

## 12. Appendix G - Special Derivations

These derivations are for electrons only. The same techniques will yield the corresponding equations for holes. All temperatures are electron temperatures and all masses are electron density of states masses.

### 12.1 Derivation 1 - Free Carrier Quantum Well Concentration

$$n_f = \int_{E_c + E_{c,top}}^{\infty} \left[ \frac{1}{2p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_c)^{\frac{1}{2}} - \frac{m}{p\hbar^2 L_{qw}} \right] \frac{1}{1 + e^{(E - E_{fn})/kT}} dE$$

Assuming Boltzmann statistics and let:

$$h = (E - E_c)/kT \quad h_c = (E_{fn} - E_c)/kT$$

yields:

$$n_f = e^{h_c} \int_{E_{c,top}/kT}^{\infty} \left[ \frac{1}{2p^2} \left( \frac{2mkT}{\hbar^2} \right)^{\frac{3}{2}} h^{\frac{1}{2}} - \frac{mkT}{p\hbar^2 L_{qw}} \right] e^{-h} dh$$

$$n_f = e^{h_c} \left[ \int_0^{\infty} \frac{2}{\sqrt{p}} N_c h^{\frac{1}{2}} e^{-h} dh - \int_0^{E_{c,top}/kT} \frac{2}{\sqrt{p}} N_c h^{\frac{1}{2}} e^{-h} dh - \int_{E_{c,top}/kT_n}^{\infty} \frac{N_{cqw}}{L_{qw}} e^{-h} dh \right]$$

$$n_f = e^{h_c} \left[ N_c \left( 1 - \frac{2}{\sqrt{p}} \frac{E_{c,top}}{kT} \right) - \frac{N_{cqw}}{L_{qw}} e^{-\frac{E_{c,top}}{kT}} \right]$$

### 12.2 Derivation 2 - Fermi-Dirac Thermionic Emission Current

$$\mathbf{J}_{n \rightarrow +}^{therm} = -q \int_{U_{c-}}^{\infty} \mathbf{v}_x g(E) f(E) dE$$

let:

$$h_c = (E_{fn} - E_c)/kT \quad E - E_c = \frac{1}{2} m \mathbf{v}^2 \quad dE = m \mathbf{v} d\mathbf{v}$$

then:

$$\mathbf{J}_{n \rightarrow +}^{therm} = -q \frac{1}{2p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_{U_{c-}}^{\infty} \frac{\mathbf{v}_x (E - E_c)^{\frac{1}{2}}}{1 + e^{(E - E_c)/kT - h_c}} dE$$

$$\mathbf{J}_{n \rightarrow +}^{therm} = -q \frac{1}{2p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{\frac{m}{2}} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \frac{\mathbf{v}_x \mathbf{v}^2}{1 + e^{m\mathbf{v}^2/2kT - h_c}} d\mathbf{v}$$

Convert from spherical to cylindrical coordinates:

$$\mathbf{J}_{n \rightarrow +}^{therm} = -q \frac{1}{4p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{\frac{m}{2}} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \int_0^{\infty} \frac{\mathbf{v}_x \mathbf{v}_{yz} e^{-m\mathbf{v}_{yz}^2/2kT}}{e^{-m\mathbf{v}_{yz}^2/2kT} + e^{m\mathbf{v}_x^2/2kT - h_c}} d\mathbf{v}_{yz} d\mathbf{v}_x$$

let:

$$y = e^{-m\mathbf{v}_{yz}^2/2kT} \quad dy = -\frac{m\mathbf{v}_{yz}}{kT} e^{-m\mathbf{v}_{yz}^2/2kT} d\mathbf{v}_{yz}$$

then:

$$\mathbf{J}_{n \rightarrow +}^{therm} = -q \frac{1}{4p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{\frac{m}{2}} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \int_1^0 \frac{-\frac{kT}{m} \mathbf{v}_x}{y + e^{m\mathbf{v}_x^2/2kT - h_c}} dy d\mathbf{v}_x$$

$$\mathbf{J}_{n \rightarrow +}^{therm} = -q \frac{1}{4p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{\frac{m}{2}} kT \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \mathbf{v}_x \ln(1 + e^{h_c - m\mathbf{v}_x^2/2kT}) d\mathbf{v}_x$$

let:

$$E_x = \frac{1}{2} m \mathbf{v}_x^2 \quad \mathbf{v}_x = \sqrt{\frac{2E_x}{m}} \quad d\mathbf{v}_x = \frac{1}{\sqrt{2mE_x}} dE_x$$

then:

$$\mathbf{J}_{n \rightarrow +}^{therm} = -A_n^* \frac{T}{k} \int_{U_{c-}}^{\infty} \ln(1 + e^{h_c - E_x/kT}) dE_x$$

This is the equation for tunneling current (include transmission probability).

let:

$$A = \frac{E_x}{kT} - h_c \quad E_x = kT(A + h_c) \quad dE_x = kT dA$$

then:

$$\mathbf{J}_{n \rightarrow +}^{therm} = -A_n^* T^2 \int_{\frac{U_{c-}}{kT} - h_c}^{\infty} \ln(1 + e^{-A}) dA$$

let:

$$z = -e^{-A} \quad dz = e^{-A} dA$$

$$\mathbf{J}_{n \rightarrow +}^{therm} = -A_n^* T^2 \int_0^{-e^{h_c - U_{c-}/kT}} \frac{\ln(1 - z)}{z} dz$$

$$\mathbf{J}_{n \rightarrow +}^{therm} = -A_n^* T^2 \text{Li}_2\left(-e^{h_c - U_{c-}/kT}\right)$$

Considerable algebra yields:

$$\mathbf{J}_{n \rightarrow +}^{therm} = -A_n^* T^2 \left\{ \text{Li}_2\left(\frac{1}{1 + e^{U_{c-}/kT - h_c}}\right) + \frac{1}{2} \left[ \ln(1 + e^{h_c - U_{c-}/kT}) \right]^2 \right\}$$

### 12.3 Derivation 3 - Boltzmann Thermionic Emission Energy Flux

$$\mathbf{S}_{n \rightarrow +}^{therm} = \int_{U_{c-}}^{\infty} \mathbf{v}_x (E - E_c) g(E) f(E) dE$$

let:

$$h_c = (E_{fn} - E_c)/kT \quad E - E_c = \frac{1}{2} m \mathbf{v}^2 \quad dE = m \mathbf{v} d\mathbf{v}$$

then assuming Boltzmann statistics:

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{1}{2p^2} \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} e^{h_c} \int_{U_{c-}}^{\infty} \mathbf{v}_x (E - E_c)^{\frac{3}{2}} e^{-(E - E_c)/kT} dE$$

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{1}{2p^2} \left(\frac{2m}{h^2}\right)^{\frac{3}{2}} \left(\frac{m}{2}\right)^{\frac{3}{2}} m e^{h_c} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \mathbf{v}_x e^{-m\mathbf{v}^2/2kT} \mathbf{v}^4 d\mathbf{v}$$

Convert to cylindrical coordinates:

$$S_{n \rightarrow +}^{therm} = \frac{m^4}{4\hbar^3 p^2} e^{h_c} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \int_0^{\infty} \mathbf{v}_x \mathbf{v}_{yz} (\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) e^{-m(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)/2kT} d\mathbf{v}_{yz} d\mathbf{v}_x$$

let:

$$a = \frac{m}{2kT}$$

then:

$$S_{n \rightarrow +}^{therm} = \frac{m^4}{4\hbar^3 p^2} e^{h_c} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \left( -\frac{\mathbf{v}_x}{2a^2} - \frac{\mathbf{v}_x (\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)}{2a} \right) e^{-a(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)} \Big|_0^{\infty} d\mathbf{v}_x$$

$$S_{n \rightarrow +}^{therm} = \frac{m^3 kT}{4\hbar^3 p^2} e^{h_c} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \left( \frac{\mathbf{v}_x}{a} + \mathbf{v}_x^3 \right) e^{-a\mathbf{v}_x^2} d\mathbf{v}_x$$

This equation can be converted into the Boltzmann tunneling energy flux.

$$S_{n \rightarrow +}^{therm} = \frac{m^3 kT}{4\hbar^3 p^2} e^{h_c} \left( -\frac{1}{a^2} - \frac{\mathbf{v}_x^2}{2a} \right) e^{-a\mathbf{v}_x^2} \Big|_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty}$$

$$S_{n \rightarrow +}^{therm} = \frac{m(kT)^2}{2\hbar^3 p^2} e^{h_c} (2kT + U_{c-}) e^{-U_{c-}/kT}$$

$$S_{n \rightarrow +}^{therm} = \frac{A_n^* kT^3}{q} \left( 2 + \frac{U_{c-}}{kT} \right) e^{h_c - U_{c-}/kT}$$

## 12.4 Derivation 4 - Fermi-Dirac Thermionic Emission Energy Flux

$$S_{n \rightarrow +}^{therm} = \int_{U_{c-}}^{\infty} \mathbf{v}_x (E - E_c) g(E) f(E) dE$$

let:

$$h_c = (E_{fn} - E_c)/kT \quad E - E_c = \frac{1}{2} m \mathbf{v}^2 \quad dE = m \mathbf{v} d\mathbf{v}$$

then:

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{1}{2p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_{U_{c-}}^{\infty} \frac{\mathbf{v}_x (E - E_c)^{\frac{3}{2}}}{1 + e^{(E - E_c)/kT - h_c}} dE$$

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{1}{2p^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \left( \frac{m}{2} \right)^{\frac{3}{2}} m \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \frac{\mathbf{v}_x \mathbf{v}^4}{1 + e^{m\mathbf{v}^2/2kT - h_c}} d\mathbf{v}$$

Convert to cylindrical coordinates:

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m^4}{4\hbar^3 p^2} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \int_0^{\infty} \frac{\mathbf{v}_x \mathbf{v}_{yz} (\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)}{1 + e^{m(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)/2kT - h_c}} d\mathbf{v}_{yz} d\mathbf{v}_x$$

let:

$$a = \frac{m}{2kT}$$

then:

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m^4}{4\hbar^3 p^2} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \frac{\mathbf{v}_x}{2} \left\{ \frac{(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)^2}{2} - \frac{(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) \ln \left( 1 + e^{a(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) - h_c} \right)}{a} \right. \\ \left. - \frac{1}{a^2} \text{Li}_2 \left( -e^{a(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) - h_c} \right) \right\} \Bigg|_0^{\infty} d\mathbf{v}_x$$

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m^4}{4\hbar^3 p^2} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \frac{\mathbf{v}_x}{2} \left\{ \frac{(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2)^2}{2} - \frac{(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) \ln \left( 1 + e^{a(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) - h_c} \right)}{a} \right. \\ \left. - \frac{1}{a^2} \text{Li}_2 \left( -e^{a(\mathbf{v}_x^2 + \mathbf{v}_{yz}^2) - h_c} \right) \right\} \Bigg|_0^{\infty} d\mathbf{v}_x$$

Considerable algebra to show that:

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m^2 (kT)^2}{4\hbar^3 p^2} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \mathbf{v}_x \left\{ h_c^2 + \frac{p^2}{3} - \ln^2 \left( e^{-a\mathbf{v}_x^2} + e^{-h_c} \right) - 2 \text{Li}_2 \left( \frac{1}{1 + e^{h_c - a\mathbf{v}_x^2}} \right) \right\} d\mathbf{v}_x$$

This equation can be converted into the Fermi-Dirac tunneling energy flux.

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m^2 (kT)^2}{4\hbar^3 \mathbf{p}^2} \int_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty} \mathbf{v}_x \left\{ \begin{aligned} &\mathbf{h}_c^2 + \frac{\mathbf{p}^2}{3} - a^2 \mathbf{v}_x^4 + 2a \mathbf{v}_x^2 \ln^2(1 + e^{a\mathbf{v}_x^2 - \mathbf{h}_c}) \\ &+ 2 \text{Li}_2(-e^{a\mathbf{v}_x^2 - \mathbf{h}_c}) \end{aligned} \right\} d\mathbf{v}_x$$

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m^2 (kT)^2}{4\hbar^3 \mathbf{p}^2} \left\{ \left( \mathbf{h}_c^2 + \frac{\mathbf{p}^2}{3} \right) \frac{\mathbf{v}_x^2}{2} - \frac{a^2 \mathbf{v}_x^6}{6} - \mathbf{v}_x^2 \text{Li}_2(-e^{a\mathbf{v}_x^2 - \mathbf{h}_c}) + \frac{2}{a} \text{Li}_3(-e^{a\mathbf{v}_x^2 - \mathbf{h}_c}) \right\} \Bigg|_{\sqrt{\frac{2U_{c-}}{m}}}^{\infty}$$

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{m(kT)^2}{4\hbar^3 \mathbf{p}^2} \left\{ \left( \mathbf{h}_c^2 + \frac{\mathbf{p}^2}{3} \right) E - \frac{E^3}{3(kT)^2} - 2E \text{Li}_2(-e^{E/kT - \mathbf{h}_c}) + 4kT \text{Li}_3(-e^{E/kT - \mathbf{h}_c}) \right\} \Bigg|_{U_{c-}}^{\infty}$$

Large amount of algebra to show that this equation evaluated at infinity is:

$$\frac{2}{3} kT \mathbf{h}_c (\mathbf{h}_c^2 + \mathbf{p}^2)$$

Even more algebra to show that:

$$\mathbf{S}_{n \rightarrow +}^{therm} = \frac{A_n^* kT^3}{q} \left[ \begin{aligned} &2 \left\{ \text{Li}_3 \left( \frac{1}{1 + e^{U_{c-}/kT - \mathbf{h}_c}} \right) + \text{Li}_3 \left( \frac{1}{1 + e^{\mathbf{h}_c - U_{c-}/kT}} \right) - \text{Li}_3(1) \right\} \\ &+ \left( \frac{U_{c-}}{kT} \right) \text{Li}_2 \left( \frac{1}{1 + e^{U_{c-}/kT - \mathbf{h}_c}} \right) \\ &+ \frac{1}{3} \mathbf{h}_c (\mathbf{h}_c^2 + \mathbf{p}^2) - \left( \frac{U_{c-}}{kT} \right) \left( \frac{\mathbf{h}_c^2}{2} + \frac{\mathbf{p}^2}{3} \right) + \frac{1}{6} \left( \frac{U_{c-}}{kT} \right)^3 \\ &- \ln(1 + e^{U_{c-}/kT - \mathbf{h}_c}) \left\{ \begin{aligned} &\frac{2}{3} \ln^2(1 + e^{U_{c-}/kT - \mathbf{h}_c}) \\ &- \left( \frac{3}{2} \frac{U_{c-}}{kT} - \mathbf{h}_c \right) \ln(1 + e^{U_{c-}/kT - \mathbf{h}_c}) \\ &+ \left( \frac{U_{c-}}{kT} \left( \frac{U_{c-}}{kT} - \mathbf{h}_c \right) - \frac{\mathbf{p}^2}{3} \right) \end{aligned} \right\} \end{aligned} \right]$$