Simulating the Stochastic Motions of Electrons and Holes inside P-N Junctions

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1 Macroscopic Description of P-N Junctions

The internal structure of diode is actually a P-N junction which is simply the P-type semiconductor concatenated with the N-type semiconductor, as shown in Figure 1. There are totally four kinds of ions inside P-N junction: mobile electrons, mobile holes, fixed and negative-charged acceptors, fixed and positive-charged donors. Inside P type semiconductor, the majority electric carriers are holes and the minority carriers are electrons. The N type semiconductor is with the opposite case.

We can consider the P-N junction as a one-dimensional rod whose length is l, with its coordinate extending from $-l/2$ to $l/2$. The fixed ions density are the acceptor $a(x)$ and donor $d(x)$ that are of homogeneous distribution respectively in P side and N side, which are responsible for the global asymmetric density distribution of mobile electrons $n(x)$ and holes $p(x)$ along the whole junction, as required by electricity neutrality. Thus density distributions of acceptor and donor are expressed as

$$a(x) = a\theta(-x), \qquad d(x) = d\theta(x), \tag{1}$$

where $a = d$, and $\theta(x)$ is Heaviside step function which is defined such that $\theta(x) = 0$ when $x < 0$ and $\theta(x) = 1$ when $x > 0$. Thus, the charge density is given by

$$\rho(x) = e[p(x) - n(x) + d(x) - a(x)]. \tag{2}$$

Considering the electrostatical interaction, diffusion process and creation-annihilation process, the steady

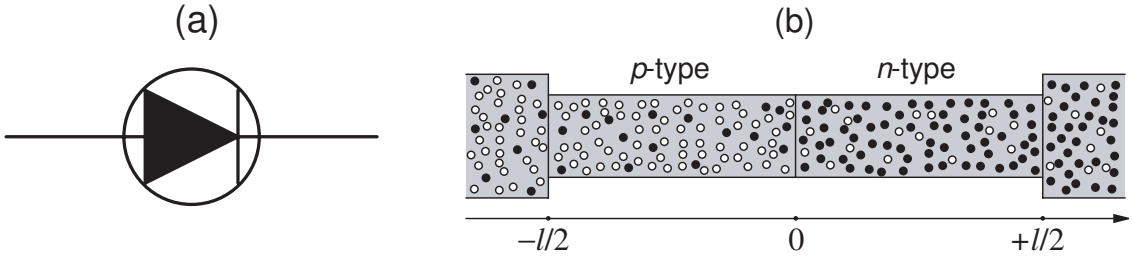

Figure 1: Schematic representation of diode (left) and P-N junction (right). In P-N junction, the black dots represent electrons and the white ones represent holes.

state of P-N junction system is described by the following coupled ordinary differential equations (ODEs):

$$\frac{dn(x)}{dx} = -\frac{J_n(x)}{D_n} - \frac{\mu_n}{D_n} en(x)\mathscr{E}(x), \tag{3}$$

$$\frac{dp(x)}{dx} = -\frac{J_p(x)}{D_p} + \frac{\mu_p}{D_p} ep(x)\mathscr{E}(x), \tag{4}$$

$$\frac{dJ_n(x)}{dx} = k_+ - k_- n(x)p(x), \tag{5}$$

$$\frac{dJ_p(x)}{dx} = k_+ - k_- n(x)p(x), \tag{6}$$

$$\frac{d\mathscr{E}(x)}{dx} = \frac{e}{\epsilon}\left[p(x) - n(x) + d(x) - a(x)\right], \tag{7}$$

$$\frac{d\phi(x)}{dx} = -\mathscr{E}(x), \tag{8}$$

with the boundary conditions $n(-l/2) = n_{\rm L}$, $p(-l/2) = p_{\rm L}$, $\phi(-l/2) = \phi_{\rm L}$, $n(l/2) = n_{\rm R}$, $p(l/2) = p_{\rm R}$, $\phi(l/2) = \phi_{\rm R}$.k_+, k_- are electron-hole pair creation and annihilation rate respectively. Here, we have Einstein's relation $\mu_n = \beta D_n$, $\mu_p = \beta D_p$, with β ($\equiv \frac{1}{k_{\rm B}T}$) being the inverse temperature. We naturally postitulate that $D_n \equiv D_p$ (therefore $\mu_n \equiv \mu_p$). Additionally, we impose the relations

$$n_{\rm L} = p_{\rm R}, \qquad\qquad n_{\rm R} = p_{\rm L}, \tag{9}$$

and

$$p_{\rm L} = n_{\rm R} + a(-l/2), \qquad\qquad n_{\rm R} = p_{\rm R} + d(l/2), \tag{10}$$

for the boundary conditions so that only the potential difference between the ends of junction is responsible for inducing particle currents. The above ODEs system is of the typical two-point value type that can not be analytically solved, however the condition for thermodynamic equilibrium in which the particle currents vanish can be easily obtained, that is

$$\beta e(\phi_{\rm L} - \phi_{\rm R}) = \ln\frac{n_{\rm L}}{n_{\rm R}} \equiv \ln\frac{p_{\rm R}}{p_{\rm L}}. \tag{11}$$

We define the applied voltage

$$V = \phi_{\rm L} - \phi_{\rm R} - \frac{1}{\beta e}\ln\frac{n_{\rm L}}{n_{\rm R}} \tag{12}$$

so that the above condition for thermodynamic equilibrium is equivalent to $V = 0$.

2 Stochastic Description of P-N Junctions

At mesoscopic level, the stochastic motions of electrons and holes can be successfully described by Markovian random process which is formulated in master equation. The fluctuations down to mesoscopic scale can be fully characterized by such process. The stochastic model we introduce here incorporates the self-consistent electric filed which is generated by the fluctuating distribution of charged ions. We now discretized the junction by dividing it into cells, each with the same volume Ω and same length Δx. Thus the cross section is given by $\sigma = \Omega/\Delta x$, and there are totally $I = l/\Delta x$ cells indexed from 1 to I. 0, $I+1$ are respectively used to refer to the left reservoir and right reservoir which impose certain boundary condition for the junction. Thus the number of electrons, holes, acceptors, donors in each cell are calculated as $N_i = n(x_i)\Omega$, $P_i = p(x_i)\Omega$, $A_i = a(x_i)\Omega$, $D_i = d(x_i)\Omega$, respectively, with $x_i = (i - 0.5)\Delta x$ ($i = 1 \cdots I$). The electron and hole number in the reservoir are N_i and P_i ($i = 0$, $I + 1$) that are maintained to be constant in time. The Poisson equation is replaced by its discretized version

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = -\frac{1}{\epsilon\Omega}(P_i - N_i + D_i - A_i), \tag{13}$$

with the boundary conditions $\phi_0 = \phi_{\rm L}$ and $\phi_{I+1} = \phi_{\rm R}$. This linear system should be solved each time when particle transition occurs. The details for solving this system is given in Appendix A.

The system state in specified by electron numbers $\{N_i\}$ and hole numbers $\{P_i\}$ in each cell which evolves in time following the network

$$\begin{array}{ccccccccccccccc}
\bar{N}_{\rm L} & \underset{W_0^{(-N)}}{\overset{W_0^{(+N)}}{\rightleftharpoons}} & N_1 & \underset{W_1^{(-N)}}{\overset{W_1^{(+N)}}{\rightleftharpoons}} & N_2 & \underset{W_2^{(-N)}}{\overset{W_2^{(+N)}}{\rightleftharpoons}} & \cdots & \underset{W_{I-2}^{(-N)}}{\overset{W_{I-2}^{(+N)}}{\rightleftharpoons}} & N_{I-1} & \underset{W_{I-1}^{(-N)}}{\overset{W_{I-1}^{(+N)}}{\rightleftharpoons}} & N_I & \underset{W_I^{(-N)}}{\overset{W_I^{(+N)}}{\rightleftharpoons}} & \bar{N}_{\rm R} \\
 & & W_1^{(+)} \updownarrow W_1^{(-)} & & W_2^{(+)} \updownarrow W_2^{(-)} & & \cdots & & W_{I-1}^{(+)} \updownarrow W_{I-1}^{(-)} & & W_I^{(+)} \updownarrow W_I^{(-)} & & \\
\bar{P}_{\rm L} & \underset{W_0^{(-P)}}{\overset{W_0^{(+P)}}{\rightleftharpoons}} & P_1 & \underset{W_1^{(-P)}}{\overset{W_1^{(+P)}}{\rightleftharpoons}} & P_2 & \underset{W_2^{(-P)}}{\overset{W_2^{(+P)}}{\rightleftharpoons}} & \cdots & \underset{W_{I-2}^{(-P)}}{\overset{W_{I-2}^{(+P)}}{\rightleftharpoons}} & P_{I-1} & \underset{W_{I-1}^{(-P)}}{\overset{W_{I-1}^{(+P)}}{\rightleftharpoons}} & P_I & \underset{W_I^{(-P)}}{\overset{W_I^{(+P)}}{\rightleftharpoons}} & \bar{P}_{\rm R}
\end{array}$$

and the probability of the system to be in certain states $\mathscr{P}(N_1,\cdots,N_I,P_1,\cdots,P_I)$ follows the master equation

$$\begin{aligned}
&\frac{d}{dt}\mathscr{P}(N_1,\cdots,N_I,P_1,\cdots,P_I)\\
&=\sum_{i=0}^{I}\Big[W_i^{(+N)}(\cdots,N_i+1,N_{i+1}-1,\cdots)\mathscr{P}(\cdots,N_i+1,N_{i+1}-1,\cdots)-W_i^{(+N)}(\cdots,N_i,N_{i+1},\cdots)\mathscr{P}(\cdots,N_i,N_{i+1},\cdots)\\
&+W_i^{(-N)}(\cdots,N_i-1,N_{i+1}+1,\cdots)\mathscr{P}(\cdots,N_i-1,N_{i+1}+1,\cdots)-W_i^{(-N)}(\cdots,N_i,N_{i+1},\cdots)\mathscr{P}(\cdots,N_i,N_{i+1},\cdots)\\
&+W_i^{(+P)}(\cdots,P_i+1,P_{i+1}-1,\cdots)\mathscr{P}(\cdots,P_i+1,P_{i+1}-1,\cdots)-W_i^{(+P)}(\cdots,P_i,P_{i+1},\cdots)\mathscr{P}(\cdots,P_i,P_{i+1},\cdots)\\
&+W_i^{(-P)}(\cdots,P_i-1,P_{i+1}+1,\cdots)\mathscr{P}(\cdots,P_i-1,P_{i+1}+1,\cdots)-W_i^{(-P)}(\cdots,P_i,P_{i+1},\cdots)\mathscr{P}(\cdots,P_i,P_{i+1},\cdots)\Big]\\
&+\sum_{i=1}^{I}\Big[W_i^{(+)}\mathscr{P}(\cdots,N_i-1,\cdots,P_i-1,\cdots)-W_i^{(+)}\mathscr{P}(\cdots,N_i,\cdots,P_i,\cdots)\\
&+W_i^{(-)}(N_i+1,P_i+1)\mathscr{P}(\cdots,N_i+1,\cdots,P_i+1,\cdots)-W_i^{(-)}(N_i,P_i)\mathscr{P}(\cdots,N_i,\cdots,P_i,\cdots)\Big],
\end{aligned}\tag{14}$$

with the transition rates

$$W_i^{(+N)}(\cdots,N_i,N_{i+1},\cdots)=\frac{D_n}{\Delta x^2}\psi(\Delta U_{i,i+1}^{(N)})N_i,\tag{15}$$

$$W_i^{(-N)}(\cdots,N_i,N_{i+1},\cdots)=\frac{D_n}{\Delta x^2}\psi(\Delta U_{i+1,i}^{(N)})N_{i+1},\tag{16}$$

$$W_i^{(+P)}(\cdots,P_i,P_{i+1},\cdots)=\frac{D_p}{\Delta x^2}\psi(\Delta U_{i,i+1}^{(P)})P_i,\tag{17}$$

$$W_i^{(-P)}(\cdots,P_i,P_{i+1},\cdots)=\frac{D_p}{\Delta x^2}\psi(\Delta U_{i+1,i}^{(P)})P_{i+1},\tag{18}$$

$$W_i^{(+)}=\Omega k_+,\tag{19}$$

$$W_i^{(-)}(N_i,P_i)=\Omega k_-\frac{N_i}{\Omega}\frac{P_i}{\Omega}.\tag{20}$$

U is the electrostatic energy stored in the system and $\Delta U_{i,i+1}$ (see Appendix A for detailed definition) is the energy difference associated with the one particle transition from cell i to cell $i+1$. The function $\psi(\Delta U)$ is defined as

$$\psi(\Delta U)=\frac{\beta\Delta U}{\exp(\beta\Delta U)-1},\tag{21}$$

which satisfies the detailed balance condition under equilibrium

$$\psi(\Delta U)=\psi(-\Delta U)\exp(-\beta\Delta U).\tag{22}$$

When the P-N junction is at equilibrium or be in nonequilibrium steady state, the mean quantities for each cell can be estimated by the time average

$$\langle X\rangle=\lim_{T\to\infty}\frac{1}{T}\int_0^T X(t)dt,\tag{23}$$

which is by ergodicity equivalent to ensemble average $\langle X\rangle = \sum_{(\mathbf{N},\mathbf{P})} X\mathscr{P}(\mathbf{N},\mathbf{P})$. Here, the quantity X can be N_i, P_i, ϕ_i, $F_i^{(N)}$, $F_i^{(P)}$, where the latter two are introduced to be the fluxes of electrons and holes between cell i and cell $i+1$, respectively. In continuum limit where $\Delta\Omega \to 0$, the densities of electrons and holes are recovered through $n(x_i) = N_i/\Delta\Omega$ and $p(x_i) = P_i/\Delta\Omega$. The derivation of total electric current including the contribution of displacement current can be found in Appendix B.

3 Numerical Simulation with Langevin's Algorithm

The Eq. (14) can be written in the following form:

$$\begin{aligned}\frac{d\mathscr{P}}{dt} =& \sum_{i=0}^{I}\Bigg[\left(\mathrm{e}^{+\partial_{N_i}}\mathrm{e}^{-\partial_{N_{i+1}}}-1\right)W_i^{(+N)}\mathscr{P}+\left(\mathrm{e}^{-\partial_{N_i}}\mathrm{e}^{+\partial_{N_{i+1}}}-1\right)W_i^{(-N)}\mathscr{P}\\ &+\left(\mathrm{e}^{+\partial_{P_i}}\mathrm{e}^{-\partial_{P_{i+1}}}-1\right)W_i^{(+P)}\mathscr{P}+\left(\mathrm{e}^{-\partial_{P_i}}\mathrm{e}^{+\partial_{P_{i+1}}}-1\right)W_i^{(-P)}\mathscr{P}\Bigg]\\ &+\sum_{i=1}^{I}\Bigg[\left(\mathrm{e}^{-\partial_{N_i}}\mathrm{e}^{-\partial_{P_i}}-1\right)W_i^{(+)}\mathscr{P}+\left(\mathrm{e}^{+\partial_{N_i}}\mathrm{e}^{+\partial_{P_i}}-1\right)W_i^{(-)}\mathscr{P}\Bigg].\end{aligned} \tag{24}$$

Introducing the probability density $\mathscr{P}$ in the limit where $N_i \gg 1$ and $P_i \gg 1$, we get

$$\begin{aligned}\partial_t\mathscr{P} \approx& \sum_{i=0}^{I}\Bigg\{-\partial_{N_i}\left[\left(W_{i-1}^{(+N)}-W_{i-1}^{(-N)}-W_i^{(+N)}+W_i^{(-N)}\right)\mathscr{P}\right]\\ &+\partial_{N_i}^2\left[\frac{1}{2}\left(W_{i-1}^{(+N)}+W_{i-1}^{(-N)}+W_i^{(+N)}+W_i^{(-N)}\right)\mathscr{P}\right]\\ &+\partial_{N_i}\partial_{N_{i+1}}\left[-\left(W_i^{(+N)}+W_i^{(-N)}\right)\mathscr{P}\right]+(N\rightleftharpoons P)\Bigg\}\\ &+\sum_{i=1}^{I}\Bigg\{-\left(\partial_{N_i}+\partial_{P_i}\right)\left[\left(W_i^{(+)}-W_i^{(-)}\right)\mathscr{P}\right]+\left(\partial_{N_i}+\partial_{P_i}\right)^2\left[\frac{1}{2}\left(W_i^{(+)}+W_i^{(-)}\right)\mathscr{P}\right]\Bigg\}.\end{aligned}$$

This shows that the variables N_i and P_i obeys stochastic differential equations of Langevin type:

$$\frac{dN_i}{dt} = F_{i-1}^{(N)} - F_i^{(N)} + R_i, \tag{25}$$

$$\frac{dP_i}{dt} = F_{i-1}^{(P)} - F_i^{(P)} + R_i, \tag{26}$$

with the following fluxes and reaction rate:

$$F_i^{(N)} = W_i^{(+N)} - W_i^{(-N)} + \sqrt{W_i^{(+N)}+W_i^{(-N)}}\,\xi_i^{(N)}(t), \tag{27}$$

$$F_i^{(P)} = W_i^{(+P)} - W_i^{(-P)} + \sqrt{W_i^{(+P)}+W_i^{(-P)}}\,\xi_i^{(P)}(t), \tag{28}$$

$$R_i = W_i^{(+)} - W_i^{(-)} + \sqrt{W_i^{(+)}+W_i^{(-)}}\,\eta_i(t), \tag{29}$$

expressed in terms of the Gaussian white noises:

$$\langle\xi_i^{(N)}(t)\rangle = \langle\xi_i^{(P)}(t)\rangle = \langle\eta_i(t)\rangle = 0, \tag{30}$$

$$\langle\xi_i^{(N)}(t)\xi_j^{(N)}(t')\rangle = \delta_{i,j}\delta(t-t'), \tag{31}$$

$$\langle\xi_i^{(P)}(t)\xi_j^{(P)}(t')\rangle = \delta_{i,j}\delta(t-t'), \tag{32}$$

$$\langle\eta_i(t)\eta_j(t')\rangle = \delta_{i,j}\delta(t-t'), \tag{33}$$

$$\langle\xi_i^{(N)}(t)\xi_j^{(P)}(t')\rangle = 0, \tag{34}$$

$$\langle\eta(t)\xi_j^{(N)}(t')\rangle = 0, \tag{35}$$

$$\langle\eta(t)\xi_j^{(P)}(t')\rangle = 0. \tag{36}$$

If we discretize the time into intervals Δt, we get

$$N_i(t+\Delta t) = N_i(t) + \left(F_{i-1}^{(N)} - F_i^{(N)} + R_i\right)\Delta t, \tag{37}$$

$$P_i(t+\Delta t) = P_i(t) + \left(F_{i-1}^{(P)} - F_i^{(P)} + R_i\right)\Delta t. \tag{38}$$

where

$$F_i^{(N)} = W_i^{(+N)} - W_i^{(-N)} + \sqrt{W_i^{(+N)} + W_i^{(-N)}}\frac{G_i^{(N)}(t)}{\sqrt{\Delta t}}, \tag{39}$$

$$F_i^{(P)} = W_i^{(+P)} - W_i^{(-P)} + \sqrt{W_i^{(+P)} + W_i^{(-P)}}\frac{G_i^{(P)}(t)}{\sqrt{\Delta t}}, \tag{40}$$

$$R_i = W_i^{(+)} - W_i^{(-)} + \sqrt{W_i^{(+)} + W_i^{(-)}}\frac{G_i^{(\mathrm{r})}(t)}{\sqrt{\Delta t}}, \tag{41}$$

with independent identically distributed normal random variables $G_i^{(N)}(t)$, $G_i^{(P)}(t)$, and $G_i^{(\mathrm{r})}(t)$, and appropriate boundary conditions at the both left and right reservoirs.

For electron, the transition rates at the boundaries are given by

$$W_0^{(+N)} = \frac{D_n}{\Delta x^2}\psi(\Delta U_{0,1}^{(N)})\bar{N}_{\mathrm{L}}, \tag{42}$$

$$W_0^{(-N)} = \frac{D_n}{\Delta x^2}\psi(\Delta U_{1,0}^{(N)})N_1, \tag{43}$$

$$W_I^{(+N)} = \frac{D_n}{\Delta x^2}\psi(\Delta U_{I,I+1}^{(N)})N_I, \tag{44}$$

$$W_I^{(-N)} = \frac{D_n}{\Delta x^2}\psi(\Delta U_{I+1,I}^{(N)})\bar{N}_{\mathrm{R}}, \tag{45}$$

with

$$\Delta U_{0,1}^{(N)} = -e(\Phi_1 - \Phi_{\mathrm{L}}) + \frac{e^2 I \Delta x^2}{2(I+1)\epsilon\Omega}, \tag{46}$$

$$\Delta U_{1,0}^{(N)} = e(\Phi_1 - \Phi_{\mathrm{L}}) + \frac{e^2 I \Delta x^2}{2(I+1)\epsilon\Omega}, \tag{47}$$

$$\Delta U_{I,I+1}^{(N)} = -e(\Phi_{\mathrm{R}} - \Phi_I) + \frac{e^2 I \Delta x^2}{2(I+1)\epsilon\Omega}, \tag{48}$$

$$\Delta U_{I+1,I}^{(N)} = e(\Phi_{\mathrm{R}} - \Phi_I) + \frac{e^2 I \Delta x^2}{2(I+1)\epsilon\Omega}, \tag{49}$$

and similar expressions for hole.

4 `PNsimulator`: A Program for Numerical Simulation

We now introduce `PNsimulator`, a C++ code implementation of the above described numerical simulation. The source files are listed in Table 1. Here, the object-orienting programming (OOP) paradigm was extensively employed in coding. We defined a class named `Cdiode`, which serves as a blueprint of the state of P-N junction recording the discretized distribution of electrons, holes, acceptors, donors, and potentials. In addition, we also defined two classes, `Cvector` and `Cmatrix`, which are used to facilitate the manipulation of vector and matrix. The operating system for `PNsimulator` is `Linux` with the following setup

- `g++`,
- `make`,
- `python3` (with `Numpy`, `Matplotlib`, `Scipy` installed),
- `gsl` (GNU Scientific Library, a C numerical package, which can be installed with the command `sudo apt-get install gsl-bin`).

Table 1: Files and Their functionalities.

File	Note
Class_vector.cpp Class_vector.h	the file containing a definition of vector class (supporting class for vector manipulation)
Class_matrix.cpp Class_matrix.h	the file containing a definition of matrix class (supporting class for matrix manipulation)
Class_diode.cpp Class_diode.h	the file containing a definition of diode (P-N junction) class
Function_random_number_generating.cpp	the file containing a function for generating random numbers
Function_diode_evolving.cpp	the file containing a function driving the evolution of diode
Function_steady_state_evaluating.cpp	the file containing a function evaluating steady state
Main.cpp	main file
Makefile	makefile
Script.py	python script file for plotting

Table 2: The artificial values of physical constants used in simulating both diode and transistor models (which can be understood in SI units). The mobilities of electrons and holes are computed according to Einstein's relation $\mu = \beta D$.

constant	value
permittivity	$\epsilon = 0.01$
inverse temperature	$\beta = 1.0$
elementary charge	$\|e\| = 1.0$
diffusion coefficient for electrons and holes	$D_n = D_p = 0.01$
generation and recombination rate constants	$k_+ = k_- = 0.01$

`Makefile` is provided to make it very convenient to compile the source code with the command `make`. We can also clean all the object file with the command `make clean`. After obtaining the executable named `Main`, we can run it with the command `./Main`. The results are the voltage-current pairs that are written into a plain text file named `I_V.out`. `Scipy.py` is a python script used to make a plot with the outputted data, and can be executed with the command `python3 Script.py`. The final figure obtained is `I_V.eps`.

The related physical constants and parameters specifying the P-N junction system are listed in Table 2 and Table 3. As we see, in the P-N junction the concentration of majority electric carriers is overwhelmingly larger than that of minority electric carriers. This is intentionally set to approaching the asymptotic situation under which the characteristics should be given by

$$I(V) = I_s \left[\exp\left(\beta e V\right) - 1\right], \tag{50}$$

which is called Shockley's equation. Here, I_s is the asymptotic electric current when P-N junction positively biased infinitely. From the results outputted in `I_V.out` (listed in Table 4), we see the applied voltages interating in the range $[-5.0, 4.0]$ with the step 0.5 and the corresponding electric currents. Figure 2 (`I_V.eps`) visualize the results, and from which we can indeed find that the relation between applied voltage and electric current can be described by Eq. (50).

Table 3: The detailed specification of discretized P-N junction.

Meaning	Value
number of cells in left region	20
number of cells in right region	20
width of each cell Δx	0.1
volume of each cell Ω	8×10^5
section area $\Sigma = \Omega / \Delta x$	8×10^6
number of electrons in left-reservoir cell	400
number of holes in left-reservoir cell	1.6×10^9
number of electrons in right-reservoir cell	1.6×10^9
number of holes in right-reservoir cell	400

Table 4: The results (voltage-current pairs) outputted in `I_V.out`.

Applied Voltage	Electric Current
-5.0000000	-8152.6886
-4.5000000	-8070.0309
-4.0000000	-7868.4078
-3.5000000	-7661.9425
-3.0000000	-7357.3122
-2.5000000	-7074.1009
-2.0000000	-6642.5810
-1.5000000	-5816.2116
-1.0000000	-4727.6563
-0.50000000	-2725.7767
0.0000000	126.89334
0.50000000	4597.1961
1.0000000	11604.314
1.5000000	23162.647
2.0000000	41470.749
2.5000000	70751.979
3.0000000	117798.43
3.5000000	192752.58
4.0000000	311466.98

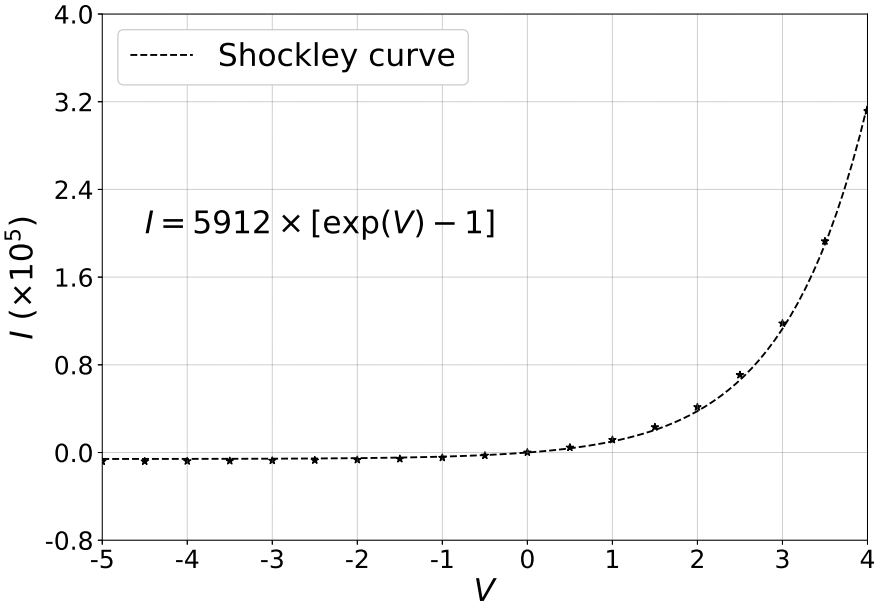

Figure 2: Characterics of P-N junction. The asterisks are the data points, with the values listed in Table 4. The dash line is obtained by fitting the data points with Shockley equation whose expression is labeled.

A Solution of discretized Possion equation

The electrostatic energy is given by

$$U = \frac{1}{2}\mathbf{\Phi}^{\mathrm{T}} \cdot \mathbf{C} \cdot \mathbf{\Phi}, \tag{51}$$

where

$$\mathbf{\Phi}^{\mathrm{T}} = (\phi_1, \cdots, \phi_i, \cdots, \phi_I) \tag{52}$$

obeys the discretized Poisson equation

$$\mathbf{C} \cdot \mathbf{\Phi} = \mathbf{Z} \tag{53}$$

with the symmetric matrix

$$\mathbf{C} = \gamma \begin{pmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & -1 & 2 & -1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{pmatrix}, \tag{54}$$

$$\gamma = \frac{\epsilon\Omega}{\Delta x^2}, \tag{55}$$

and

$$\mathbf{Z}^{\mathrm{T}} = e\,(P_1 - N_1 + D_1 - A_1, \cdots, P_i - N_i + D_i - A_i, \cdots, P_I - N_I + D_I - A_I) + \gamma(\phi_{\mathrm{L}}, 0, \cdots, 0, \cdots, 0, \phi_{\mathrm{R}}). \tag{56}$$

The electrostatic potential is given by

$$\mathbf{\Phi} = \mathbf{C}^{-1} \cdot \mathbf{Z} \tag{57}$$

with

$$\left(\mathbf{C}^{-1}\right)_{ij} = \begin{cases} \frac{i}{\gamma(I+1)}(I+1-j) & \text{if} \quad i \leq j, \\ \frac{j}{\gamma(I+1)}(I+1-i) & \text{if} \quad i > j. \end{cases} \tag{58}$$

The change of electrostatic energy during the transition of a electron of charge $-e$ from the i^{th} to the $(i+1)^{\text{th}}$ cell is given by

$$\Delta U^{(N)}_{i,i+1} = \frac{1}{2}\left(\mathbf{Z'}^{\mathrm{T}} \cdot \mathbf{C}^{-1} \cdot \mathbf{Z'} - \mathbf{Z}^{\mathrm{T}} \cdot \mathbf{C}^{-1} \cdot \mathbf{Z}\right) \tag{59}$$

where

$$Z'_k = Z_k + e\delta_{k,i} - e\delta_{k,i+1}. \tag{60}$$

Since hole have the charge $+e$, we thus have that

$$\Delta U^{(N)}_{i,i+1} = -e(\Phi_{i+1} - \Phi_i) + \frac{e^2}{2}\Big[\left(\mathbf{C}^{-1}\right)_{i,i} - 2\left(\mathbf{C}^{-1}\right)_{i,i+1} + \left(\mathbf{C}^{-1}\right)_{i+1,i+1}\Big], \tag{61}$$

$$\Delta U^{(P)}_{i,i+1} = +e(\Phi_{i+1} - \Phi_i) + \frac{e^2}{2}\Big[\left(\mathbf{C}^{-1}\right)_{i,i} - 2\left(\mathbf{C}^{-1}\right)_{i,i+1} + \left(\mathbf{C}^{-1}\right)_{i+1,i+1}\Big]. \tag{62}$$

Using equation (58), we find that

$$\Delta U^{(N)}_{i,i+1} = -e(\Phi_{i+1} - \Phi_i) + \frac{e^2 I \Delta x^2}{2(I+1)\epsilon\Omega}, \tag{63}$$

$$\Delta U^{(P)}_{i,i+1} = +e(\Phi_{i+1} - \Phi_i) + \frac{e^2 I \Delta x^2}{2(I+1)\epsilon\Omega}. \tag{64}$$

We notice that, for transitions at the boundaries, these expressions should be modified according to the values of the potentials in the reservoirs (see below).

B Total Electric Current

We now give the calculation of total current which includes the contribution from the displacement current. By definition, we have total current

$$\mathscr{I}(t) \equiv \int d\boldsymbol{\sigma} \cdot [e(\mathbf{j}_p - \mathbf{j}_n) + \epsilon\, \partial_t \boldsymbol{\mathscr{E}}] \tag{65}$$

with a surface integral over the section area $\sigma = \Omega/\Delta x$. By spatial discretization, we get

$$\sigma\epsilon\partial_t \mathscr{E}_{x,i} \simeq -\frac{e\epsilon\sigma}{\Delta x}\sum_{j=0}^{L}\left[(\mathbf{C}^{-1})_{i+1,j+1} - (\mathbf{C}^{-1})_{i+1,j} - (\mathbf{C}^{-1})_{i,j+1} + (\mathbf{C}^{-1})_{i,j}\right](F^{(P)}_j - F^{(N)}_j). \tag{66}$$

Since

$$(\mathbf{C}^{-1})_{i+1,j+1} - (\mathbf{C}^{-1})_{i+1,j} - (\mathbf{C}^{-1})_{i,j+1} + (\mathbf{C}^{-1})_{i,j} = \frac{L}{\gamma(L+1)}\,\delta_{ij} - \frac{1}{\gamma(L+1)}\,(1-\delta_{ij}) \tag{67}$$

and

$$e\int d\boldsymbol{\sigma} \cdot (\mathbf{j}_p - \mathbf{j}_n) \simeq e\left(F^{(P)}_i - F^{(N)}_i\right), \tag{68}$$

we find that

$$\mathscr{I}(t) \simeq \frac{e}{L+1}\sum_{j=0}^{L}\left(F^{(P)}_j - F^{(N)}_j\right) \tag{69}$$

independently of the location i.

References

[1] Jiayin Gu and Pierre Gaspard, *Stochastic Approach and Fluctuation Theorem for Charge Transport in Diodes*, Phys. Rev. E **97**, 052138 (2018). (selected as **Editors' Suggestion**).