

Two-Particle Monte Carlo for TCAD: Fermionic Treatment of Electron–Electron Scattering

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Abstract—This paper presents a model for treating electron–electron scattering (EES) in Monte Carlo (MC) transport calculations for microelectronic device simulation. Conventional MC transport in Technology Computer-Aided Design (TCAD) is predominantly based on single-particle approaches, where scattering events affect only the electron whose trajectory is sampled. Within such a framework, EES can only be incorporated through iterative schemes. Since EES fundamentally involves the interaction of two carriers, a two-particle description appears more appropriate. The scattering rates are evaluated using Fermi’s golden rule. In contrast to earlier approaches based on products of single-particle states, the present work derives the relevant expressions from antisymmetric two-particle wave functions that reflect the fermionic nature of electrons. Results from device simulations of the implementation are presented.

Index Terms—electron-electron scattering, TCAD, Monte Carlo transport.

I. INTRODUCTION

The advancement of modern microelectronics strongly relies on TCAD simulation tools. Besides supporting performance-oriented design decisions, TCAD also plays an important role in enhancing reliability of these increasingly complex devices.

A key reliability concern in MOSFETs is hot-carrier degradation, which requires a detailed understanding of the carrier energy distribution function (EDF) inside the device. Carriers with high kinetic energy are most likely to break atomic bonds at the semiconductor-insulator interface, making the high-energy tail of the distribution particularly relevant.

The two-particle model proposed in this work influences the high-energy regime and therefore provides valuable input for physically based hot-carrier degradation (HCD) models [1].

II. TWO-PARTICLE MONTE CARLO TRANSPORT

The model was reported in previous contributions [2]. In brief, instead of a single-particle trajectory, two trajectories are propagated simultaneously. Each electron can scatter individually with phonons or mutually via EES. In device simulations, the domain is divided into cells. Each *resting cell* holds one electron, whereas the *cell under simulation* hosts two electrons, propagated until one of them reaches a cell edge. Then, the cell under simulation is updated and the process is repeated.

III. EES TREATMENT

In MC transport simulations, the rate at which the system changes from its current (initial) state $|\mathbf{k}_1, \mathbf{k}_2\rangle$ to one final state $|\mathbf{k}'_1, \mathbf{k}'_2\rangle$ is determined by Fermi’s golden rule

$$W_{\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k}'_1, \mathbf{k}'_2} = \frac{2\pi}{\hbar} |M|^2 \delta(\underbrace{\varepsilon_{\mathbf{k}'_1} + \varepsilon_{\mathbf{k}'_2} - \varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_2}}_{\Sigma}). \quad (1)$$

Rate Calculation: The key novelty of this work lies in the evaluation of the matrix element M entering the scattering rate. In previous approaches, this term has often been evaluated using states given by products of two plane waves (2a).

However, electrons are fermions and must obey the Pauli principle. To account for this, symmetric (2b, +) and antisymmetric (2b, -) states must be considered, which is a standard procedure in quantum mechanics [3].

$$|\mathbf{k}_1, \mathbf{k}_2\rangle = \frac{1}{\Omega} e^{i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)} \quad (2a)$$

$$|\mathbf{k}_1, \mathbf{k}_2\rangle_F = \frac{1}{\sqrt{2}\Omega} \left[e^{-i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)} \pm e^{-i(\mathbf{k}_2 \cdot \mathbf{r}_1 + \mathbf{k}_1 \cdot \mathbf{r}_2)} \right] \quad (2b)$$

As a consequence, for fermions, the simple matrix element 3a needs to be evaluated for both symmetric and antisymmetric states to obtain M_{sym} and M_{asym} , respectively. Finally, due to spin degeneracy, a triplet of states (spin-symmetric) and one singlet (spin-antisymmetric) state exist. This implies that the spatial part of the wave function is antisymmetric in 3/4 of the cases and symmetric in 1/4 of the cases, leading to the averaged matrix element in 3b.

$$M = \langle \mathbf{k}'_1, \mathbf{k}'_2 | V | \mathbf{k}_1, \mathbf{k}_2 \rangle \quad (3a)$$

$$|M|_F^2 = (3|M_{asym}|^2 + |M_{sym}|^2)/4 \quad (3b)$$

As perturbation V , a screened Coulomb interaction is assumed, where β denotes the inverse Thomas-Fermi screening length:

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^2}{4\pi\epsilon_s} \frac{e^{-\beta|\mathbf{r}_1 - \mathbf{r}_2|}}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad \beta^2 = \frac{e^2 n}{\epsilon_s k_B T} \frac{F_{-1/2}(\eta)}{F_{1/2}(\eta)}, \quad (4)$$

and η is defined as $\eta = (E_F - E_C)/(k_B T)$.

Conventional and fermionic matrix elements are written as

$$|M|^2 = \frac{e^4}{\epsilon^2 \Omega^2} \delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2} \frac{1}{(q^2 + \beta^2)^2} \quad (5a)$$

$$|M|_F^2 = \frac{e^4}{\epsilon^2 \Omega^2} \delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2} \times \left[\frac{1}{(q^2 + \beta^2)^2} + \frac{1}{(p^2 + \beta^2)^2} - \frac{1}{(q^2 + \beta^2)(p^2 + \beta^2)} \right] \quad (5b)$$

with $q = |\mathbf{q}| = |\mathbf{k}'_1 - \mathbf{k}_1| = |\mathbf{k}'_2 - \mathbf{k}_2|$ and $p = |\mathbf{p}| = |\mathbf{k}'_2 - \mathbf{k}_1|$. Momentum conservation $\delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2}$ in (5a) and energy conservation $\delta(\Sigma)$ in (1) constrain the allowed transitions to a constant energy surface in $\mathbf{k}$ -space, which is a sphere for parabolic dispersions. The scattering rate Γ is the sum of all transition rates originating from an initial state $|\mathbf{k}_1, \mathbf{k}_2\rangle$. In semiconductors, a continuum of states is assumed, thus instead the transition rate is integrated over the constant energy surface, weighted by the density of states. Conventional and fermionic scattering rates write as

$$\Gamma = \frac{me^4}{4\pi\hbar^3\epsilon^2} \frac{n}{K(K^2 + \beta^2)} \frac{K^2}{\beta^2} \quad (6a)$$

$$\Gamma_F = 2\Gamma - \frac{me^4}{2\pi\hbar^3\epsilon^2} \frac{n}{K(K^2 + 2\beta^2)} \ln\left(1 + \frac{K^2}{\beta^2}\right) \quad (6b)$$

Final State Selection: Having evaluated the scattering rate for a given initial state $|\mathbf{k}_1, \mathbf{k}_2\rangle$, a final state $|\mathbf{k}'_1, \mathbf{k}'_2\rangle$ must be drawn randomly such that, when sampled repeatedly, the resulting distribution reproduces the transition rate distribution, illustrated in Figure 1.

The surface of final states is best described in spherical coordinates, with the polar axis aligned with $\mathbf{K} = \mathbf{k}_2 - \mathbf{k}_1$ running through the centre of the sphere $\mathbf{k}_0 = (\mathbf{k}_1 + \mathbf{k}_2)/2$ and the poles at $\mathbf{k}_1$ and $\mathbf{k}_2$. The transition rate depends only on $\theta = \angle(\mathbf{q}, \mathbf{K})$, with $q = K \cos(\theta)$ and $p = K \sin(\theta)$. Random polar angles θ_r can then be drawn as follows:

The fermionic matrix element comprises three terms $T_{s,1}$, $T_{s,2}$, and T_a . Dominated by the first two terms, an inversion method for $T_{s,1}$ is set up first via $CDF = F(\theta_r)/F(\theta = \pi/2)$

$$F(\theta) = \int_0^{2\pi} \int_0^\theta T_{s,1} \delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2} \delta(\sigma_\epsilon) d\theta' d\phi \quad (7a)$$

$$\theta_r = \arccos \sqrt{\frac{r \beta^2}{K^2 - r K^2 + \beta^2}} \quad (7b)$$

Since $T_{s,1}$ and $T_{s,2}$ are related by particle exchange, mirroring $\theta_r \leftarrow \pi - \theta_r$ in 50% of cases yields their combined distribution. T_a is then handled via acceptance-rejection with probability

$$A(\theta_r) = \frac{T_{s,1} + T_{s,2} - T_a}{T_{s,1} + T_{s,2}} \quad (8)$$

In case of rejection, θ_r is redrawn until acceptance is achieved. Due to azimuthal symmetry, a random angle ϕ_r is drawn uniformly from $[0, 2\pi)$. The final states are given by $\mathbf{k}'_1 = \mathbf{k}_1 + \mathbf{q}(\theta_r, \phi_r)$ and $\mathbf{k}'_2 = \mathbf{k}_2 - \mathbf{q}(\theta_r, \phi_r)$.

IV. DISCUSSION OF TRANSITION RATES

The fermionic matrix element (5b) introduces two additional terms with respect to its conventional counterpart (5a), altering the angular transition rate distribution and almost doubling the overall scattering rate (6b). Figure 1 illustrates this distribution for the interaction of a hot (1 eV) and a cold ($k_B T$) electron, resembling a ballistic channel electron scattering with a thermal drain electron in a MOSFET. Hence $\epsilon_{\text{hot}} \gg \epsilon_{\text{thermal}}$, $\mathbf{K} \approx \mathbf{k}_{\text{hot}}$ was assumed. Varying the parameters n and

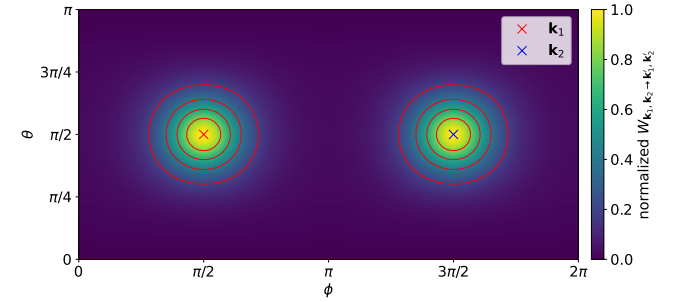


Fig. 1: transition rate distribution over the Fermi surface. $n = 1 \times 10^{19} \text{ cm}^{-3}$, $\epsilon_{\text{hot}} = 1 \text{ eV}$, $T = 300 \text{ K}$.

ϵ_{hot} shows that the transition rate distribution broadens with increasing n and decreasing ϵ_{hot} , as illustrated in Figure 2. Contrary the total scattering rate increases with decreasing n and increasing ϵ_{hot} , as shown in Figure 3. Higher total rates indicate stronger effects on transport, whereas narrower transition-rate distributions suggest the opposite. In the limit of a δ -like distribution, the effect of EES vanish, since particle states can only be interchanged or remain unchanged. Thus the overall transport behavior is nontrivial to predict.

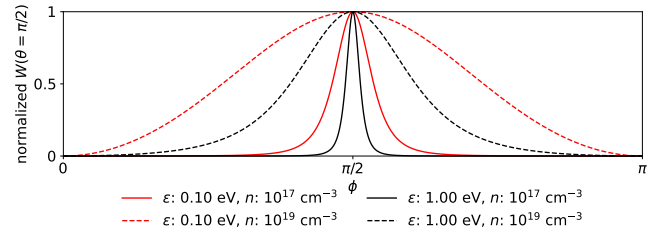


Fig. 2: The transition rate distribution broadens with increasing n and decreasing ϵ_{hot} .

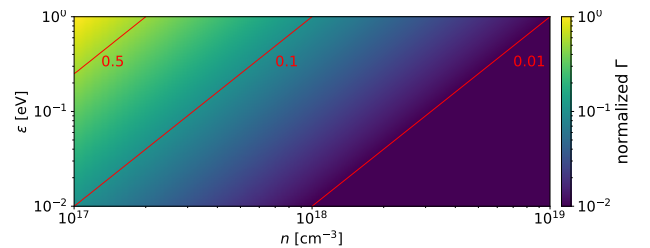


Fig. 3: The total scattering rate increases with ϵ_{hot} and decreases with n .

V. 1D TRANSPORT SIMULATIONS

In order to study the implications of EES on transport characteristics, we developed a two-particle Monte Carlo transport simulator, which is an open-source code [4] written in Python.

Here we employed our code base to simulate a parametrizable benchmark potential. This allows for easy parametric variation of the maximum electric field and the drain voltage, in order to study their influences in a controlled manner.

Potential: The electrostatic potential is modeled by a sigmoidal function:

$$\varphi(x) = \frac{-V_D \alpha}{1 + \exp(B(x - x_c))}. \quad (9)$$

For $\alpha = 1$, the parameter $B = -4E_{\max}/V_D$ can be chosen to enforce a maximum electric field $E_{\max}$ at the inflection point x_c . The simulation domain length is chosen such that the targeted potential drop is almost V_D . Then the small correction factor α is used to ensure that the potential drop is exactly V_D , while approximately preserving the prescribed maximum electric field. This way four potential energy profiles $\varepsilon_{\text{pot}} = -e\varphi$ are generated, shown in Figure 4.

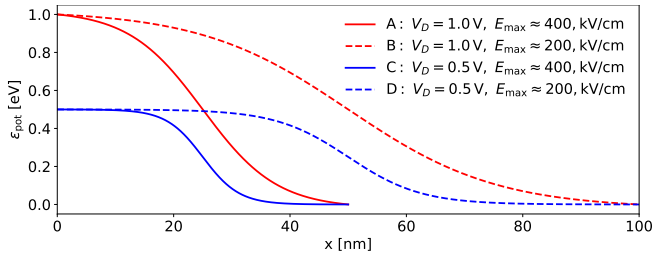


Fig. 4: Benchmark potential profiles

Mean Energy: Averaged quantities within the cells are computed from samples taken at the cell edges:

$$\langle \varepsilon_{\text{kin}} \rangle = \frac{\sum_i w_i \varepsilon_{\text{kin},i}}{\sum_i w_i} \quad (10)$$

The individual samples i are taken at the cell exits, weighted by the inverse of the absolute normal velocity $w_i = 1/|v_{x,i}|$.

Figures 5 shows the mean energy along the channel. For relative comparison, the position is normalized to the total length L_D .

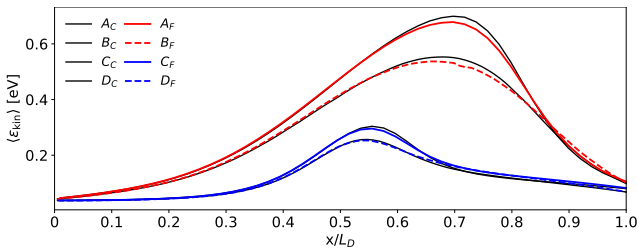


Fig. 5: Average energy as function of the channel position. Simulated for fermionic and conventional Matrix elements. Results are shown for $n = 1 \times 10^{19} \text{ cm}^{-3}$ and $T = 300 \text{ K}$.

Energy Distribution: To obtain the EDF, a histogram is constructed for each cell. At each sampling event, the bin corresponding to the electron's energy is incremented by the weight w_i . In the end, the total weight in each bin is divided by the square root of the energy at the bin center, $\sqrt{\varepsilon_c}$, to account for the three-dimensional density of states.

Figures 6 and 7 show the EDF for two different benchmark potentials, A and C, respectively. The EDF is then normalized by its maximum value such that the maximum equals unity.

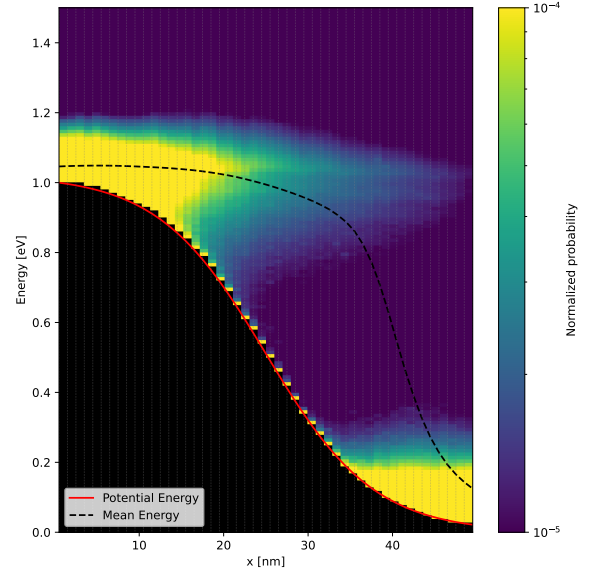


Fig. 6: Energy distribution for potential profile A. Simulated using fermionic matrix elements. Results are shown for $n = 1 \times 10^{19} \text{ cm}^{-3}$ and $T = 300 \text{ K}$.

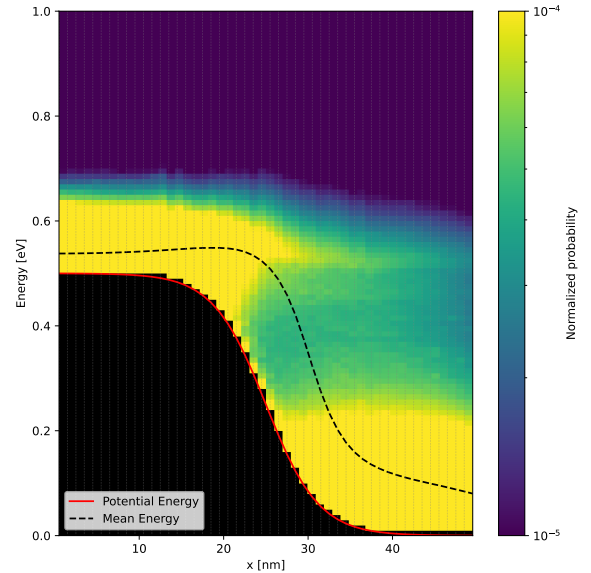


Fig. 7: Energy distribution for potential profile C. Simulated using fermionic matrix elements. Results are shown for $n = 1 \times 10^{19} \text{ cm}^{-3}$ and $T = 300 \text{ K}$.

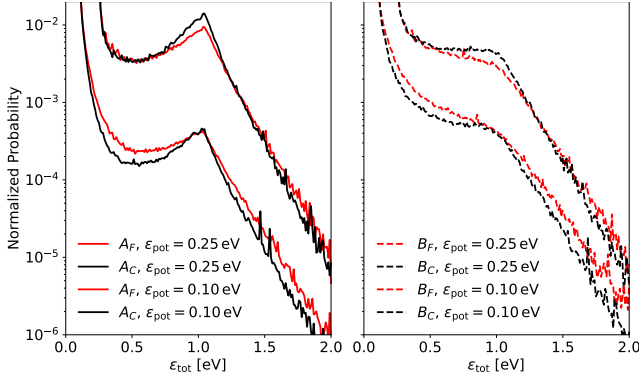


Fig. 8: Energy distribution at the drain for potential profiles A (left) and B (right), evaluated at the positions where the potential energy decreases to 25% and 10% of its maximum. Results are shown for $n = 1 \times 10^{19} \text{ cm}^{-3}$ and $T = 300 \text{ K}$.

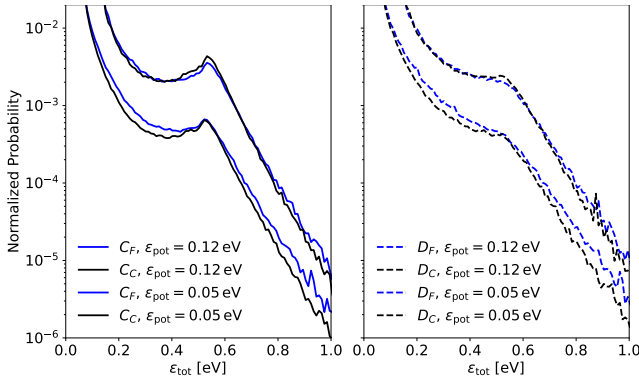


Fig. 9: Energy distribution at the drain for potential profiles C (left) and D (right), evaluated at the positions where the potential energy decreases to 25% and 10% of its maximum. Results are shown for $n = 1 \times 10^{19} \text{ cm}^{-3}$ and $T = 300 \text{ K}$.

VI. RESULTS AND DISCUSSION

Figure 5 shows that average energy increases with increasing drain voltage V_D and increasing maximum electric field E_{max} . Interestingly, increasing E_{max} maintain the shape of the energy profile, while increasing V_D shifts the energy maximum toward the drain and broadens the high-energy region. Moreover, the higher scattering rates originating from the fermionic treatment lead to a slightly lower average energy, as scattering events occur more frequently.

Figures 6 and 7 compare the EDFs for potential profiles A ($V_D = 1.0 \text{ V}$) and C ($V_D = 0.5 \text{ V}$), respectively. The EDF corresponding to the higher drain voltage exhibits a substantially sparser population at the drain in the energy range $\varepsilon \in [0.25V_D, 0.75V_D]$ and a more pronounced ballistic stream originating from the source. This was additionally highlighted by setting maximum value of the colorbar to the values in the ballistic stream and the minimum only one decade lower. In contrast, the EDF for the lower drain voltage is distributed more uniformly over the energy region and does not form such

a drastic gap. This indicates more efficient relaxation, which is also visible by comparing the mean energies.

Figures 8 and 9 present the EDFs evaluated for the four potential profiles at two different positions. Comparing the high-field cases to the low-field cases, A to B and C to D, shows that the ballistic peak is significantly reduced at lower fields. This is likely due to a combination of lower carrier velocities and longer simulation domains, which allow for more efficient energy relaxation. In all cases, the increased scattering rates resulting from the fermionic treatment enhance the high-energy tail, as expected. Another effect, visible for all profiles but most pronounced for profile A, is the higher population of fermionic EDFs at intermediate energies below the ballistic peak. This effect is particularly evident for the EDF of potential A evaluated closest to the drain ($\varepsilon_{\text{pot}} = 0.1 \text{ eV}$).

Comparing the results to previous work [5]–[7], it is found that EES enhances the high-energy tail, in agreement with earlier studies. In addition, the tail shape differs from that reported in [5], [6], where a more pronounced deviation from a Maxwellian-like distribution is observed. In contrast, the present results exhibit an approximately linear decay on a logarithmic scale above the ballistic peak.

Direct quantitative comparison of EDFs is limited, as different studies employ different potentials and simulation conditions. Nevertheless, physically based modelling is essential for capturing hot-carrier distributions [7] and enabling their use in HCD models, thereby supporting the identification of trade-offs between performance and reliability.

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