ME 595M: Monte Carlo Simulation

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Monte Carlo Simulation

- BTE solutions are often difficult to obtain
  - Closure issues force the use of BTE moments
    - Inherent approximations
  - Ballistic transport is often not described well by perturbed equilibrium distributions
- Instead, seek to track representative carriers and use statistical averaging to predict transport behavior
  - Monte Carlo methods are essentially averaging or integration tools
- In neither case can we easily incorporate quantum (wave) effects

Scattering

- Treatment of scattering underlies almost all MC methods
- Consider electron scattering mechanisms
  - Acoustic deformation potential (ADP)

$$\frac{1}{\tau_1} = \left(2 \times 10^{13}\right)\sqrt{E(p)/q}$$

  - Intervalley scattering by phonon absorption

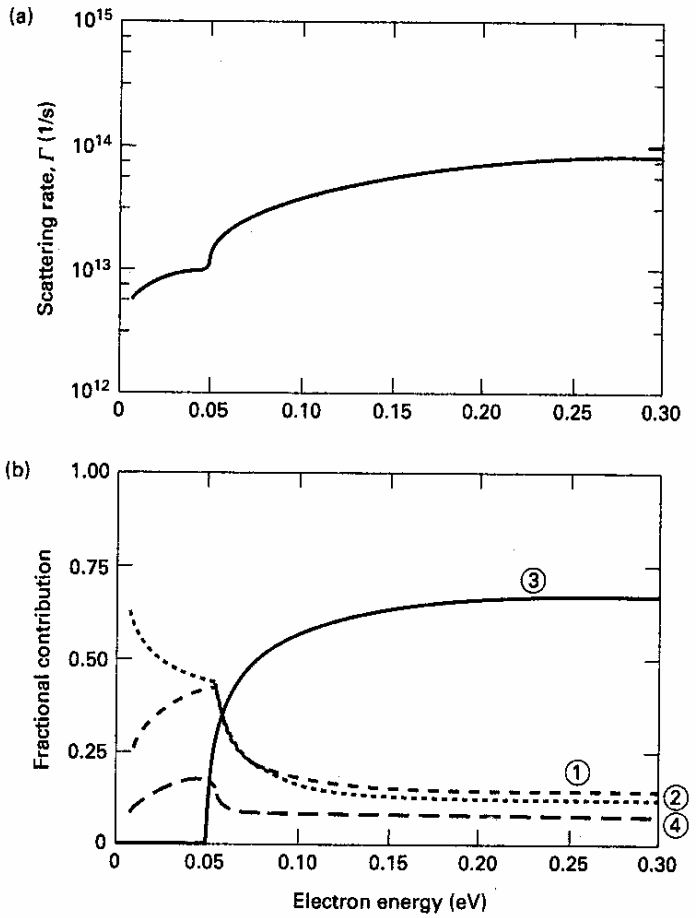
$$\frac{1}{\tau_2} = \left(1.5 \times 10^{13}\right)\sqrt{E(p)/q + 0.050}$$

  - Others (τ_3^{-1}, τ_4^{-1}, …)
- Combine with Mathiessen's rule

$$\Gamma(p) = \sum_i \frac{1}{\tau_i(p)}$$

(Effective Scattering Rate)

Combining Scattering Events



Lundstrom Fig. 6.1

Fig. 6.1 (a) Total scattering rate versus energy for the model semiconductor. (b) Fractional contribution versus energy that each of the four scattering processes makes to the total scattering rate. 1: ADP, 2: intervalley absorption, 3: intervalley emission, and 4: ionized impurity with $N_I = 10^{16}\,cm^{-3}$.

Equation of Motion

- The most complex transport equation employed in most MC simulations is Newton's law, F=ma

$$\mathbf{F_e} = \frac{d\mathbf{p}}{dt} = -q\mathbf{E}$$

- Collision times are typically much smaller than free-flight times
  - Collisions are treated as instantaneous events
- Carrier position can be expressed as an integral of velocity

$$\mathbf{r}(t) = \mathbf{r}(0) + \int_0^t \mathbf{v}(t')dt'$$

Free Flight

- Consider an electron under the action of an electric field directed along the z-axis

$$p_x(t) = p_x(0)$$

$$p_y(t) = p_y(0)$$

$$p_z(t) = p_z(0) + (-q)\mathbf{E}_z t$$

- Position relations become

$$x(t) = x(0) + \frac{p_x(0)}{m^*} t$$

$$y(t) = y(0) + \frac{p_y(0)}{m^*} t$$

$$z(t) = z(0) + \frac{E(t) - E(0)}{(-q)\mathbf{E}_z}$$

E in numerator is energy

last equality derives from the parabolic energy band assumption

Ensemble Scattering

- Consider a collection of carriers of concentration n_{CF} that have not undergone scattering since time t=0
- Assume a constant scattering rate Γ_0 (for now)
- The time evolution of n_{CF} is expressed mathematically as

$$\frac{dn_{CF}}{dt} = -\Gamma_0 n_{CF}$$

  - solution

$$n_{CF}(t) = n_{CF}(0)e^{-\Gamma_0 t}$$

Scattering Probability and Time

- Probability that an electron survives until time t without scattering is

$$\frac{n_{CF}(t)}{n_{CF}(0)} = e^{-\Gamma_0 t}$$

- Probability that a carrier undergoes its first collision between t and t+dt is the scattering rate times the survival probability

$$P(t)dt = \Gamma_0 e^{-\Gamma_0 t} dt$$

Random Selection

- Now we wish to choose a random number such that the probability of choosing a number between r and r+dr equals the probability of selecting a collision time between t and t+dt

$$P(r)dr = P(t)dt$$

let P(r) = 1 for a random number generator between 0 and 1

$$\rightarrow dr = \Gamma_0 e^{-\Gamma_0 t} dt$$

$$\rightarrow r_c = 1 - e^{-\Gamma_0 t_c}$$

$$\rightarrow t_c = -\frac{1}{\Gamma_0}\ln(1 - r_c) = -\frac{1}{\Gamma_0}\ln(r_1)$$

- Note that r_1 is also a uniformly distributed random number between 0 and 1
- Foregoing equation relates random numbers to collision times

Self-Scattering

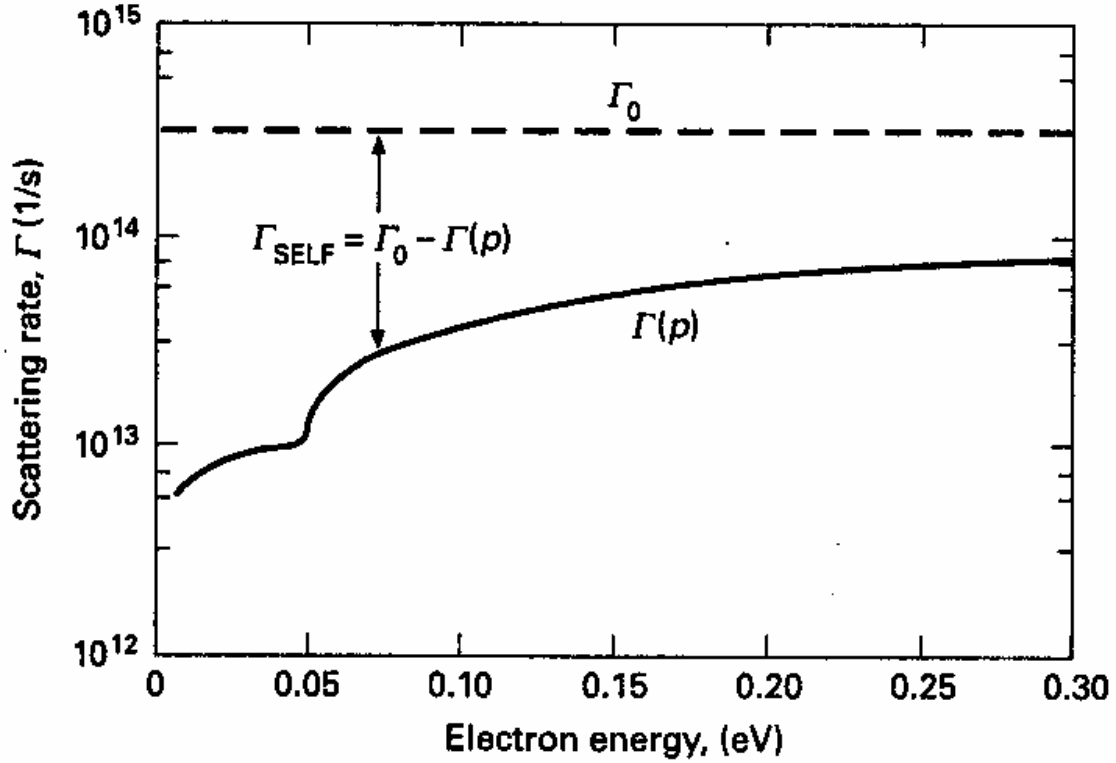
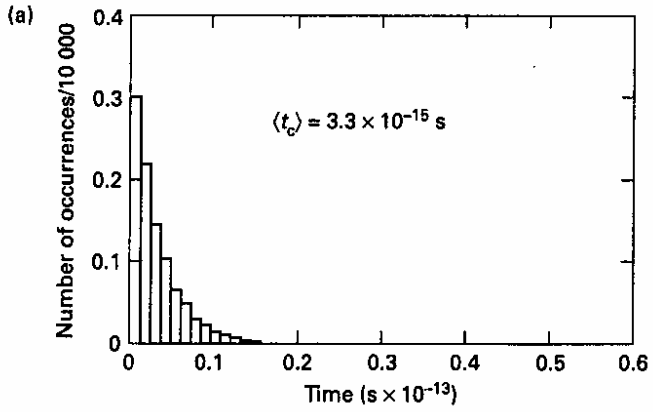


Fig. 6.4 Total scattering rate versus energy for electrons in the model semiconductor. An approximation that assumes $\Gamma(p) = \Gamma_0$ is also displayed.

- **Lundstrom Fig. 6.4**

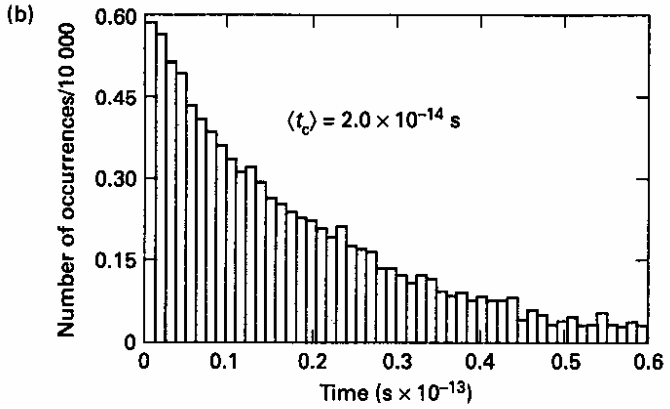
Collision Distributions

t_c based on all scattering events (including self-scattering)



$$\langle t_c \rangle \approx \frac{1}{\Gamma_0}$$

t_c based on only real scattering events (not including self-scattering)



$$\langle t_c \rangle \approx \frac{1}{\Gamma(p)}$$

Fig. 6.5 Histogram of (a) 10 000 free flight durations for a semiconductor with $\Gamma(p) = \Gamma_0$ and (b) 10 000 real free flight durations (those terminated by a real scattering event) for the model semiconductor. The times were computed from eq. (6.17) assuming $\Gamma_0 = 3 \times 10^{14}\,s^{-1}$ by summing the times for successive random numbers until a real scattering event was detected. The electron's kinetic energy was assumed to be 0.15 eV. The times were computed from eq. (6.17).

Lundstrom Fig. 6.5

Identification of Scattering Events

- After selecting the duration of free flight (t_c), we must properly choose the type of scattering event that occurs
- Each scattering mechanism can alter the particle's momentum (direction and magnitude) differently
- Ultimately, the choices must be proportional to the relative likelihoods of occurrence

Cumulative Scattering Probabilities

- Consider *k* possible scattering mechanisms
- Imagine a cumulative bar chart that includes a sum of the fractional probabilities of each type
- Choose a uniformly distributed random number r_2 between 0 and 1
- Select scattering event l if the following holds

$$\frac{\sum_{i=1}^{l-1} \frac{1}{\tau_i(p)}}{\Gamma_0} \leq r_2 < \frac{\sum_{i=1}^{l} \frac{1}{\tau_i(p)}}{\Gamma_0}$$

Graphical Interpretation

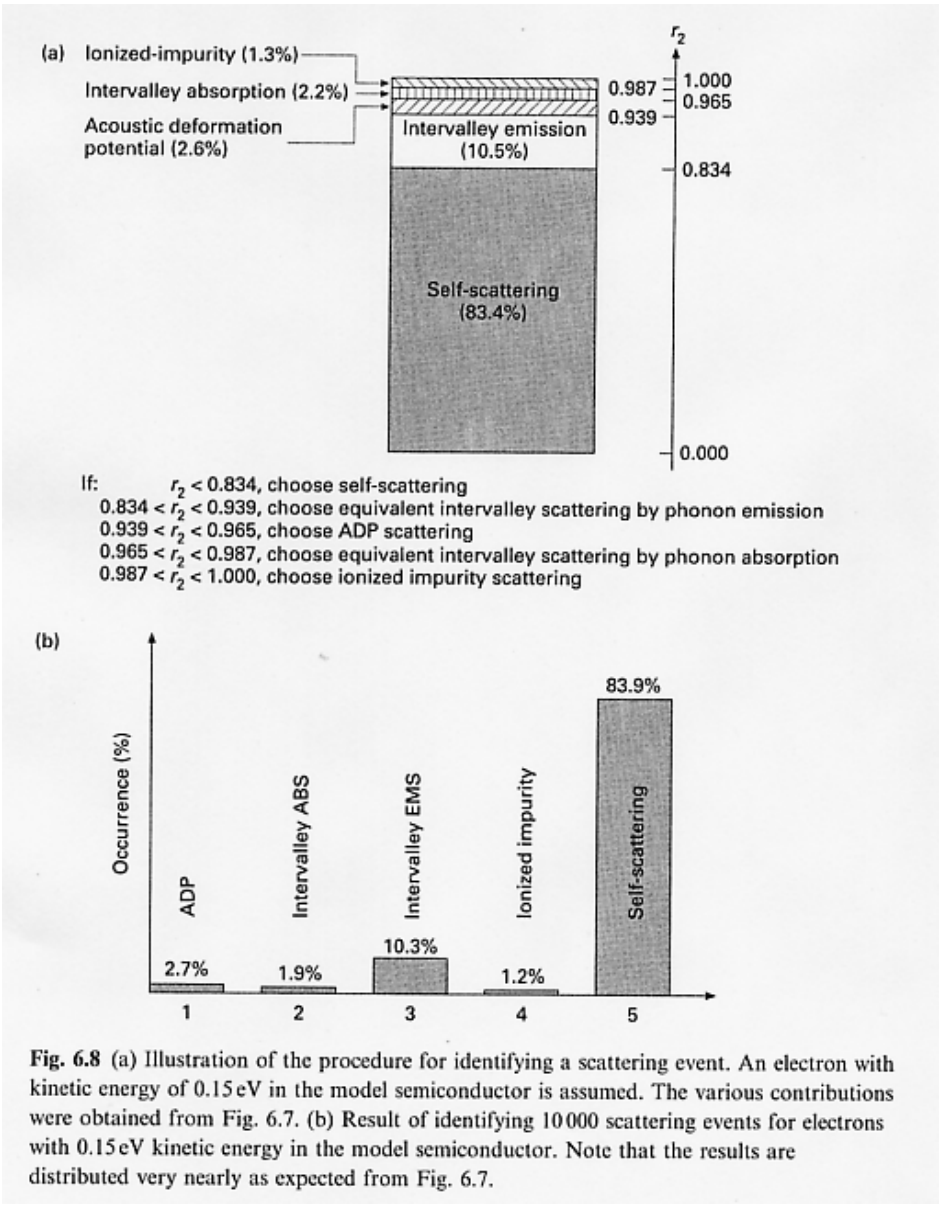


Fig. 6.8 (a) Illustration of the procedure for identifying a scattering event. An electron with kinetic energy of 0.15 eV in the model semiconductor is assumed. The various contributions were obtained from Fig. 6.7. (b) Result of identifying 10 000 scattering events for electrons with 0.15 eV kinetic energy in the model semiconductor. Note that the results are distributed very nearly as expected from Fig. 6.7.

- Lundstrom, Fig. 6.8

Selecting a Final State

- Generally the most expensive part of the computation
- Must select the final magnitude of momentum (energy) and its direction
- Consider particle states immediately before (t_c^-) and after (t_c^+) scattering

$$p(t_c^+) \equiv p' = \sqrt{2m^*\left[E\left(t_c^-\right) + \Delta E\right]}$$

  - assumes parabolic energy bands
  - ΔE is a fundamental characteristic of the scattering event (e.g., $\Delta E=0$ for elastic scattering, $\Delta E \sim \hbar\omega$ for events involving phonons)

Selecting a Final Direction

- Align local coordinate system with initial momentum vector **p**
- Assume azimuthal invariance

$$\int_0^{2\pi} P(\beta)d\beta = 1 \rightarrow P(\beta)d\beta = \frac{1}{2\pi}d\beta$$

- Thus, we can select azimuthal angle from a uniformly distributed random number r_3 as $\beta = 2\pi r_3$

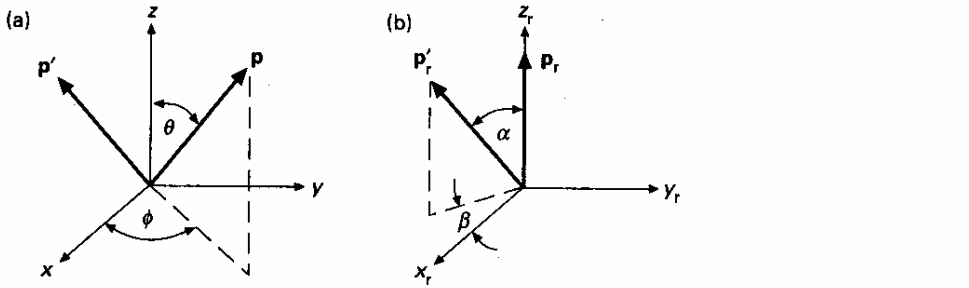


Fig. 6.9 (a) Scattering event in the $(\hat{x}, \hat{y}, \hat{z})$ coordinate system. The incident momentum is **p** and the scattered momentum, **p**′. (b) The same scattering event in the rotated coordinate system, $(\hat{x}_r, \hat{y}_r, \hat{z}_r)$, which is obtained by rotating $(\hat{x}, \hat{y}, \hat{z})$ by an angle of ϕ about the $\hat{z}$-axis, then θ about the $\hat{y}$-axis. In the rotated system, the incident momentum is $\mathbf{p}_r$ and the scattered momentum $\mathbf{p}'_r$.

- **Lundstrom Fig. 6.9**

Determination of the Polar Angle

- Scattering often depends on the polar angle; hence, its treatment is more complicated

$$\int_0^{\pi} P(\alpha)d\alpha = 1 \rightarrow P(\alpha)d\alpha = \frac{\sin\alpha d\alpha \int_0^{\infty}\int_0^{2\pi} S(\mathbf{p},\mathbf{p}')d\beta p'^2 dp'}{\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} S(\mathbf{p},\mathbf{p}')\sin\alpha d\alpha d\beta p'^2 dp}$$

- If we assume a simple delta-function scattering mechanism [S~δ(E'-E)], then

$$P(\alpha)d\alpha = \frac{\sin\alpha d\alpha}{2}$$

Final Polar Angle

- Now we seek another uniformly distributed random number r_4 between 0 and 1 to satisfy

$$P(r)dr = P(\alpha)d\alpha = \frac{\sin\alpha d\alpha}{2} \rightarrow P(r) = 1$$

$$\rightarrow \int_0^{r_4} dr = \frac{1}{2}\int_0^{\alpha} \sin\alpha' d\alpha' = \frac{1}{2}(1-\cos\alpha) \rightarrow \cos\alpha = 1 - 2r_4$$

- Finally, we find **p'** in the local coordinate system as

$$\mathbf{p'} = \begin{pmatrix} p'\sin\alpha\cos\beta \\ p'\sin\alpha\sin\beta \\ p'\cos\alpha \end{pmatrix}$$

- Last step involves transformation from local to global coordinates

Other Monte Carlo Topics

- Ensemble vs. incident flux approaches
  - Ensemble follows particles in parallel in a time-stepping procedure
    - Uses “superelectron” approximation
  - Incident flux follows each particle sequentially from beginning to end
- Treatment of Coulomb effects
  - Charged particles alter the local field through Coulomb interactions
  - Can be handled by summing individual contributions
  - If foregoing is too onerous, then particle-in-cell-type methods can be applied
  - Must ensure that the size of the time step does not exceed natural fluctuations at the plasma frequency

Relation between Monte Carlo Simulation at the BTE

- Consider a 1D slab on infinitesimal thickness that contains a single particle trajectory

$$\delta n_i(\mathbf{r},t) = \delta(\mathbf{r}-\mathbf{r_i}), \quad \text{and}$$

$$\delta f_i(\mathbf{r},\mathbf{p},t) = \delta(\mathbf{r}-\mathbf{r_i}(t))\delta(\mathbf{p}-\mathbf{p_i}(t))$$

- Apply the chain rule

$$\frac{\partial \delta f_i}{\partial t} = \nabla_{r_i}\delta f_i \cdot \frac{d\mathbf{r_i}}{dt} + \nabla_{p_i}\delta f_i \cdot \frac{d\mathbf{p_i}}{dt}$$

$$= \nabla_{r_i}\delta f_i \cdot \mathbf{v} + \nabla_{p_i}\delta f_i \cdot \left(-q\mathbf{E} + \left.\frac{\partial \mathbf{p_i}}{\partial t}\right|_{coll} \right)$$

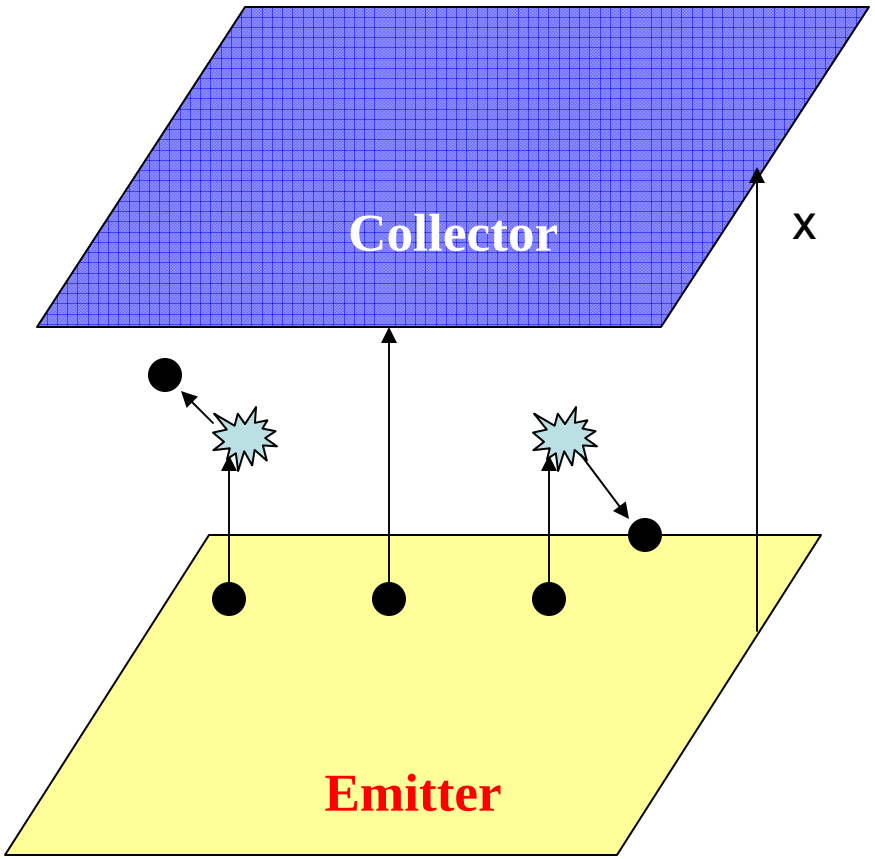
but we notice that $\nabla_{r_i,p_i}\delta f = -\nabla_{r,p}\delta f$

and $\nabla_{p_i}\delta f_i \cdot \left(\left.\frac{\partial \mathbf{p_i}}{\partial t}\right|_{coll} \right) = \left.\frac{\partial \delta f_i}{\partial t}\right|_{coll}$

now sum over all trajectories

$$\frac{\partial f}{\partial t} + \nabla_r f \cdot \mathbf{v} - q\mathbf{E}\cdot\nabla_p f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

Homework Problem



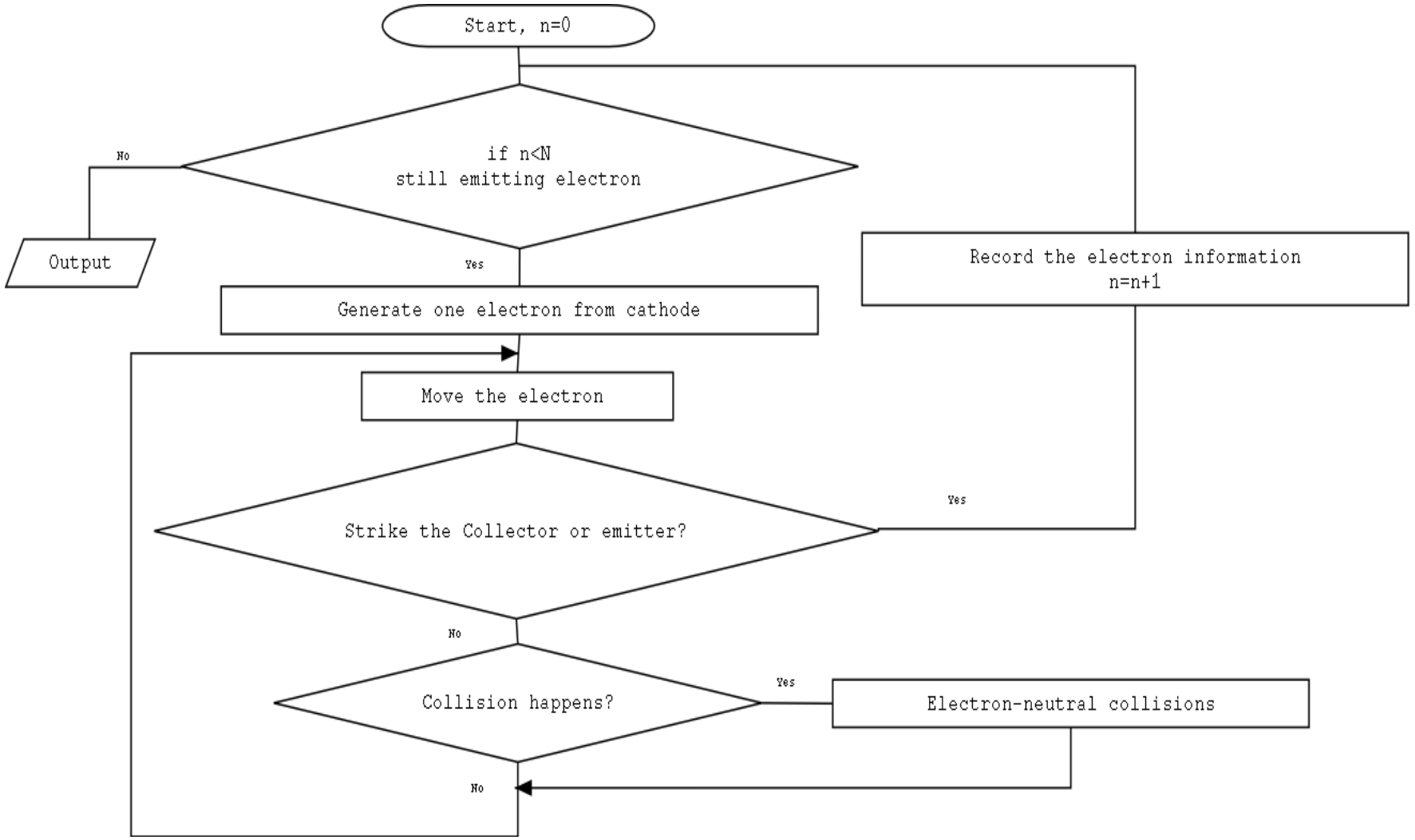
1. Two parallel infinite plates
2. Particles leave the same spot on the source plate at a fixed initial velocity
3. Assume no interactions among particles, i.e. neglect the force between particles
4. Particles scatter with a constant cross section
5. Post-collision velocity will be determined by the model provided
6. The spacing is so small that, for each particle, at most one collision would occur
7. Determine the radial and angular distributions on the collector, and the total number of collisions

Code Breakdown

- Data structure:
  - What do we use to represent a particle?
    - Something to bind together all the interesting kinetic properties of particles
    - A “particle” class in C++
    - A “particle” structure in C
    - A n by 7 array in C/C++, matlab, or Fortran 77

1	V_x	V_y	V_z	x	y	z
2	V_x	V_y	V_z	x	y	z
3	V_x	V_y	V_z	x	y	z

Algorithm


Start, n=0
if n<N
still emitting electron
No
Output
Yes
Generate one electron from cathode
Move the electron
Strike the Collector or emitter?
Yes
Record the electron information
n=n+1
No
Collision happens?
Yes
Electron-neutral collisions
No

Algorithm Breakdown

- Generate the particles at the emitter
  - Set the V_x according to the initial energy, assuming y, z velocity components of particles are neligible
  - Set X,Y,Z to zero

$$V_x = \sqrt{2E/m}, V_y = 0, V_z = 0$$

$$X = 0, Y = 0, Z = 0$$

Move particles

- What time step to use?

$$P(\Delta t) = 1 - \exp(-n\sigma\upsilon\Delta t) < 0.1$$

- Recommendation: ~ 1 femtosecond or less

$$L > \upsilon\Delta t$$

Position Updates

$$x^{n+1} - x^n = \upsilon_x dt$$

$$y^{n+1} - y^n = \upsilon_y dt$$

$$z^{n+1} - z^n = \upsilon_z dt$$

Collision

- Calculate the probability:

$$P(\Delta t) = 1 - \exp(-n\sigma\upsilon\Delta t)$$

$$r \in [0,1]$$

- Select a random number
- If r<P, then a collision occurs
- See notes about polar scattering angle and azimuthal angle
- See notes about post-collision velocity

Parameters

- Number of particles: N=50,000
- Initial kinetic energy of all particles: E=5eV

$$E = \frac{1}{2} m_e \upsilon^2$$

- Gap: L = 10 nm
- Cross-section, $\sigma = 10^{-18}$ m^2
- Number density of media (target particles), $n = 2.5 \times 10^{25}$ m^{-3}
- Assume that all scattering is elastic

Record the particle information

- When the particle hits the collector or the emitter, we assume it is absorbed without other side effects
- The final particle positions should be stored only for particles that have collided