**Introduction**

This document gives a brief discussion about quasi-Fermi levels (QFLs), which are often referenced and used in semiconductor modeling but seldom receive sufficient coverage in a single document. I put together a few sources, highlights, and derivations so that other readers can explore QFLs and decide if their use is right for their own application. It is important both to understand the math behind QFLs and know how to avoid misuse. The level of detail in this document is aimed at those who are using drift-diffusion style models of carrier transport in semiconductors and who are already familiar with Fermi levels and band gaps.

**What is a quasi-Fermi level?**

The use of Fermi levels in device engineering is widely established and accepted, and is nearly essential in understanding device physics in equilibrium conditions. It is a highly useful property that a single number (the fermi level) can describe an entire probability distribution.

[graphics and equations can go here in a later edition]

The Fermi level and the Fermi-Dirac distribution together describe the equilibrium conditions of a semiconductor. Once thermal equilibrium is disrupted by the application of bias or temperature, the Fermi level no longer describes the concentration of electrons and holes. Instead, these concentrations can be described by a pair of quasi-Fermi levels (QFLs), which are independent of each other and exist within the band gap for non-degenerate semiconductors.

In my limited research, the earliest reference I found to quasi-Fermi levels was in William Shockley’s 1949 paper called “The Theory of p-n Junctions in Semiconductors and p-n Junction Transistors.” The concept is not explicitly presented as novel, but it isn’t cited from another paper, so I can’t be sure if he originally came up with the idea. Shockley defines QFLs as

This is a similar form as presented in Siegfried Selberherr’s 1984 textbook called “Analysis and Simulation of Semiconductor Devices.” However in Selberherr’s form, the equation is presented with the intrinsic concentration ni replaced with an effective intrinsic concentration nie meant to fit “moderate heavy doping effects,” as he described them. Selberherr also uses slightly different terminology, with “quasi-Fermi potential” referring to phi in the equation, and “quasi-Fermi level” referring to a quantity with units of energy. I’ll use Shockley’s notation here.

Shockley’s equations can be reversed to give the QFL in terms of the potential psi and carrier concentration p and n.

QFLs are useful when graphing the band structure of a 1D device. Since QFLs rest within the band gap for non-degenerate semiconductors, they will bend along with the band edges as bias is applied across a semiconductor. Carrier concentrations normally cannot be plotted alongside the potential and band edges because they span many orders of magnitude, but QFLs serve as a useful visual stand-in for these values. Additionally, the gradient of the QFL can be used to describe the rate of flow of a particular type of charge carrier.

[later edition can show QFLs in a band gap]

To use QFLs with the drift-diffusion model, first the partial current densities Jp and Jn are given as

Where J is the current density in current per area, q is the unit charge, D is the diffusion coefficient for a carrier type, nabla is the gradient operator, p and n are carrier concentrations, psi is the potential, and µ is the carrier mobility. Subscripts p and n are implicit in the coefficents D and µ but are omitted for the sake of brevity.

The gradients of the carrier concentrations can be replaced with the following derivation:

This uses the chain rule to calculate the derivative (gradient) of an exponential function

These are then substituted into the current equations. For holes, the current relation is found as follows:

D can be removed if it is exchangeable with µ0 by the relation

The final form of the current equation is:

 For electrons, the current relation is given by:

D can be removed if it is exchangeable with µ0 by the relation

The final form of the current equation is:

Note that there are two forms to the current equation. The first form is a more general form which uses a carrier mobility µ which can vary with the magnitude of the electric field, as is commonly encountered in simulations. The mobility denoted as µ0 gives the value which can be found from Einstein’s relation. It describes the mobility when the electric field is very small.

In the special case where the electric field is small and µ=µ0, then

These are the forms which are generally cited in literature. However, they don’t mention the stipulation that Einstein’s relation must apply.

**Use of quasi-Fermi levels in simulations**

COMSOL’s semiconductor module enables the use of QFLs in its simulations. On page 28, the manual for this says “The quasi-Fermi level formulation use the quasi-Fermi levels as the dependent variable, instead of the carrier concentrations. This formulation is advantageous in some cases, for example for near-equilibrium systems at very low temperatures.”

Selberherr describes how to use QFLs in simulations and presents its several advantages, but concludes that he ultimately prefers to use the independent variables (ψ, n, p) over (ψ, ϕn, ϕp).

Some advantages mentioned are:

* “The gradient of the quasi-Fermi potential always points in the direction of the flow of the corresponding current density.”
* “the electric field and the gradient of the quasi-Fermi potentials are almost parallel in critical device areas.”

Drawbacks include:

* “Only to first order is the carrier transport driving force the gradient of the quasi Fermi potential. Away from equilibrium the electric field vector will become important.”
* “Higher order derivatives of the quasi-Fermi potentials have been neglected. This means that we transform a non-local solution of the Boltzmann equation into an approximate one depending only upon the local gradient of the quasi-Fermi potential.”

Ultimately, it seems that simulations with the drift-diffusion model are best left to tracking the carrier concentrations and electric potential. QFLs are a useful visual tool and can greatly simplify problems whenever the electric field is small, but whenever Einstein’s relation cannot be applied, then QFLs simply represent a change of coordinates and do not simplify the problem at all.