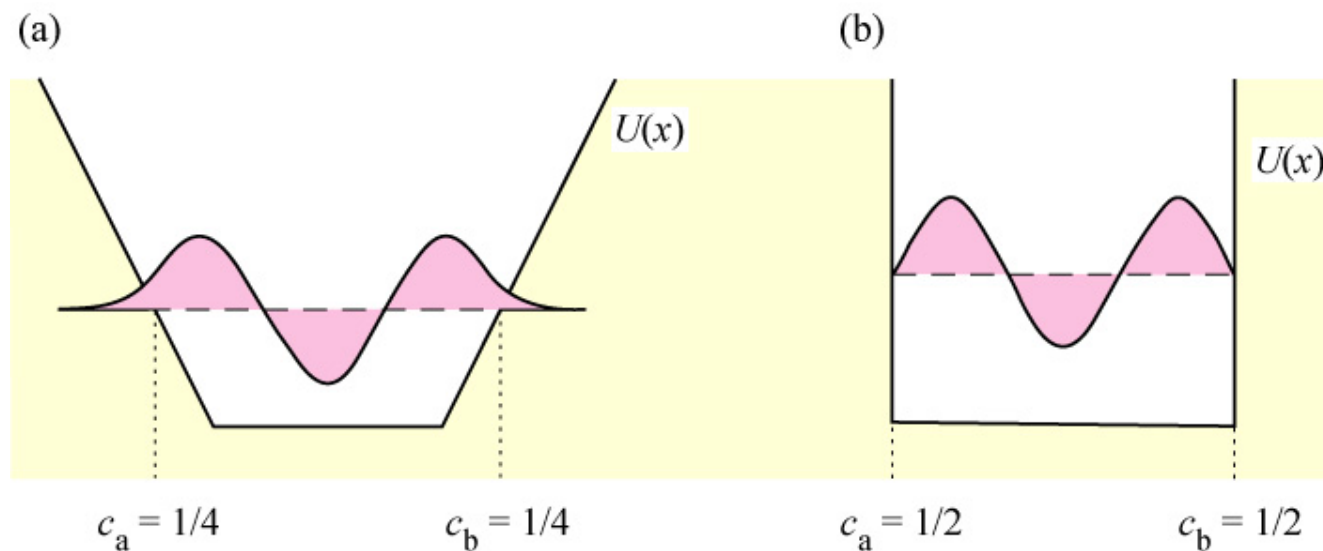


Fig. 9.6. Phase changes  $c_a 2\pi$  and  $c_b 2\pi$  of wave functions in quantum wells for a potential energy  $U(x)$  varying (a) linearly and (b) discontinuously at the classical turning points.

We now consider the case in which the turning points are at a *discontinuous change* of  $U(x)$ , as illustrated in **Fig. 9.6(b)**. Assuming that the walls of the potential well are infinitely high, the wave function must vanish at the turning

point. Hence the change in phase incurred by the wave at the turning point must be  $\pi$ , i. e.  $c_a = c_b = (1/2)$ . Using this value in Eq. (9.34), one obtains

$$\int_a^b p(x) dx = (n + 1) \pi \hbar \quad \text{for } n = 0, 1, 2 \dots \quad (9.35)$$

which is identical to the one-dimensional Bohr-Sommerfeld quantization condition given in Eq. (1.3.36). This is not surprising: In the Bohr-Sommerfeld model, the electron trajectory around the nucleus is a rigid circle or ellipse, and hence the wave function vanishes for radii larger than the Bohr radius.

We summarize the phase changes of the quantum mechanical wave for a linear and a discontinuous potential energy  $U(x)$  at the turning point:

$$\text{If } U(x) = \text{linear function, then } c_a = \frac{1}{4} \quad (9.36)$$

$$\text{If } U(x) = \text{discontinuous, then } c_a = \frac{1}{2} . \quad (9.37)$$

The same applies to  $c_b$ .

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**Exercise: *The WKB approximation for bound states.*** Calculate the energies of the allowed states of a particle with mass  $m^*$  in a one-dimensional

**infinite square-shaped** quantum well by using the WKB approximation. The potential energy of the infinite square well is given by  $U(x) = 0$  for  $|x| < L_{\text{QW}}/2$  and  $U(x) = \infty$  for  $x = \pm L_{\text{QW}}/2$ .

$$\text{Solution: } E_n = (n + 1)^2 \frac{\hbar^2 \pi^2}{2 m^* L_{\text{QW}}^2} \quad \text{for } n = 0, 1, 2 \dots \quad (9.38)$$

Calculate the energies of the allowed states of a particle with mass  $m^*$  in a one-dimensional **triangular-shaped** quantum well by using the WKB approximation. The potential energy of the triangular-shaped well is given by  $U(x) = e \mathcal{E} x$  for  $x \geq 0$  and  $U(x) = \infty$  for  $x < 0$ .

$$\text{Solution: } E_n = \left( \frac{3 \pi}{2} \left( n + \frac{3}{4} \right) \right)^{2/3} \left( \frac{e^2 \hbar^2 \mathcal{E}^2}{2 m^*} \right)^{1/3} \quad \text{for } n = 0, 1, 2 \dots \quad (9.39)$$

Calculate the energies of the allowed states of a particle with mass  $m^*$  in a one-dimensional **V-shaped** quantum well by using the WKB approximation. The potential energy of the V-shaped well is given by  $U(x) = e \mathcal{E} |x|$ .

$$\text{Solution: } E_n = \left( \frac{3\pi}{4} \left( n + \frac{1}{2} \right) \right)^{2/3} \left( \frac{e^2 \hbar^2 \mathcal{E}^2}{2 m^*} \right)^{1/3} \quad \text{for } n = 0, 1, 2 \dots \quad (9.40)$$

Calculate the energies of the allowed states of a particle with mass  $m^*$  in a one-dimensional **parabolic-shaped** quantum well by using the WKB approximation. The potential energy of the parabolic-shaped well is given by  $U(x) = (1/2) m \omega^2 x^2$ .

$$\text{Solution: } E_n = \left( n + \frac{1}{2} \right) \hbar \omega \quad \text{for } n = 0, 1, 2 \dots \quad (9.41)$$


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## 9.4 The variational method

The variational method is a versatile method to calculate approximate wave functions and eigenstate energies of a potential. The starting point of the variational method is an educated guess for the wave function of a given quantum mechanical potential. Having made such an initial guess, it is not clear that the wave function given by the educated guess is a good wave function, *i. e.*, if it matches well the true wave function of the potential.

Therefore, we call the approximate wave function based on the guess the trial wave function or **trial function**. The trial function may contain one or several trial parameters whose selection allows for an optimization of the wave function. Assuming that the normalized trial function for a one-dimensional problem is then given by  $\psi(x, \alpha)$ , where  $x$  is the spatial coordinate and  $\alpha$  is the trial function parameter or **trial parameter**, whose value must yet be determined.

The expectation value for the total energy of a quantum mechanical particle, described by the trial function  $\psi(x, \alpha)$ , is given by

$$\langle E \rangle = \langle \psi(x, \alpha) | H | \psi(x, \alpha) \rangle \quad (9.42)$$

Like ordinary particles, quantum mechanical particles assume a state in which their total energy is minimized. This fact can be used to find an optimum value for the trial parameter. Thus the condition

$$\frac{d}{d\alpha} \langle E \rangle = \frac{d}{d\alpha} \langle \psi(x, \alpha) | H | \psi(x, \alpha) \rangle = 0 \quad (9.43)$$

can be used to determine the optimum value for  $\alpha$ . Of course the quality of

the wave function and of the eigenstate energy will also depend on the quality of the trial function, *i. e.*, on the initial educated guess. Finally, the insertion of the optimum value for  $\alpha$  into Eq. (9.42) yields the eigenstate energy.

If the trial function has more than one trial parameter, the condition of Eq. (9.43) needs to be applied several times, *i. e.* for each trial parameter. Whereas the quality of the wave function can improve with the number of trial parameters, so does the computational effort. The variational method thus allows one to calculate the wave function and the eigenstate energy of particles in a quantum mechanical potential. **With a good trial function, the accuracy of the eigenstate energy can be better than 1%, even if only a single trial parameter is used.**

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**Exercise: *The Fang-Howard wave function.*** In this exercise, the ground-state wave function and energy of a triangular potential well are calculated by the variational method. The potential occurring in the semiconductor of a MIS structure has a triangular shape, as shown in **Fig. 9.7**. The potential energy in the semiconductor is given by  $U(x) = E_{\text{pot}}(x) = e \mathcal{E} x$ . Use the trial function  $\psi(x, \alpha) = A x e^{-\alpha x}$  where  $A$  is a normalization constant and  $\alpha$  is the trial parameter. This trial function was introduced by Fang and Howard (1966).

First calculate the normalization constant  $A$  by using the normalization condition. Then calculate the expectation value of the total energy as a function of  $\alpha$ . Determine the trial parameter  $\alpha$  by minimizing the expectation value of the total energy with respect to  $\alpha$ , *i. e.*  $(d/d\alpha) \langle E(\alpha) \rangle = 0$ . Finally calculate the expectation value for the total energy,  $E_0$ .

Results: Application of the normalization condition yields:

$$A = 2\alpha^{3/2} \quad (9.44a)$$

Minimizing the energy expectation value yields:

$$\alpha = [(3/2) e E m^* / \hbar^2]^{1/3} \quad (9.44b)$$

Calculation of the total energy expectation value yields:

$$E_0 = (3/2)[(3/2) e E \hbar / (m^*)^{1/2}]^{2/3} \quad (9.44c)$$

Draw the band diagram of a GaAs metal insulator semiconductor (MIS) structure for negative, zero, and positive bias. Then assume that the electric field in the GaAs is  $\mathcal{E} = 7 \times 10^4$  V/cm in the positively-biased case. Calculate the ground state energy of electrons in the GaAs ( $m^* = 0.067 m_0$ ) by using the Fang-Howard wave function.

Result:  $E_0 = 75 \text{ meV}$ .

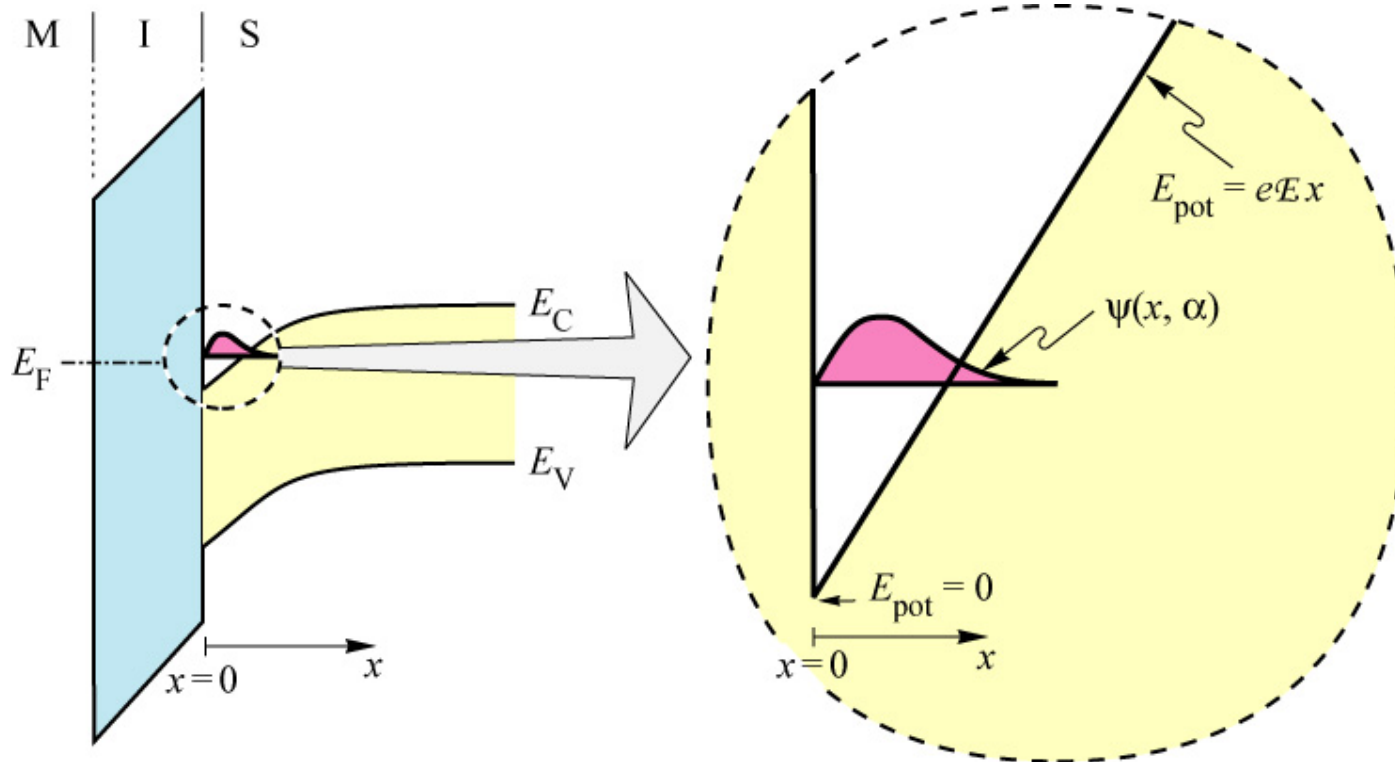


Fig. 9.7. Band diagram of an triangular-shaped electron channel of a metal-insulator-semiconductor structure. Also shown is the Fang-Howard wave function.

**Exercise: Variational wave functions in a V-shaped potential well.** In this

exercise, the ground-state wave function and two excited-state wave functions and the state energies of a V-shaped potential well are calculated by the variational method. The potential and wave functions are shown in **Fig. 9.8**. The potential energy in the semiconductor is given by  $U(x) = E_{\text{pot}}(x) = e E x$  for  $x \geq 0$  and  $U(x) = E_{\text{pot}}(x) = -e E x$  for  $x \leq 0$ . Develop trial wave functions of the lowest three states taking into account that the lowest three wave functions have 0, 1, and 2 nodes. Also take into account the *even* symmetry of the  $n = 0$  and  $n = 2$  states, and the *odd* symmetry of the  $n = 1$  state.

Solution:

There are several possible solutions to this exercise. One possible set of trial wave functions is:

$$\psi_0(x) = A_0 (1 + \alpha_0 x) e^{-\alpha_0 x} \quad \text{for } x \geq 0 \quad (9.45a)$$

$$\psi_0(x) = A_0 (1 - \alpha_0 x) e^{\alpha_0 x} \quad \text{for } x < 0 \quad (9.45b)$$

$$\psi_1(x) = A_1 x e^{-\alpha_1 x} \quad \text{for } x \geq 0 \quad (9.45c)$$

$$\psi_1(x) = A_1 x e^{\alpha_1 x} \quad \text{for } x < 0 \quad (9.45d)$$

$$\psi_2(x) = A_2 (\alpha_2^2 x^2 - 1)(1 + \alpha_2 x) e^{-\alpha_2 x} \quad \text{for } x \geq 0 \quad (9.45e)$$

$$\psi_2(x) = A_2 (\alpha_2^2 x^2 - 1)(1 - \alpha_2 x) e^{\alpha_2 x} \quad \text{for } x < 0 \quad (9.45f)$$

The normalization constants of the trial wave functions are determined by using the normalization condition. One obtains

$$A_0 = \sqrt{(2/5) \alpha_0} \quad (9.46a)$$

$$A_1 = \sqrt{2 \alpha_1^3} \quad (9.46b)$$

$$A_2 = \sqrt{(4/63) \alpha_2} \quad (9.46c)$$

Minimizing the expectation value of the energy yields the variational parameters

$$\alpha_0 = \left(\frac{9}{4}\right)^{1/3} \left(e \mathcal{E} 2 m^* / \hbar^2\right)^{1/3} \quad (9.47a)$$

$$\alpha_1 = \left(\frac{3}{4}\right)^{1/3} \left(e \mathcal{E} 2 m^* / \hbar^2\right)^{1/3} \quad (9.47b)$$

$$\alpha_2 = \left(\frac{47}{12}\right)^{1/3} \left(e \mathcal{E} 2 m^* / \hbar^2\right)^{1/3} \quad (9.47c)$$

The eigenstate energies are then given by

$$E_0 = \frac{3}{10} \left(\frac{81}{2}\right)^{1/3} \left(\frac{e^2 \hbar^2 \mathcal{E}^2}{2 m^*}\right)^{1/3} \quad (9.48a)$$

$$E_1 = \frac{3}{2} \left(\frac{9}{2}\right)^{1/3} \left(\frac{e^2 \hbar^2 \mathcal{E}^2}{2 m^*}\right)^{1/3} \quad (9.48b)$$

$$E_2 = \frac{9}{7} \left( \frac{47}{12} \right)^{2/3} \left( \frac{e^2 \hbar^2 \mathcal{E}^2}{2 m^*} \right)^{1/3} \quad (9.48c)$$

The agreement of the eigenstate energies with the numerically evaluated correct values is generally quite good. The difference between approximation and correct value is typically just a few percent.

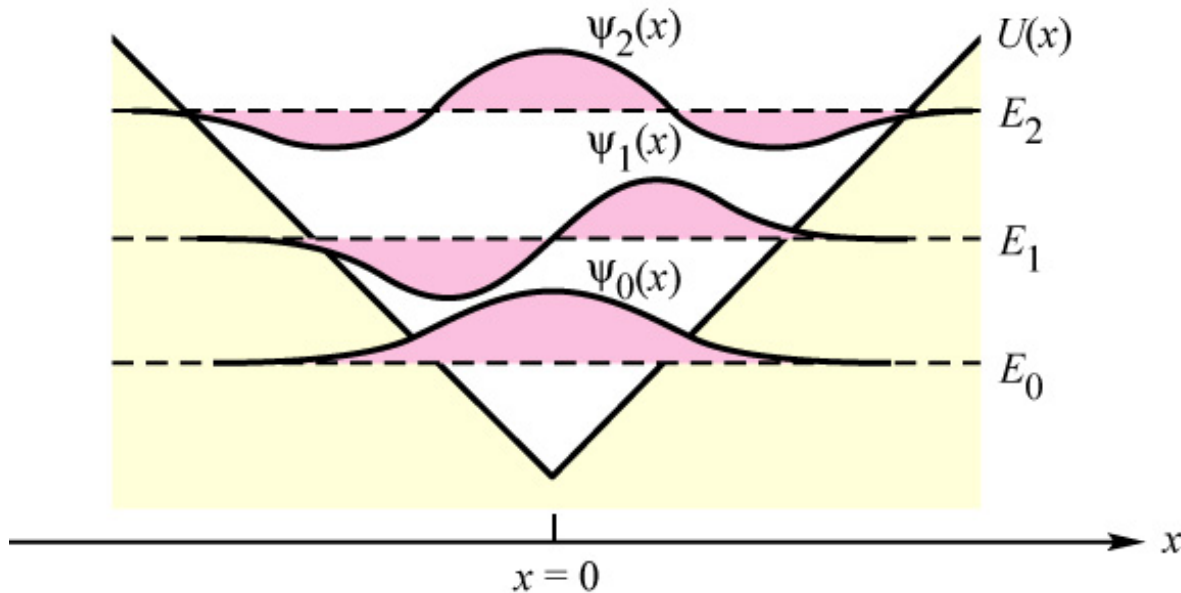


Fig. 9.8. Potential energy diagram and schematic wave functions of a V-shaped quantum well.