Diffusion models for atomic scale electron currents in semiconductor, p-n junction

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Abstract—While semiconductor electronics is at heart of modern world, and now uses 5nm or smaller processes of single atoms, it seems there are missing models of actual electron currents in these scales - which could help with more conscious design of future electronics. This article proposes such practical methodology allowing to model approximated electron flows in semiconductor, nonlinear Ohm law in p-n junction, and hopefully more complex systems e.g. built of transistors. It assumes electron hopping between atoms using Maximal Entropy Random Walk based diffusion - chosen accordingly to (Jaynes) maximal entropy principle, this way leading to the same stationary probability density as quantum models. Due to Anderson-like localization in nonhomogeneous lattice of semiconductor, electrons are imprisoned in entopic wells, requiring to exceed a potential barrier for conductance.

Keywords: diffusion, maximal entropy random walk, semiconductor, conductance, p-n junction

I. INTRODUCTION

While historically electronics was focused on much larger scales and heuristic models ([1], [2], [3]), modern processors use e.g. 5nm process with perspective of further reductions, what means scales of single atoms - suggesting to include also quantum effects into considerations. Literature search for such conductance models was unsuccessful, complete quantum modelling is extremely costly from computational perspective, hence there is proposed relatively inexpensive intermediate modelling framework, which includes quantum stationary probability distribution, which is usually localized (Anderson [4]).

Specifically, we focus on Maximal Entropy Random Walk (MERW) type diffusion - chosen accordingly to the (Jaynes) maximal entropy principle. While for a regular lattice its predictions would be the same as for standard diffusion, referred here as Generic Random Walk (GRW), for defected lattice e.g. semiconductor with dopants as exchanged single atoms, predictions are very different as we can see in examples in Fig. 1. While GRW leads to nearly uniform stationary probability density, MERW predicts stationary density as quantum mechanics - with strong Anderson-like localization property, confirmed experimentally for semiconductor with STM (scanning tunneling microscope) [5].

For defected lattice of semiconductor crystal, without such localization (GRW) tiny potential would already lead to electron conductance with (linear) Ohm law. In contrast, in reality this conductance is often blocked - here with Anderson-like localization, requiring some breakdown voltage to overcome the localization to allow for electron flow, getting very nonlinear voltage-current dependence.

This article extends on [6] MERW/GRW conductance sim-
labor, among others by mean-field self-interaction (MFSI) inclusion of potential created by electron density, reflective boundary conditions allowing for flat boundary potentials in equilibrium, and finally application to practical systems like diode as p-n junction.

II. MAXIMAL ENTROPY RANDOM WALK (MERW)

This section contains brief introduction to MERW [7], which now has many applications (≈ 200 citations), for example can be imagined as random walk along Ising sequence [8]. The basic formulas (also standard GRW) are gathered in Fig. 2.

Deeper discussion can be found e.g. in [9] - also for possible expansions of framework here, like continuous limit leading to Schrödinger equation, or potentials varying in time for high expansions of framework here, like continuous limit leading to formulas (also standard GRW) are gathered in Fig. 2.

Imagine a graph given by adjacency matrix \( M \) which has single maximum:

\[
\sum_{i \neq j} M_{ij} = \sum_{i \neq j} (1) = n - 1
\]

for vertex \( i \). Random walk as uniform path ensemble

\[
\sum_{i \neq j} \sum_{\gamma} S_{ij} \ln(S_{ij}) = \lim_{l \to \infty} \frac{1}{l} \sum_{H} \Pr(\gamma) \ln(\Pr(\gamma))
\]

Entropy is maximized for unified ensemble, this time of possible paths - hence MERW is equivalently uniform ensemble among paths on given graph.

C. Used weighted MERW as Boltzmann path ensemble

To add weights we go from uniform to Boltzmann ensemble - here of paths, exactly as for random walk along Ising sequence (useful e.g. to find its pattern distributions [8]).

Let us define \( V_{ij} \) as energy of \( i \)-j pair of vertices, e.g. \( V_{ij} = (V_i + V_j)/2 \) for point potential \( V \). It allows to define energy of path \( \gamma \) with discrete time \( t \in \mathbb{Z} \) as \( E(\gamma) = \sum_t V_{\gamma_{t-1} \gamma_t} \).

Entropy maximization (2) now requires to subtract mean energy \( \sum_{ij} p_i S_{ij} \) Inverting sign it becomes minimization of Gibbs free energy \( G \) per step:

\[
\min_{S} G = \sum_{ij} p_i S_{ij} (\ln(S_{ij}) + \beta V_{ij})
\]

Which is minimized for Boltzmann ensemble - now among paths. Its partition function \( Z \) can be expressed with power
of (analogous to minus tight-binding Hamiltonian) popular in statistical mechanics (e.g. [11])

\begin{equation}
M_{ij} := \exp(-\beta V_{ij})
\end{equation}

Asymptotically the right hand side behaves dominant eigenvalue of $M$. Finally equation (1) allows to express free energy per step as:

\begin{equation}
\beta G = - \lim_{l \to \infty} \frac{\ln(Z_l)}{l} = -\ln(\lambda)
\end{equation}

\(D. Sketch of combinatorial derivation of S, \rho formulas\)

As in Fig. 3 let us present sketch of derivation of MERW as random walk given by Boltzmann ensemble of paths, exactly like for random walk along Ising-like sequence. Deeper discussion and expansions can be found e.g. in [9].

As mentioned, powers of transfer matrix $M_{ij} := \exp(-\beta V_{ij})$ contain Boltzmann path ensemble:

\begin{equation}
(M^l)_{ij} = \sum_{\gamma_0 \cdots \gamma_l} \exp \left( - \beta \sum_{t=1}^{l} V_{\gamma_{t-1} \gamma_t} \right)
\end{equation}

Assuming connected aperiodic graph, Frobenius-Perron theorem says that $M$ has unique dominant left/right eigenvalues:

\begin{equation}
\max: \quad M \psi = \lambda \psi \quad \phi^T M = \lambda \phi^T
\end{equation}

getting asymptotic $M^l \approx \lambda^l \phi \psi^T$, which allows to calculate $S_{ij} = \Pr(\gamma_t = j | \gamma_{t-1} = i)$ like in Fig. 3 (for any k):

\[ S_{ij} = \frac{\Pr(ij)}{\Pr(i)} = \lim_{l \to \infty} \frac{M_{ij}(M^l)_{ik}}{\lambda^l \psi_i} \]

and analogously stationary probability density from statistics inside such sequences (for any $j, k$):

\[ \rho_i = \Pr(i) \propto \lim_{l \to \infty} (M^l)_{ij} (M^l)_{ik} \propto \phi_i \psi_i \]

\(E. Sketch of optimization derivation of S, \rho formulas\)

Alternatively, we could treat this problem as maximization with 3 sets of constraints - for simplicity using $\beta = 1$:

\begin{equation}
\min_{S,\rho} G(S, \rho) \quad \text{for} \quad G = \sum_{ij} \rho_i S_{ij} (\ln(S_{ij}) + V_{ij})
\end{equation}

\[ \forall i \sum_j S_{ij} = 1 \quad \forall i \rho_j = \sum_j \rho_i S_{ij} \quad \sum_i \rho_i = 1 \]

Denoting the 3 types of Lagrange multipliers as $(\xi_i)$, $(\eta_j)$ and $\theta$, equating $S_{ij}$ derivative to 0 we get:

\[ \ln(S_{ij}) = \frac{\xi_i}{\rho_i} - V_{ij} - 1 + \eta_j \]

Substituting it to $\rho$, derivative equated to zero, we get:

\[ \theta = \eta_i + \sum_j S_{ij}(\ln(S_{ij}) + V_{ij} - \eta_j) = \eta_i + \sum_j S_{ij} \left( \frac{\xi_j}{\rho_j} - 1 \right) \]

Using $\sum_j S_{ij} = 1$ assumption we can simplify:

\[ \theta = \eta_i + \xi_i/\rho_i - 1 \]

Denoting $\psi_i = \exp(\eta_i)$, $\phi_i = \rho_i \exp(\xi_i/\rho_i)$, $\lambda = \exp(-\theta)$, $M_{ij} = \exp(-\beta V_{ij})$, the constraints equations become left/right eigenequations, leading to formulas as before.

We have minimization here, but focus only on eigenvectors as exponents - enforcing positive coordinates, leading to dominant eigenvectors as before.

\(III. Defected lattice and self-interaction\)

Let us now expand and apply discussed MERW methodology to electron conductance, [6] contains simplified simulator.

\(A. Electron conductance on lattice e.g. crystal\)

As the graph for our walker we would like to focus on lattices - with nodes representing single atoms, or maybe discretized larger systems. We work on 2D regular lattice (analogously in 3D) of size $n_x \times n_y$ hence containing $n = n_x n_y$ nodes.

The previously used vertex indices $i, j$ correspond to such 2 (or higher) dimensional lattice vectors $i \equiv (x, y)$.

For simplicity we assume the walker can only jump to a nearest neighbor (4 in 2D, 6 in 3D) or stay in a given node: all but $M_{x,y}(x,y)$, $M_{x,y}(x \pm 1,y)$, $M_{x,y}(x,y \pm 1)$ terms of $n \times n$ matrix $M$ are zero - it is sparse matrix, of degree 5 in 2D, with cyclic boundary conditions especially in x conductance direction to close the circuit.

Transfer matrix $M_{ij} = \exp(-\beta V_{ij})$ is nonzero only for these allowed jumps, the remaining can be imagined as corresponding to infinite energy $V_{ij} = \infty$.

The potential here has 3 types of contributions:

\[ V = V^v + V^e + V^d \]

- $V^v$ describes potential characteristic for a given vertex e.g. as atoms of various types like dopants, ideally to be chosen based e.g. on orbital structures,
- $V^e$ corresponds to attached external voltage stimulating electron flow for conductance,
- $V^d$ describes potential resulting from electron density - while in literature it is usually chosen arbitrarily, here in the
Figure 4. Visualized MERW electron densities $\rho$ and $V^d(\rho)$ potentials they produce (from Poisson equation) for $40 \times 40$ lattice with cyclic boundary conditions and different strengths of self-interaction $\gamma$. All use the same randomly chosen defect pattern: n-type dopants (red dots of -0.5 potential, diagrams on left), and p-type dopants (green dots of +0.5 potential, diagrams on right). As expected, strong self-interaction $\gamma$ makes density more uniform due to Coulomb repulsion.

next subsection we include such self-interaction in electron density optimization.

The $V^v$ and $V^d$ contributions usually can be included as point-like e.g.: $V^v_{ij} = (V^v_i + V^v_j)/2$. We could also include direction dependence e.g. for Lorentz force in Hall effect.

In contrast $V^e$ rather requires special treatment. Naively it needs linear potential dependence like $V^e(x) = xU/n_x$ for attached external voltage $U$. However, it has problem when closing the circuit to allow circulation of electrons ($M$ needs cyclic boundary conditions in $x$) - requiring some analogue of e.g. battery. To avoid saw-like potential, we can subtract mean potential for each vertex, leaving constant gradient preferring jumps in one direction e.g.:

$$V^e(x,y) = \exp(\mp \beta U/n_x)$$

(12)

This term preferring jumps in one direction requires nonsymmetric $M$, what corresponds to non-Hermitian Hamiltonian [12].

B. Adding mean-field self-interaction (MFSI)

The discussed random walk has imagined single walker. However, in conductance we have multiple charged walkers: electrons, which Coulomb repulsion should make density more uniform, as presented in Fig. 4.

Hence we should interpret $\rho_i = \phi_i \psi_i$ stationary probability distribution also as representing charge density, bringing additional $V^d(\rho)$ contribution to potential, which can be calculated using Poisson equation: $\Delta V \propto -\rho$. Working on discrete lattice, we can discretize the Laplacian - e.g. in 2D use:

$$V^d_{x-1,y} + V^d_{x+1,y} + V^d_{x,y-1} + V^d_{x,y+1} - 4V^d_{x,y} = \gamma (\rho_{xy} - \rho^0_{xy})$$

(13)

for some constant $\gamma$, and $\rho^0$ charge density without the conductance electrons - for simplicity assumed as uniform $\rho^0_{xy} = 1/n$.

These are $n = n_x n_y$ linear equation, we can find inverse of such discretized Laplacian as $n \times n$ matrix, finally getting:

$$V = V^0 + \gamma \Delta^{-1} \rho$$

(14)

containing vertex potential describing node e.g. atom types ($V^v$) and external voltage ($V^e$).

Choosing boundary conditions is a subtle problem - while for $M$ at least in $x$ direction cyclic are required, for Laplacian $\Delta$ there are used as in Fig. 5.

- Vertical ($y$): cyclic boundary conditions,
- Horizontal ($x$): reflective boundary conditions treating edge as self-loop, this way pretending there are reflected charges
behind it, what allows flat potential boundary behavior, different for both boundaries (for built-in voltage).
The \( \mathbf{n} \times \mathbf{n} \) matrix \( \Delta \) is singular here, what corresponds to freedom of choice of absolute potential. To invert this issue, we can e.g. add 1 to all coordinates, what means adding 1 to the only 0 eigenvalue (to uniform eigenvector).

Numerical search of dominant left/right eigenvalue can be formulated as finding fixed point:

\[
\rho_i = \phi_i \psi_i \quad \phi, \psi : \text{eigenvectors of } M(\rho) \tag{15}
\]

including \( V^d \) containing linear \( \rho \) dependence.

A natural inexpensive approach is starting with some \( \phi^0, \psi^0 \) e.g. as uniform (or for assumed approximation of potential) and iterate \( t \rightarrow t + 1 \) until some convergence condition:

\[
\rho_{i}^{t} = \phi_{i}^{t} \psi_{i}^{t} \quad \phi^{t+1}, \psi^{t+1} : \text{eigenvectors of } M^{t} = M(\rho^{t}) \tag{16}
\]

where e.g. dominant eigenvectors can be improved with single steps of power method like \( \psi^{t+1} \propto M^{t} \psi^{t} \) and normalize. In practice it usually converges, however e.g. often oscillating, what suggests e.g. using some fractional steps, also in this moment there is no convergence guarantee. Generally, numerical approaches for MFSI require further work, alternative one by directly satisfying \( 2n + 1 \) constraints (2 eigenequations and normalization) is presented in Appendix.

There could also used some inexpensive approximations, like assuming parametrized family of potential only dependent on \( x \).

Fig. 1, 6, 7 present calculated example of p-n junction using such iteration until convergence, we can see voltage-current plot as expected for diode. Electrons are (Anderson) localized in p part in equilibrium, and their density becomes more uniform when attaching external voltage, weakening built-in voltage, more easily for forward bias.

The flow diagrams show fixed positions of p (green) and n (red) type dopants as atoms of different potential. Grayness presents electron densities. There are also arrows representing local currents as:

\[
\rho_{xy}(S_{xy},(x+1,y) - S_{xy},(x-1,y), S_{xy},(x,y+1) - S_{xy},(x,y-1)) \tag{17}
\]

In reverse bias we can see kind of domain wall travelling with voltage - it has minimal density with symmetric diffusion in both directions, allowing for conductance when reaching junction.

**IV. CONCLUSIONS AND FURTHER WORK**

There was presented initial framework for modelling electron conductance e.g. in atomic scale, which is planned to be further developed, for example:

- There was only presented simple diode example - should be also considered more complex e.g. transistor, trying to find applications of such models to improve technology e.g. by better control of defect distribution.
- Presented inexpensive framework is kind of between classical and quantum - recreates (localized) quantum stationary probability distribution, but neglects interference - there is required comparison with complete quantum models (like tight-binding) and experiments (e.g. temperature dependence, STM like [5]), understanding inaccuracies and hopefully compensate them in inexpensive ways.
- The atomic potentials are very simple now, final models might require including atomic orbital structures, maybe

![Figure 6. Example of p-n junction conductance dependence for 60 \times 20 lattice and various attached potential difference \( \Delta V \). All use the same defect pattern: red dots denote +0.5 potential, green -0.5 (\( \beta = 10, \gamma = 1 \)). Plotted arrows represent local electron currents (17). We can see strong localization for low \( \Delta V \) which prevents conductance, with equalizing density for larger \( |\Delta V| \) (weakening built-in voltage), especially in n \( \rightarrow \) p forward bias direction.](image-url)
multiple vertices per node corresponding to involved orbitals of given atom.
- There is assumed nearest-neighbors jumping between atoms, what seems reasonable for low voltage, but generally might require more complex modelling, up to more dense lattice and adding electron velocities like in Langevin model.
- There was discussed static modelling: of stabilized electron flows. In practice electronics often works with very high frequencies. MERW for varying potential is discussed in [9] and should be considered in the future.
- Better numerical methods are yet to be developed.

APPENDIX

To numerically include self-interaction, there was suggested cyclically updating potentials (Poisson equation) and dominant eigenvectors, hoping for some convergence. While it is inexpensive thanks to working on sparse matrices, there is no convergence guarantee. Hence here is proposed alternative numerical approach based on constraint satisfaction, however, it requires to work on dense matrices due to $\Delta^{-1}$ being dense. As in optimization derivation [11-13], to focus on dominant eigenvectors let us enforce them to have positive coordinates by directly optimizing their logarithms: $\Phi_i = \ln(\phi_i)$, $\Psi_i = \ln(\psi_i)$.

A. Fixed potential

For fixed $M_{ij} = \exp(-\beta V_{ij})$ we could just use standard numerical library to find dominant left/right eigenvectors $\phi$, $\psi$. To prepare for self-interaction, let us do it through iteration to satisfy the $n + 1$ constraints $C = 0$:

$$C = \left( (\lambda\psi_i - (M\psi)_i)_{i=1..n}, 1 - \sum_k \psi_k^2 \right)$$

for $\psi = \exp(\Psi_i)$, the Jacobian $J$ made of derivatives is:

$$J_{i=1..n+1}, j=1..n := \partial_{\Psi_j} C = \left( (\lambda\delta_{ij}\psi_j - M\psi_j)_i, 1 - 2\psi_i^2 \right)$$

$$J_{i=1..n+1}, n+1 := \partial_{\lambda} C = (\psi_{i=1..n}, 0)$$

Suggesting iteration (in practice with linear solve):

$$\begin{align*}
\tag{18} \Psi, \lambda & \rightarrow (\Psi, \lambda) - J^{-1}C
\end{align*}$$

Experimentally in 3-4 such steps $\|C\|$ usually gets from uniform $\psi$ down to $\sim 10^{-13}$ for random positive terms matrices of various sizes - for dense matrices allowing to approximate dominant eigenvectors of positive terms matrices a few times faster than standard Mathematica library with Arnoldi method.

B. Plus self-interaction

We are now ready to add self-interaction: with no longer constant $M_{ij} = \exp(-\beta V_{ij})$; but this time depending on charge density $V = V(\rho)$ for

$$\rho_i = \phi_i\psi_i = \exp(\Phi_i + \Psi_i) \quad \text{normalized to} \quad \sum_i \rho_i = 1$$

As discussed, self-interaction from Poisson equation, denoting $T = \gamma(\Delta)^{-1}/2$, can be written as:

$$V_{ij}(\rho) = V_{ij}^0 + \sum_k (T_{ik} + T_{jk})\rho_k \quad \tag{19}$$

For non-symmetric matrix here we need to use both eigenvectors, the constraint becomes $2n + 1$ dimensional $C = 0$:

$$C = \left( (\lambda\phi_i - \phi^T M)_i, (\lambda\psi - M\psi)_i, 1 - \sum_k \phi_k\psi_k \right) \quad \tag{20}$$

We can analogously construct $2n + 1 \times 2n + 1$ Jacobian from derivatives:

$$\partial_{\Phi_k} M_{ij} = \partial_{\Phi_k} \exp(-\beta V_{ij}) = -\beta M_{ij}(T_{ik} + T_{jk})\rho_k = \partial_{\Phi_k} M_{ij}$$

$$\partial_{\Phi_k} (\lambda\phi_i - \phi^T M)_i = \delta_{ik}\phi_i - \phi_k M_{ki} - \sum_j \phi_j (\partial_{\Phi_k} M_{ij})$$

$$\partial_{\Phi_k} (\lambda\psi - M\psi)_i = -\sum_j (\partial_{\Phi_k} M_{ij})\psi_j$$

$$\partial_{\Phi_k} (\lambda\psi - M\psi)_i = \lambda\delta_{ik}\psi_i - M_{ik}\psi_k - \sum_j (\partial_{\Phi_k} M_{ij})\psi_j$$

$$\partial_{\Phi_k} \left( 1 - \sum_i \phi_i\psi_i \right) = \partial_{\Phi_k} \left( 1 - \sum_i \phi_i\psi_i \right) = -\phi_k\psi_k$$

We can analogously perform step [18], but this time it requires more caution e.g. changing step size until $\|C\|_2$ is indeed reduced, or use gradient method e.g. for $\|C\|_2$.

REFERENCES

[1] S. M. Sze, *Semiconductor devices: physics and technology*. John wiley & sons, 2008.
[2] B. G. Streetman, S. Banerjee *et al.*, *Solid state electronic devices*. Pearson/Prentice Hall Upper Saddle River, NJ, 2006, vol. 10.
[3] R. S. Muller, T. I. Kamins, M. Chan, and P. K. Ko, *Device electronics for semiconductor devices: physics and technology*. Wiley New York, 1986.
[4] A. Lagendijk, B. Van Tiggelen, and D. S. Wiersma, “Fifty years of Anderson localization,” *Phys. Today*, vol. 62, no. 8, pp. 24–29, 2009.
[5] A. Richardella, P. Roushan, S. Mack, B. Zhou, D. A. Huse, D. D. Awschalom, and A. Yazdani, “Visualizing critical correlations near the metal-insulator transition in Ga1-xMnxAs,” *Science*, vol. 327, no. 5966, pp. 665–669, 2010.
[6] J. Duda, “Electron conductance models using maximal entropy random walks.” [Online]. Available: http://demonstrations.wolfram.com/author.html?author=Jarek+Duda/.
[7] Z. Burda, J. Duda, J.-M. Luck, and B. Waclaw, “Localization of the maximal entropy random walk,” *Physical review letters*, vol. 102, no. 16, p. 160602, 2009.
[8] J. Duda, “Nearly accurate solutions for ising-like models using maximal entropy random walk,” *arXiv preprint arXiv:1912.13300*, 2019.
[9] ——, “Extended maximal entropy random walk,” Ph.D. dissertation, Jagiellonian University, 2012. [Online]. Available: http://www.fais.uj.edu.pl/documents/41628/6d3bcb07-cb71-4eba-8a5a-d974256dd065.
[10] E. T. Jaynes, “Information theory and statistical mechanics,” *Physical review*, vol. 106, no. 4, p. 620, 1957.
[11] R. J. Baxter, *Exactly solved models in statistical mechanics*. Elsevier, 2016.
[12] F. Bagarello, R. Passante, and C. Trapani, “Non-hermitian hamiltonians in quantum physics,” *Springer Proceedings in Physics*, vol. 184, 2016.
Figure 7. Higher voltage resolution of flows as in Fig. 6, showing e.g., interesting domain wall shift before breakdown voltage in reverse bias.