Evolution of Charge Carriers Through Time and Space

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***Abstract*—The physics underlying semiconductor devices must be understood to effectively design new devices and experiments. While equations can be provided to model phenomena such as propagation of carriers through a channel or device, or the evolution of current in the device with time, conducting the derivation of these equations from parent equations and phenomena may be highly informative. In this report, we present the derivation of equations for carrier concentrations as a function of time and space within a device; these equations are then used to model the behavior of charge carriers and the resulting current within a device. An app has been developed that allows for visualization and interaction with these equations. The app is available at https://pat-trinity-ralph-carrier-propagation-devicephysics-unm.streamlit.app/.**

I. Introduction

The current passing through a device, usually within a channel, controlled by a gate voltage within a MOSFET (Metal-Oxide-Semiconductor Field-Effect Transistor) is a critical parameter. The current is influenced by many factors, but principally arises from the movement of charge carriers, electrons and holes. Understanding and modeling this movement of carriers and thereby the current is necessary to informatively design a device. We therefore set out to derive the relevant equations.

II. Derivation of Carrier Concentration and Current

A. Green's Functions and Fourier Transform

We start with Green's functions for the partial derivatives of electrons and holes as functions of space and time, $n(x,t)$ and $p(x,t)$, respectively:

For electrons:

$$\frac{\partial^2 G_n(x,t)}{\partial x^2} - \left(\frac{\nu_n}{D_n}\right)\frac{\partial G_n(x,t)}{\partial x} + \frac{1}{D_n}\frac{\partial G_n(x,t)}{\partial t} + \frac{1}{\tau_n D_n}G_n(x,t) = \frac{1}{D_n}\,\delta(x-x_0)\,\delta(t-t_0)$$

For holes:

$$\frac{\partial^2 G_p(x,t)}{\partial x^2} - \left(\frac{\nu_p}{D_p}\right)\frac{\partial G_p(x,t)}{\partial x} + \frac{1}{D_p}\frac{\partial G_p(x,t)}{\partial t} + \frac{1}{\tau_p D_p}G_p(x,t) = \frac{1}{D_p}\,\delta(x-x_0)\,\delta(t-t_0)$$

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The generation terms, G_n and G_p, for electrons and holes respectively:

$$G_n = G_p = \left(\frac{P_0 N}{h\nu}\right)e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}$$

Were input to the above Green's equations, resulting in the equations below. For electrons:

$$\frac{\partial\left(\frac{P_0N}{h\nu}e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right)}{\partial x^2} - \left(\frac{\nu_n}{D_n}\right)\frac{\partial\left(\frac{P_0N}{h\nu}e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right)}{\partial x} + \frac{1}{D_n}\frac{\partial\left(\frac{P_0N}{h\nu}e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right)}{\partial t} + \frac{1}{\tau_n D_n}\left(\frac{P_0N}{h\nu}e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right) = \frac{1}{D_n}\,\delta(x-x_0)\,\delta(t-t_0)$$

For holes:

$$\frac{\partial^2\left(\frac{P_0N}{h\nu}\,e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right)}{\partial x^2} - \left(\frac{\nu_n}{D_n}\right)\frac{\partial\left(\frac{P_0N}{h\nu}\,e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right)}{\partial x} + \frac{1}{D_n}\frac{\partial\left(\frac{P_0N}{h\nu}\,e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right)}{\partial t} + \frac{1}{\tau_n D_n}\left(\frac{P_0N}{h\nu}\,e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}\,e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}\right) = \frac{1}{D_n}\,\delta(x-x_0)\,\delta(t-t_0)$$

We can define constants:

$$A = e^{-\frac{(t-t_0)^2}{\delta(t-t_0)}}B = e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}C = \frac{P_0N}{h\nu}$$

Rewriting the equation, initially focusing on the electron equation:

$$AC\frac{\partial(e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}})}{\partial x^2} - \left(\frac{\nu_n}{D_n}AC\right)\frac{\partial(e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}})}{\partial x} + \frac{1}{D_n}AC\frac{\partial(e^{-\frac{(x-x_0)^2}{\delta(x-x_0)}})}{\partial t} + \frac{1}{\tau_n D_n}ACe^{-\frac{(x-x_0)^2}{\delta(x-x_0)}}) = \frac{1}{Dn}\delta(x-x_0)\delta(t-t_0)$$

Breaking the equation into portions, we take advantage of the linearity property of the Fourier transform.

B. Fourier Transform

$$\mathcal{F}\left[C \cdot A \cdot \frac{\partial^2 B}{\partial x^2}\right]$$

We can then bring out the constants A and C, and take the fourier transform of B using the law of exponents.

$$C \cdot A \cdot \mathcal{F}\left[\frac{\partial^2}{\partial x^2}\left(e^{-\frac{2(x-x_0)}{\delta(x-x_0)}}\right)\right]$$

Defining a new constant, expanding the exponent and then taking the Fourier transform of the first section yields:

$$d = \frac{2}{\delta(x-x_0)}$$
$$C \cdot A \cdot e^{dx_0} \cdot \mathcal{F}\left[\frac{\partial^2}{\partial x^2}\left(e^{-dx}\right)\right]$$
$$C \cdot A \cdot e^{dx_0} \cdot [(jw)^2 \cdot \frac{2d}{d^2+\omega^2}]$$

Continuing the Fourier for the following sections and bringing them all together:

$$C \cdot \left(\frac{2d}{d^2+\omega^2}\right) \cdot$$
$$A \cdot \left(e^{dx_0}(j\omega)^2 - \frac{v_n}{D_n}(j\omega) + \frac{1}{D_n}\frac{\partial}{\partial t} + \frac{1}{\tau_n D_n}\right)$$
$$= \frac{1}{D_n} e^{-j\omega x_0} \delta(t-t_0)$$

C. Laplace Transform

Once the Fourier Transform was obtained for both equations, the Laplace Transform was taken to get $G_n(k,s)$ and $G_p(k,s)$.

$$G_n(j\omega, s) = \frac{\frac{1}{D_n * \sqrt{2\pi}} e^{-j\omega x_0}}{\left(e^{dx_0}(j\omega)^2 - \frac{v_n}{D_n}(j\omega) + \frac{s}{D_n} + \frac{1}{\tau_n D_n}\right)}$$

$$G_p(j\omega, s) = \frac{\frac{1}{D_p} e^{-j\omega x_0}}{\left(e^{dx_0}(j\omega)^2 - \frac{v_p}{D_p}(j\omega) + \frac{s}{D_p} + \frac{1}{\tau_p D_p}\right)}$$

The following expressions can be simplified by multiplying the denominator by D_n and D_p respectivly as well as $\frac{1}{\sqrt{2\pi}}$

$$G_n(k,s) = \frac{1}{\sqrt{2\pi}} * \frac{e^{-j\omega x_0}}{\cdot\left(D_n(k)^2 - v_n(k) + s + \frac{1}{\tau_n}\right)}$$

$$G_p(k,s) = \frac{1}{\sqrt{2\pi}} * \frac{e^{-j\omega x_0}}{\cdot\left(D_p(k)^2 - v_n(k) + s + \frac{1}{\tau_n}\right)}$$

D. Apply Inverse Laplace Transform

After applying the Fourier and Laplace transforms, we now have the following expressions:

$$G_n(k,s) = \frac{1}{\sqrt{2\pi}} \, \frac{e^{ikx_0}}{D_n k^2 - ik\nu_n + \frac{1}{\tau_n} + s}$$

$$G_p(k,s) = \frac{1}{\sqrt{2\pi}} \, \frac{e^{ikx_0}}{D_p k^2 + ik\nu_p + \frac{1}{\tau_p} + s}$$

These equations are valid but we desire to understand and model the charge carrier and current behavior within the real time and space domains. Therefore, we first convert back to the time domain by applying the inverse Laplace transform.

Define:

$$a \;=\; D_p\,k^2 \;+\; i\,k\,V_p \;+\; \frac{1}{\tau_p}$$

Since,

$$\mathcal{L}^{-1}\Big\{\frac{1}{s+a}\Big\}(t) = e^{-at}$$

The inverse Laplace transform of $G_p(k,s)$ is given by:

$$\mathcal{L}^{-1}\{G_p(k,s)\}(t) = \frac{1}{\sqrt{2\pi}}\, e^{ikx_0}\, \mathcal{L}^{-1}\Big\{\frac{1}{s+a}\Big\}(t)$$
$$= \frac{1}{\sqrt{2\pi}}\, e^{ikx_0}\, e^{-a\,t}$$

E. Inverse Fourier Transform

And now to convert back to space domain, we apply the inverse Fourier transform. We begin by defining $\alpha(t)$ to allow us to match the form of the inverse Fourier transform:

Define:

$$\alpha(t) = \frac{1}{2\pi}\frac{e^{-t/\tau_p}}{\sqrt{2\pi}}$$

Then,

$$g(x,t) = \alpha(t)\int_{-\infty}^{\infty} \exp\big[ikx_0 - D_p\,k^2\,t - i\,k\,\nu_p\,t\big] e^{ikx}\,dk$$
$$= \alpha(t)\int_{-\infty}^{\infty} \exp\big[-D_p\,t\,k^2 + k\,i(\nu_p\,t - x - x_0)\big]\,dk$$

To complete the square in the exponent, define the following constants **which are not the same as the previous definitions**:

$$A = D_p\,t$$

$$B = i(\nu_p\,t - x - x_0)$$

$$C = 0$$

so that

$$-D_p\,t\,k^2 + k\,i(\nu_p\,t - x - x_0) = -\big(A\,k^2 + B\,k + C\big)$$

Plugging into our expression above, we achieve:

$$g(x,t) = \alpha(t)\,\int_{-\infty}^{\infty} \exp\big[-\big(A\,k^2 + B\,k\big)\big]\,dk$$

Where,

$$\alpha(t) = \frac{e^{-t/\tau_p}}{\sqrt{2\pi}}, \quad A = D_p\, t, \quad B = i(\nu_p\, t - x - x_0)$$

The definition of "completing the square", or standard Gaussian-integral result is:

$$\int_{-\infty}^{\infty} e^{-\left(ax^2+bx+c\right)}\, dx \; = \; \sqrt{\frac{\pi}{a}}\; \exp\!\Big(\frac{b^2}{4a} - c\Big)$$

Plugging in all expressions for AB, C and $\alpha(t)$ and expanding results in:

$$G_n(x,t) = \frac{1}{2\pi\sqrt{2\, D_n\, t}} \exp\!\Big(-\frac{(x - x_0 - \nu_n\, t)^2 + \frac{t}{\tau_n}}{4\, D_n\, t}\Big),$$

$$G_p(x,t) = \frac{1}{2\pi\sqrt{2\, D_p\, t}} \exp\!\Big(-\frac{(x - x_0 + \nu_p\, t)^2 + \frac{t}{\tau_p}}{4\, D_p\, t}\Big)$$

Final Integration

In this step, we must integrate the generation terms, the result of the above, with the Source term, defined the same for holes and electrons as:

$$S_p = S_n = \frac{P_0\, \eta}{h\nu} \exp\!\Big[-\frac{(x-x_0)^2}{\sigma_x^2}\Big] \exp\!\Big[-\frac{(t-t_0)^2}{\sigma_t^2}\Big]$$

In fact, the delta function results in the exponents in the Source dropping out. This will be seen shortly.

From the above, we can reorganize the generation terms as:

$$G_n(x,t) = e^{-t/\tau_n} \sqrt{\frac{1}{4\pi\, D_n\, t}} \exp\!\Big[-\frac{\big(x - x_0 - \nu_n\, t\big)^2}{4\, D_n\, t}\Big],$$

$$G_p(x,t) = e^{-t/\tau_p} \sqrt{\frac{1}{4\pi\, D_p\, t}} \exp\!\Big[-\frac{\big(x - x_0 + \nu_p\, t\big)^2}{4\, D_p\, t}\Big]$$

The relevant delta function property is:

$$\int_{-\infty}^{\infty} f(x)\, \delta(x-a)\, dx = f(a)$$

Starting with the integration of G_n, which results in our expression for electron concentration as a function of space and time $n(x,t)$:

$$n(x,t) \; = \; \int Gn(x,t)\, S_n\, dx \; = \; \dots$$

Within the integral, we have:

$$\begin{aligned} G_n(x,t)\, S_n(x,t) = e^{-t/\tau_n} \sqrt{\frac{1}{4\pi\, D_n\, t}}\; \frac{P_0\, \eta}{h\nu} \\ \exp\!\Big[-\frac{(x - x_0 - \nu_n\, t)^2}{4\, D_n\, t}\Big] \\ \exp\!\Big[-\frac{(x-x_0)^2}{\sigma_x^2}\Big]\; \exp\!\Big[-\frac{(t-t_0)^2}{\sigma_t^2}\Big] \end{aligned}$$

However, latter two exponents drop out, because of the delta function property; if one inputs x_0 and t_0, these terms both become $exp(0)$ which goes to 1.

Therefore, the product of $G_n(x,t)$ and $S_n(x,t)$ becomes:

$$G_n(x,t)\, S_n(x,t) = e^{-t/\tau_n} \sqrt{\frac{1}{4\pi\, D_n\, t}}\; \frac{P_0\, \eta}{h\nu}\; \exp\!\Big[-\frac{(x - x_0 - \nu_n\, t)^2}{4\, D_n\, t}\Big]$$

The overall integral becomes:

$$\begin{aligned} n(x,t) &= \int G_n(x,t)\, S_n(x,t)\, dx \\ &= \int e^{-t/\tau_n} \sqrt{\frac{1}{4\pi\, D_n\, t}}\; \frac{P_0\, \eta}{h\nu}\; \exp\!\Big[-\frac{((x - x_0) - \nu_n\, t)^2}{4\, D_n\, t}\Big]\, dx \end{aligned}$$

Define:

$$\alpha \; = \; e^{-t/\tau_n} \sqrt{\frac{1}{4\pi\, D_n\, t}}\; \frac{P_0\, \eta}{h\nu}$$

Then the carrier density can be written as:

$$\begin{aligned} n(x,t) &= \int_x^{\infty} G_n(x,t)\, S_n(x)\, dx \\ &= \alpha \int_x^{\infty} \exp\!\Big[-\frac{((x - x_0) - \nu_n t)^2}{4\, D_n\, t}\Big]\, dx \end{aligned}$$

Where x and ∞ are defined as the bounds of a carrier; i.e. one can calculate the concentration from x_0 up to infinitely far from the x_0 location.

With this result, we now apply the power of a power rule, yielding:

Then the carrier density can be written as

$$= \alpha \int_x^{\infty} \exp\!\Big[-\frac{2((x - x_0) - \nu_n t)}{4\, D_n\, t}\Big]\, dx$$

We can factor out the $\nu_n\ t$ term, finally giving:

$$= \alpha \exp\!\left(\frac{2\nu t}{4 D_n t}\right) \int_x^{\infty} \exp\!\Big[-\frac{2(x - x_0)}{4\, D_n\, t}\Big]\, dx$$

This integral can be solved with u-substitution. Where

$$u = \frac{-2(x-x_0)}{4 D_n t}$$

and

$$du = -\frac{2}{4 D_n t} dx$$

And bounds are appropriately shifted, and defining constants, **again with different values than the previous definitions**:

$$u(\infty) \; = \; -\frac{2(\infty - x_0)}{4 D_n t} \implies -\infty \; = \; B$$

$$u(x) \; = \; -\frac{2(x - x_0)}{4 D_n t} \; = \; A$$

$$= \alpha\; \exp\!\Big(\frac{2\, \nu_n\, t}{4\, D_n\, t}\Big) \int_A^B e^{\,u}\, du$$

III. Results

A. Carrier Concentrations $n(x, t)$ and $p(x, t)$

Evaluating this integral and applying the power of a power rule again, we arrive at our final answer.

$$n(x,t) = \frac{P_0\,\eta}{h\nu}\,e^{-t/\tau_n}\,\sqrt{\frac{1}{4\pi\,D_n\,t}}\,\exp\Bigl[-\frac{\bigl((x-x_0)+\nu_n\,t\bigr)^2}{4\,D_n\,t}\Bigr]$$

Similarly for holes:

$$p(x,t) = \frac{P_0\,\eta}{h\nu}\,e^{-t/\tau_p}\,\sqrt{\frac{1}{4\pi\,D_p\,t}}\,\exp\Bigl[-\frac{\bigl((x-x_0)-\nu_p\,t\bigr)^2}{4\,D_p\,t}\Bigr]$$

B. Partial Derivatives of (n(x,t)) and (p(x,t))

After a **trivial** derivation involving the chain rule in (x), we find:

$$\frac{\partial n(x,t)}{\partial x} = -\frac{P_0\,\eta}{h\nu}\,e^{-t/\tau_n}\,\sqrt{\frac{1}{4\pi\,D_n\,t}}\,\frac{x-x_0+\nu_n\,t}{2\,D_n\,t}\,\exp\Bigl[-\frac{\bigl((x-x_0)+\nu_n\,t\bigr)^2}{4\,D_n\,t}\Bigr]$$

Similarly for holes,

$$\frac{\partial p(x,t)}{\partial x} = -\frac{P_0\,\eta}{h\nu}\,e^{-t/\tau_p}\,\sqrt{\frac{1}{4\pi\,D_p\,t}}\,\frac{x-x_0-\nu_p\,t}{2\,D_p\,t}\,\exp\Bigl[-\frac{\bigl((x-x_0)-\nu_p\,t\bigr)^2}{4\,D_p\,t}\Bigr]$$

We developed a Python-based web-app that plots these carrier concentrations and current, as dependent on their concentrations. The user can define many relevant parameters such as carrier mobilities or the strength of an applied electric field and observe these parameters' influence on carrier propagation and current. The app may be found at https://pat-trinity-ralph-carrier-propagation-devicephysics-unm.streamlit.app/.

IV. Conclusion

We derived expressions for charge carriers concentrations, beginning from Green's functions and applying Fourier and Laplace transforms. The derived equations are used in a web app modeling these phenomena. The web app is interactive and visualizes the effect of many parameters on carrier concentrations and current. Overall, we find that although lengthy, the derivation was highly informative; and that the model and app developed are highly extensible and informative in demonstrating the physics discussed in this class.