

Let a and b be the classical turning points for a particle moving with the energy E across a potential barrier $U(x)$. In other words, in the region $a < x < b$, one has $U(x) > E$. The WKB wave function is of the form:

$$x < a: \quad \psi = \frac{2}{\sqrt{v}} \cos \left[\frac{1}{\hbar} \int_a^x p \, dx + \frac{\pi}{4} \right] \tag{1}$$

$$= \frac{1}{\sqrt{v}} e^{\frac{i}{\hbar} \int_a^x p \, dx + \frac{i\pi}{4}} \quad (\text{incident})$$

$$+ \frac{1}{\sqrt{v}} e^{-\frac{i}{\hbar} \int_a^x p \, dx - \frac{i\pi}{4}} \quad (\text{reflected})$$

$$x > b: \quad \psi = \left[\frac{D}{v} \right]^{\frac{1}{2}} e^{\frac{i}{\hbar} \int_b^x p \, dx + \frac{i\pi}{4}} \quad (\text{transmitted}) \tag{2}$$

where D is the density of flux in the transmitted wave, $p = \sqrt{2m[E - U(x)]}$, and $v(x) = p/m$. The incident wave is normalized to unit flux density and so D coincides with the transmission coefficient. It is given by:

$$D(E) = e^{-\frac{2}{\hbar} \int_a^b |p| \, dx} = e^{-\frac{2}{\hbar} \int_a^b \sqrt{2m[U(x) - E]} \, dx} \tag{3}$$

Inside the barrier the wave function is of the form†

$$a < x < b: \quad \psi = \left[\frac{D}{v} \right]^{\frac{1}{2}} e^{\frac{1}{\hbar} \left| \int_x^b p \, dx \right|} = \left[\frac{1}{v} \right]^{\frac{1}{2}} e^{-\frac{1}{\hbar} \left| \int_a^x p \, dx \right|} \tag{4}$$

Example: Parabolic barrier $U(x) = -\frac{1}{2}\kappa x^2$. Take $E = -\frac{1}{2}\kappa a^2$. Equation (3) gives:

$$D = e^{-\frac{4}{\hbar} \int_0^a \sqrt{m\kappa(a^2 - x^2)} \, dx} = e^{-\frac{\pi}{\hbar} a^2 \sqrt{m\kappa}} \equiv e^{\frac{2\pi E}{\hbar\omega}}, \quad \text{where } \omega \equiv \sqrt{\kappa/m} \tag{5}$$

The parabolic potential barrier admits of an exact solution (see L&L, §50, not a quasi-classical approximation), valid for arbitrary values of E , including $E > 0$ (above-barrier transmission):

† Following Landau and Lifshitz, I placed the absolute value bars outside the integral in Eq. (4), rather than inside as in (3). This is perhaps to emphasize that the inside the barrier there may be regions where p is real and regions where p is imaginary, so that $\left| \int \dots \right| \neq \int | \dots |$. I am not sure if that is what L&L had in mind; but in ordinary barriers the phase of p is not varying (always $\pi/2$) and one would not make a distinction between $\left| \int \dots \right|$ and $\int | \dots |$.

$$D = \frac{1}{1 + e^{-2\pi\varepsilon}}, \quad \text{where } \varepsilon \equiv \frac{E}{\hbar\omega}. \quad (6)$$

Obviously, the exact solution agrees with (5) for a large negative E . Equation (6) can be used when considering tunneling near the top of any smooth barrier. Thus, consider a band-bending curve between the source and the drain of a short-channel (length L) field-effect transistor. Suppose, we know only the height of the barrier ϕ_p relative to the source and the source-drain bias V . Assuming

$$\phi(x) = -\frac{1}{2} \kappa (x - x_p)^2, \quad (7)$$

we can express κ and x_p in the form:

$$x_p = \frac{L \phi_p}{V} [(1 + V/\phi_p)^{1/2} - 1]; \quad \kappa = \frac{2\phi_p}{x_p^2}. \quad (8)$$

Lateral tunneling current between two 2-dimensional gases. Let θ be the angle between the incident \mathbf{k} and the direction normal to the barrier. If E is the total energy of incident particle then the transmission coefficient equals $D(E \cos^2 \theta)$, where $D(E)$ is given by Eq. (3). The current J per unit width of the source is given by

$$J = \frac{eE_F \sqrt{2m E_F}}{\pi^2 \hbar^2} \int_0^1 du \sqrt{1-u} D(uE_F), \quad (9)$$

$$\frac{eE_F \sqrt{2m E_F}}{\pi^2 \hbar^2} = 4.00 \frac{\text{mA}}{\text{mm}} \left[\frac{m}{m_0} \right]^{1/2} \left[\frac{E_F}{[1 \text{ meV}]} \right]^{3/2}$$

where E_F is the Fermi energy. In equilibrium, an equal and opposite current flows from the drain electrode. If δV is an infinitesimal drain voltage, then $J = G \delta V$ and the conductance G per unit source width in equilibrium is

$$G \equiv \frac{\partial J}{\partial V} = \frac{e^2 \sqrt{2m E_F}}{\pi^2 \hbar^2} \int_0^1 du D[E_F(1-u^2)]. \quad (10)$$

Analogous formulae for tunneling between two 3D electron gases. Current J per unit area of the diode:

$$J = \frac{em}{2\pi^2 \hbar^3} \int_0^{E_F} dE \int_0^E D(\xi) d\xi = \frac{em}{2\pi^2 \hbar^3} \int_0^{E_F} (E_F - E) D(E) dE. \quad (11)$$

Equilibrium conductance per unit area:

$$G = \frac{e^2 m}{2\pi^2 \hbar^3} \int_0^{E_F} D(E) dE. \quad (12)$$

Derivation of Eqs. (9) and (10):

$$n [\text{cm}^{-2}] = \frac{2}{(2\pi)^2} \int_0^{k_F} k dk \int_{-\pi}^{\pi} d\theta .$$

The linear current density is $\int e n(\mathbf{k}) v(\mathbf{k}) D(\mathbf{k})$:

$$\begin{aligned} J &= \frac{e}{2\pi^2} \int_{-\pi/2}^{\pi/2} \cos\theta d\theta \int_0^{k_F} k dk \frac{\hbar k}{m} D\left[\frac{\hbar^2 k^2 \cos^2\theta}{2m}\right] \\ &= \frac{e}{2\pi^2 \hbar^2} \int_{-\pi/2}^{\pi/2} \cos\theta d\theta \int_0^{E_F} \sqrt{2mE} D(E \cos^2\theta) dE \quad \text{set } x = E \cos^2\theta \quad (*) \\ &= \frac{e}{2\pi^2 \hbar^2} \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\cos^2\theta} \int_0^{E_F \cos^2\theta} \sqrt{2m x} D(x) dx \quad \text{integrate by parts} \\ &= \frac{e}{2\pi^2 \hbar^2} \int_{-\pi/2}^{\pi/2} d\theta \tan\theta E_F 2 \cos\theta \sin\theta \sqrt{2m E_F \cos^2\theta} D(E_F \cos^2\theta) dx \\ &= \frac{e E_F \sqrt{2m E_F}}{\pi^2 \hbar^2} \int_{-1}^1 dt t^2 D[E_F(1-t^2)] = \frac{e E_F \sqrt{2m E_F}}{\pi^2 \hbar^2} \int_0^1 du \sqrt{1-u} D(u E_F) \end{aligned}$$

Differentiating this equation in the form (*) with respect to E_F , we arrive at Eq. (10). Derivation of Eq. (11)[†] is quite similar:

$$\begin{aligned} n [\text{cm}^{-3}] &= \frac{2}{(2\pi)^3} \int_0^{k_F} k^2 dk \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \\ J &= \frac{2e 2\pi}{(2\pi)^3} \int_0^{k_F} k^2 dk \frac{\hbar k}{m} \int_0^{\pi/2} \sin\theta d\theta \cos\theta D\left[\frac{\hbar^2 k^2 \cos^2\theta}{2m}\right] \\ &= \frac{em}{2\hbar^3 \pi^2} \int_0^{E_F} E dE \int_0^1 dx D(xE) = \frac{em}{2\pi^2 \hbar^3} \int_0^{E_F} dE \int_0^E dx D(x) \quad (**) \\ &= \frac{em E_F^2}{2\pi^2 \hbar^3} \int_0^1 (1-u) D(u E_F) du . \end{aligned}$$

Transition between two last lines is obtained via integration by parts.

In 1D case, $n [\text{cm}^{-1}] = (2/2\pi) \int_0^{k_F} dk$, and

$$J = \frac{e}{\pi \hbar} \int_0^{E_F} dE D(E) ; \quad G = \frac{e^2}{\pi \hbar} D(E_F) ,$$

in agreement with the Landauer formula (for two spin channels).

[†] The result agrees with that quoted by A. A. Grinberg and S. Luryi, "Fine structure in the energy dependence of current density and oscillations in the current-voltage characteristics of tunnel junctions", *Phys. Rev. B* **42**, 1705-1712 (1990)

Example: parabolic barrier: peak at x_p ; peak energy relative to energy at $x=0$ is ϕ_p . Therefore, energy E ranges from 0 to E_F and $\varepsilon \equiv (E - \phi_p)/\hbar\omega$. Assuming that $|2\pi\varepsilon_F| \gg 1$, we can use Eq. (5) rather than (6):

$$D = e^{2\pi(E - \phi_p)/\hbar\omega} \quad (13)$$

Substitute (13) in Eq. (9) and integrate (neglecting E_F compared to ϕ_p):

$$J = \frac{2eE_F\sqrt{2mE_F}}{3\pi^2\hbar^2} e^{-\frac{2\pi\phi_p}{\hbar\omega}} = \frac{2eE_F\sqrt{2mE_F}}{3\pi^2\hbar^2} e^{-\frac{\pi}{\hbar}\sqrt{2m\phi_p}x_p}.$$

Finite temperature: In a 3D case (and, of course, 1D case too) it is possible to reduce the current density to one quadrature also at finite temperatures. Equation (11) is replaced by

$$J = \frac{em}{2\pi^2\hbar^3} \int_0^\infty \Phi(E, E_F, T) D(E) dE, \quad (14)$$

where

$$\Phi(E, E_F, T) \equiv kT \ln \left[1 + e^{\frac{E_F - E}{kT}} \right]. \quad (15)$$

Derivation: Note that the function (15) is an indefinite integral of the Fermi function:

$$f(E) \equiv \frac{1}{1 + e^{(E - E_F)/kT}} = -\frac{d\Phi}{dE}.$$

Rewrite formula (**) on p. 3 in the form

$$J = \frac{em}{2\pi^2\hbar^3} \int_0^\infty f(E) dE \int_0^E dx D(x) = \frac{em}{2\pi^2\hbar^3} \int_0^\infty d\Phi \int_0^E dx D(x)$$

and integrate by parts, noting that $\Phi(E)$ vanishes as $E \rightarrow \infty$. At low temperatures, Eq. (14) goes over into (11) since

$$\Phi(E, E_F, T) \xrightarrow{T \rightarrow 0} (E_F - E) \Theta(E_F - E),$$

where $\Theta(x)$ is the step function ($\Theta=0$ for $x < 0$ and $\Theta=1$ otherwise).

Tunneling into a quantum well: In this case the transmission coefficient can be written in the form:

$$D(E) = 2\pi\hbar v(E) \delta(E - E_0), \quad (16)$$

where $v(E)$ has the dimensionality sec^{-1} and describes the tunneling rate into a discrete level in a 1D problem (see the example on next page). Substituting (16) into (14), we have

$$J = \frac{em}{\pi\hbar^2} \Phi(E_0, E_F, T) v(E_0) \Theta(E_0). \quad (17)$$

Payne† has calculated the current into (or out of) a 1D quantum well of size a bounded by rectangular barriers of thickness b and height U . His result is of the form:

$$j_{1 \rightarrow \text{QW}} = 2e v(E_0) [f_1(E_0) - f_{\text{QW}}(E_0)], \quad (18)$$

where

$$v(E) = \frac{8 [E(U - E)]^{3/2}}{U^2 [\hbar + a \sqrt{m(U - E)}]} e^{-2b \sqrt{2m(U - E)}} \quad (19)$$

(I have included the spin degeneracy factor of 2, omitted by Payne). Defining $D(E)$ as in Eq. (16), and calculating the 1D current by

$$j_{1 \rightarrow \text{QW}} = \int_0^\infty dE D(E) [f_1(E) - f_{\text{QW}}(E)],$$

we arrive at Payne's formula (provided $E_0 > 0$). Since our derivation of Eq. (14) was unrestricted to any particular form of the transmission coefficient, we can use $D(E) = 2\pi\hbar v(E) \delta(E - E_0)$ in Eq. (14). This leads to the following result (In Eq. 17, we had omitted the reverse flux) for the net current density:

$$J_{1 \rightarrow \text{QW}} = \frac{em}{\pi\hbar^2} v_1(E_0) \Theta_1(E_0) kT \ln \frac{1 + e^{(E_F^{(1)} - E_0)/kT}}{1 + e^{(E_F^{(\text{QW})} - E_0)/kT}}, \quad (20)$$

Similarly, for the tunneling current out of the well:

$$J_{\text{QW} \rightarrow 2} = \frac{em}{\pi\hbar^2} v_2(E_0) \Theta_2(E_0) kT \ln \frac{1 + e^{(E_F^{(\text{QW})} - E_0)/kT}}{1 + e^{(E_F^{(2)} - E_0)/kT}}, \quad (21)$$

where the functions $\Theta_{1,2}$ are the step functions relative to the conduction-band edge $E_C^{(1,2)}$ in the respective electrode, $\Theta_i(E) \equiv \Theta(E - E_C^{(i)})$, and $v_1(E)$ and $v_2(E)$ are the tunneling rates through the emitter and the collector barriers, respectively. A reasonable approximation for the tunneling rates v_i is to take them in the form (19) with both U and E defined relative to the conduction band edge in the respective electrode. The magnitude of U should be replaced by the average barrier heights U_1 and U_2 , see the Figure.

To include transitions through the second level in the QW, we add to Eq. (20) another term which has E_0 replaced by E_1 . No harm will be done if we add a similar term to Eq. (21), but this term is small because in our model the level E_1 is not appreciably populated.

The sheet charge density inside the quantum well σ satisfies

$$\frac{d\sigma}{dt} = J_{1 \rightarrow \text{QW}} - J_{\text{QW} \rightarrow 2}, \quad (22)$$

(the current continuity equation); also from Gauss' law we have

$$\frac{\sigma}{\epsilon} = F_2 - F_1 \quad (23)$$

where F_1 and F_2 are the electric fields in the barriers 1 and 2, respectively.

† M. C. Payne, "Transfer Hamiltonian description of resonant tunneling", *J. Phys. C* **19**, 1145-1155 (1986)

Energy levels in the potential well of width a bounded by the barriers of height U_1 and U_2 are given by, approximately:

$$E_n = \frac{\pi^2 \hbar^2 (n+1)^2}{2ma^2} (1 - \sqrt{2\hbar^2/ma^2 U_1} - \sqrt{2\hbar^2/ma^2 U_2}), \quad n = 0, 1, \dots \quad (24)$$

This formula is valid for low-lying levels in the limit $ma^2 U_{1,2} \hbar^2 \gg 1$. Corrections due to a non-flat potential $\delta V(x)$ inside the well, calculated quasi-classically, are the same for all levels:

$$\delta E_n = \frac{1}{a} \int_{-a/2}^{a/2} \delta V dx = \frac{e \sigma}{\varepsilon} \frac{a^2}{8}, \quad (25)$$

where the last expression is obtained assuming all the QW charge placed in the middle of the well. Note that if δV is expanded in the Taylor series about the midpoint of the well, then only even powers of x will contribute a correction. This would be also true in a rigorous (non-quasiclassical) perturbation calculation: the unperturbed wave functions have a definite parity with respect to reflections in the midplane and hence the expectation values of odd powers of x vanish.

Distribution inside QW. Expression (20) above is written on the assumption that the density of electrons in the QW is given by the equilibrium statistics, characterized by a Fermi level $E_F^{(QW)}$:

$$\frac{d\sigma}{dE} = \frac{em}{\pi\hbar^2} f_{QW}(E) \quad \rightarrow \quad \sigma = \frac{em}{\pi\hbar^2} \Phi(E_0, E_F^{(QW)}, T). \quad (26)$$

This is undoubtedly a good approximation near equilibrium, when $E_F^{(1)} - E_F^{(QW)} \leq kT$, and, generally, when the inelastic scattering time τ_{in} inside QW is short, $\tau_{in} v_{1,2}(E_0) \ll 1$ (e.g., for thick and high barriers). In this case, Eq. (22) becomes an equation for $E_F^{(QW)}(t)$:

$$\frac{d\sigma}{dt} = \frac{em}{\pi\hbar^2} f_{QW}(E_0) \frac{E_F^{(QW)}}{dt} = J_{1 \rightarrow QW}(E_F^{(QW)}) - J_{QW \rightarrow 2}(E_F^{(QW)}). \quad (27)$$

In the opposite limit, $\tau_{in} v_{1,2}(E_0) \gg 1$, a better approximation is to assume a "friable" distribution in the QW, that replicates the distribution in the emitter – multiplied by a filling factor $\xi < 1$:

$$\frac{d\sigma}{dE} = \frac{em}{\pi\hbar^2} \xi f_1(E) \quad \rightarrow \quad \sigma = \frac{em}{\pi\hbar^2} \xi \Phi(E_0, E_F^{(1)}, T). \quad (28)$$

In this case, Eqs. (20) and (22) will be replaced by

$$J_{1 \rightarrow QW} = \frac{em}{\pi\hbar^2} \left[v_1(E_0) \Theta(E_0) \Phi(E_0, E_F^{(1)}, T) (1 - \xi) \right], \quad (29)$$

$$J_{QW \rightarrow 2} = \frac{em}{\pi\hbar^2} \left[v_2(E_0) \Theta(E_0) [\xi \Phi(E_0, E_F^{(1)}, T) - \Phi(E_0, E_F^{(2)}, T)] \right].$$

Equation (22) thus becomes an equation for $\xi(t)$.

Procedure:

Setting $d\sigma/dt = 0$ in Eq. (22) determines the unknown parameter $E_F^{(QW)}$. All quantities of interest can be expressed in terms of $E_F^{(QW)}$.

$$\sigma = \frac{em}{\pi\hbar^2} \left[\Phi(E_0, E_F^{(QW)}, T) + \Phi(E_1, E_F^{(QW)}, T) \right].$$

1. Calculate the potential distribution in the absence of tunneling (only thermionic leakage). Express F_1 and F_2 in terms of $E_F^{(QW)}$.

2. Determine the effective emitter barrier height and the energy levels relative to the conduction band edge in the emitter:

$$U_1 = U_1^{(0)} - eF_1 \frac{b_1}{2};$$

$$E_0 = \frac{\pi^2\hbar^2}{2ma^2} \left(1 - \sqrt{2\hbar^2/ma^2 U_1} - \sqrt{2\hbar^2/ma^2 U_2} \right) - F_1 (b_1 + a/2) + \frac{e\sigma}{\varepsilon} \frac{a^2}{8};$$

$$E_1 = \frac{4\pi^2\hbar^2}{2ma^2} \left(1 - \sqrt{2\hbar^2/ma^2 U_1} - \sqrt{2\hbar^2/ma^2 U_2} \right) - F_1 (b_1 + a/2) + \frac{e\sigma}{\varepsilon} \frac{a^2}{8}.$$

3. Calculate the tunneling rates $v_1(E_0)$ and $v_1(E_1)$ from Eq. (19), substituting U_1 for U .

4. Calculate $J_{1 \rightarrow QW}$, taking into account tunneling into both levels E_0 and E_1 :

$$J_{1 \rightarrow QW} = \frac{em}{\pi\hbar^2} \left[v_1(E_0) \Theta(E_0) [\Phi(E_0, E_F^{(1)}, T) - \Phi(E_0, E_F^{(QW)}, T)] + v_1(E_1) \Theta(E_1) [\Phi(E_1, E_F^{(1)}, T) - \Phi(E_1, E_F^{(QW)}, T)] \right].$$

5. Determine the effective collector barrier height and the energy levels relative to the conduction band edge in the collector:

$$U_2 = U_2^{(0)} + eF_2 \frac{b_2}{2};$$

$$E_0 = \frac{\pi^2\hbar^2}{2ma^2} \left(1 - \sqrt{2\hbar^2/ma^2 U_1} - \sqrt{2\hbar^2/ma^2 U_2} \right) + F_2 (b_2 + a/2) + \frac{e\sigma}{\varepsilon} \frac{a^2}{8};$$

$$E_1 = \frac{4\pi^2\hbar^2}{2ma^2} \left(1 - \sqrt{2\hbar^2/ma^2 U_1} - \sqrt{2\hbar^2/ma^2 U_2} \right) + F_2 (b_2 + a/2) + \frac{e\sigma}{\varepsilon} \frac{a^2}{8}.$$

6. Calculate the tunneling rates $v_2(E_0)$ and $v_2(E_1)$ from Eq. (19), substituting U_2 for U .

7. Calculate $J_{QW \rightarrow 2}$, taking into account tunneling from both levels E_0 and E_1 :

$$J_{QW \rightarrow 2} = \frac{em}{\pi\hbar^2} \left[v_2(E_0) \Theta(E_0) [\Phi(E_0, E_F^{(QW)}, T) - \Phi(E_0, E_F^{(2)}, T)] + v_2(E_1) \Theta(E_1) [\Phi(E_1, E_F^{(QW)}, T) - \Phi(E_1, E_F^{(2)}, T)] \right].$$