Effect of Electron-Electron Scattering on the Energy Distribution in Semiconductor Devices

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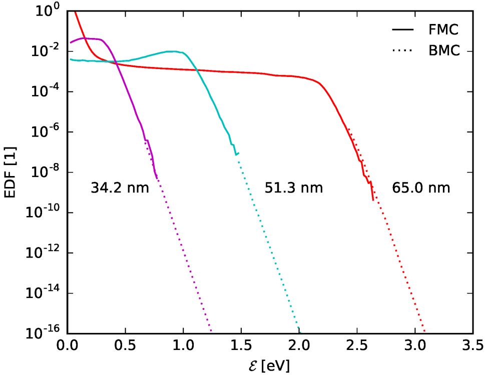
Motivation

Why electron-electron scattering (EES)?

- Thermalization of channel hot electrons in the drain region
- Modeling of hot carrier degradation:

  EES enhances the high-energy tail of the distribution function[1]



[1] P. Childs, C. Leung, J. Appl. Phys., 79, 222 (1996)

Outline

- Motivation
- Two-particle kinetic equation
- Two-particle Monte Carlo method
- Results and discussion
- Conclusion

Single-particle Formulation

- Boltzmann equation for electrons in a bulk semiconductor

$$\left(\frac{\partial}{\partial t} + \frac{e}{\hbar}\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}_1}\right) f(\boldsymbol{k}_1, t) = (Q_{\text{one}} + Q_{\text{ee}})[f](\boldsymbol{k}_1, t)$$

- Single-particle scattering operator (interactions with phonons, impurities, alloy disorder)

$$Q_{\text{one}}[f](\boldsymbol{k}_1, t) = \int [S(\boldsymbol{k}_1|\boldsymbol{k}_1')f(\boldsymbol{k}_1', t) - S(\boldsymbol{k}_1'|\boldsymbol{k}_1)f(\boldsymbol{k}_1, t)]\,\mathrm{d}\boldsymbol{k}_1'$$

- Two-particle scattering operator

$$Q_{\text{ee}}[f](\boldsymbol{k}_1, t) = \iiint S_{\text{ee}}(\boldsymbol{k}_1, \boldsymbol{k}_2|\boldsymbol{k}_1', \boldsymbol{k}_2')\left[f(\boldsymbol{k}_1', t)f(\boldsymbol{k}_2', t) - f(\boldsymbol{k}_1, t)f(\boldsymbol{k}_2, t)\right]\mathrm{d}\boldsymbol{k}_2\,\mathrm{d}\boldsymbol{k}_2'\,\mathrm{d}\boldsymbol{k}_1'$$

Two-particle Formulation

- Two-particle kinetic equation

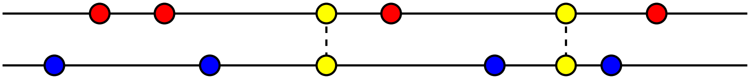
$$\left(\frac{\partial}{\partial t} + \frac{e}{\hbar}\left(\boldsymbol{E}\cdot\nabla_1 + \boldsymbol{E}\cdot\nabla_2\right)\right) g(\boldsymbol{k}_1,\boldsymbol{k}_2,t) = (Q_{\text{one}} + 2Q_{\text{ee}})[g](\boldsymbol{k}_1,\boldsymbol{k}_2,t)$$

- Two-particle scattering operator is linear in the two-particle distribution function

$$Q_{\text{ee}}[g](\boldsymbol{k}_1,\boldsymbol{k}_2,t) = \iint S_{\text{ee}}(\boldsymbol{k}_1,\boldsymbol{k}_2|\boldsymbol{k}_1',\boldsymbol{k}_2')\left[g(\boldsymbol{k}_1',\boldsymbol{k}_2',t) - g(\boldsymbol{k}_1,\boldsymbol{k}_2,t)\right] \mathrm{d}\boldsymbol{k}_1'\,\mathrm{d}\boldsymbol{k}_2'$$

- Augmentation of the single-particle scattering rate

$$S_{\text{one}}(\boldsymbol{k}_1,\boldsymbol{k}_2|\boldsymbol{k}_1',\boldsymbol{k}_2') = S(\boldsymbol{k}_1|\boldsymbol{k}_1')\,\delta(\boldsymbol{k}_2' - \boldsymbol{k}_2) + \delta(\boldsymbol{k}_1' - \boldsymbol{k}_1)\,S(\boldsymbol{k}_2|\boldsymbol{k}_2')$$



Stationary Two-particle MC Method

- Total scattering rate

$$\Gamma(\boldsymbol{k}_1,\boldsymbol{k}_2) = \Gamma_{\text{one}}(\boldsymbol{k}_1) + \Gamma_{\text{one}}(\boldsymbol{k}_2) + 2\,\Gamma_{\text{ee}}(\boldsymbol{k}_2 - \boldsymbol{k}_1)$$

- Electron-electron scattering rate is constant during a free flight

$$\Gamma_{\text{ee}}(\boldsymbol{k}_2 - \boldsymbol{k}_1) = \frac{ne^4 m}{4\pi\hbar^3\varepsilon_s^2\beta_s^2}\frac{|\boldsymbol{K}|}{|\boldsymbol{K}|^2 + \beta_s^2}, \qquad \boldsymbol{K} = \boldsymbol{k}_2(t) - \boldsymbol{k}_1(t) = \text{const}$$

- Self-scattering rate is added only to the single-particle rate

$$\Gamma_{\text{one}}^{\text{max}} = \Gamma_{\text{one}}(\boldsymbol{k}) + \Gamma_{\text{self}}(\boldsymbol{k})$$

- Free flight time calculation using self-scattering

$$\Gamma_{\text{max}} = 2\,\Gamma_{\text{one}}^{\text{max}} + 2\,\Gamma_{\text{ee}}(\boldsymbol{k}_2 - \boldsymbol{k}_1), \qquad t_{\text{f}} = -\frac{1}{\Gamma_{\text{max}}}\log(1-r)$$

Stationary Two-particle MC Method

- Probability distribution of the magnitude of the momentum transfer $q = |\boldsymbol{q}|$

$$p(q) = C\frac{q}{(q^2+\beta_s^2)^2}, \qquad 0 \le q \le K$$

- Generation of a random momentum transfer vector

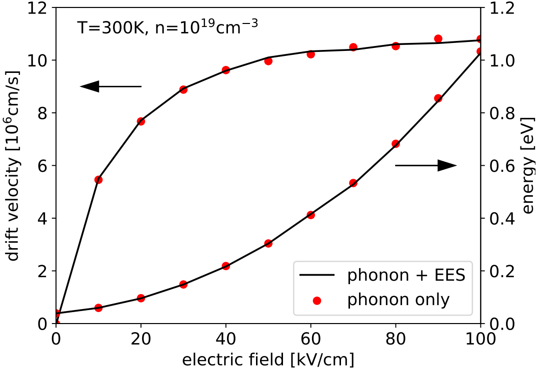
$$q^2 = \frac{r_1 K^2 \beta_s^2}{K^2(1-r_1)+\beta_s^2}, \qquad \cos\vartheta = \frac{q_r}{K}, \qquad \varphi = 2\pi r_2$$

- Wave vectors after electron-electron scattering

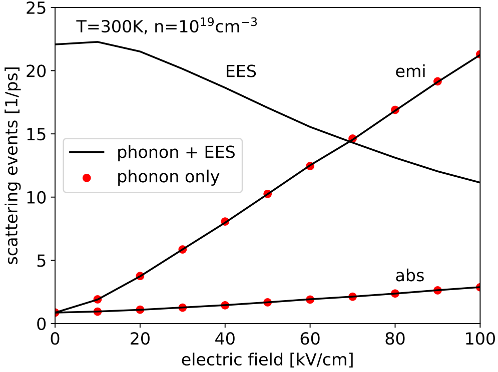
$$\boldsymbol{k}_1' = \boldsymbol{k}_1 + \boldsymbol{q}, \qquad \boldsymbol{k}_2' = \boldsymbol{k}_2 - \boldsymbol{q}$$

Exact conservation of momentum and energy!

Results for Bulk Silicon

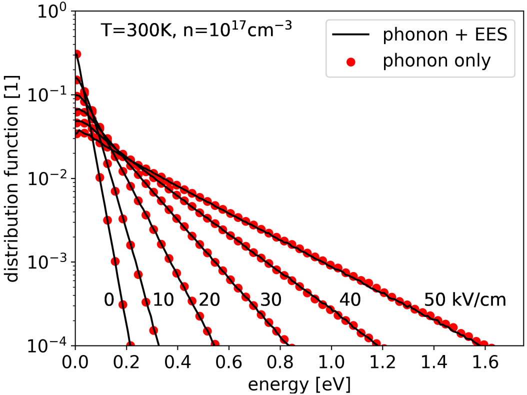


Mean velocity and mean energy versus electric field



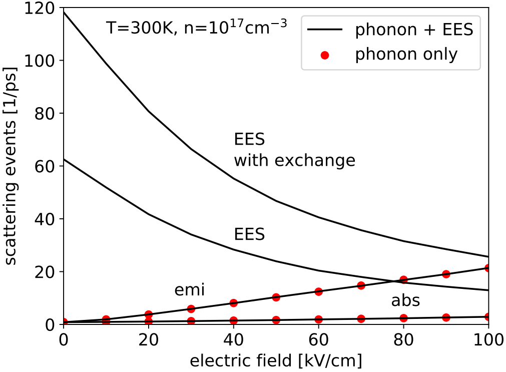
Number of scattering events in a given time interval

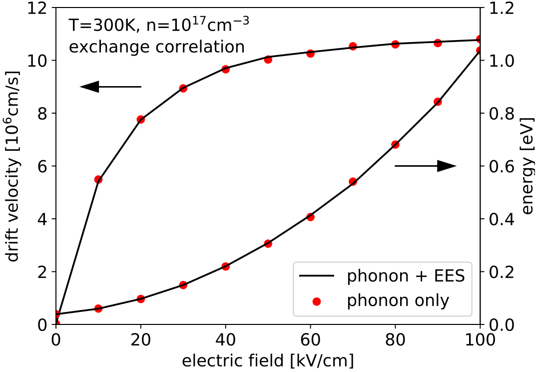
Results for Bulk Silicon



Distribution functions for uniform electric field

Effect of Exchange Correlation

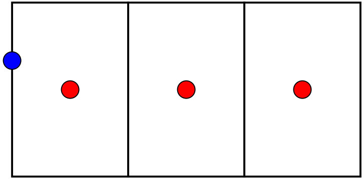




Position-dependent Two-particle MC Method

- Piece-wise constant approximation of $g(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{r})$ in real space
- Use bulk MC algorithm in each mesh cell
- Store initial state of a partner electron in each cell
- The following properties are used
  - Time invariance of the stationary equation
  - Markov property: duration of the remaining free flight is independent of the past

initial



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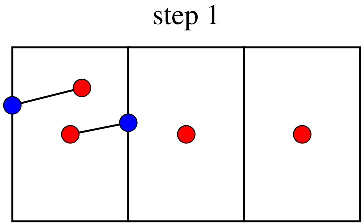

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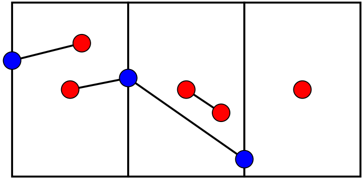
step 2



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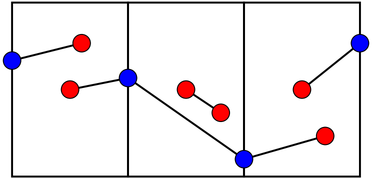

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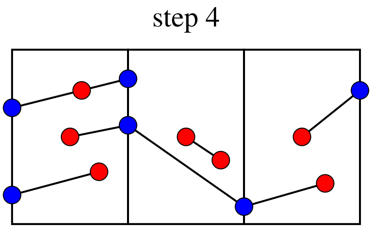

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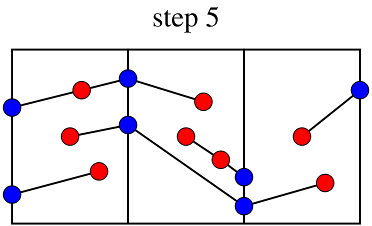

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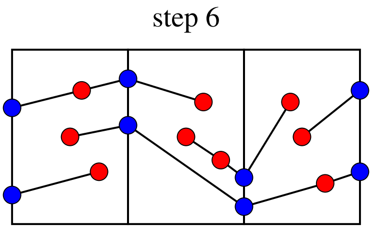
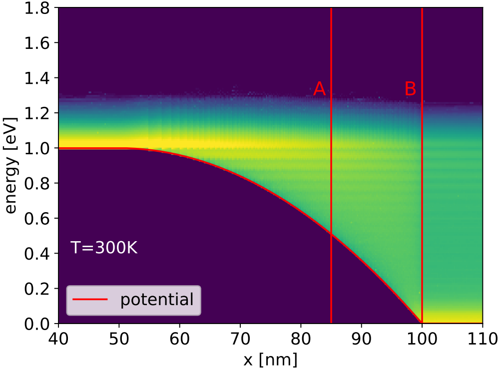
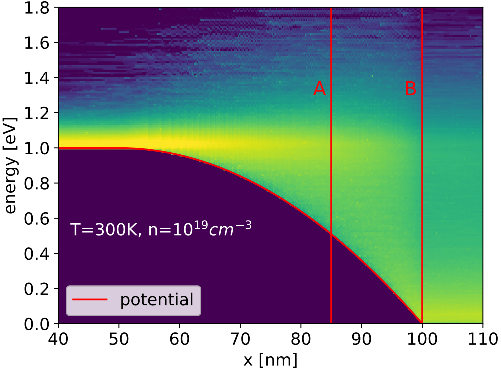


Distribution Function in a FET Channel

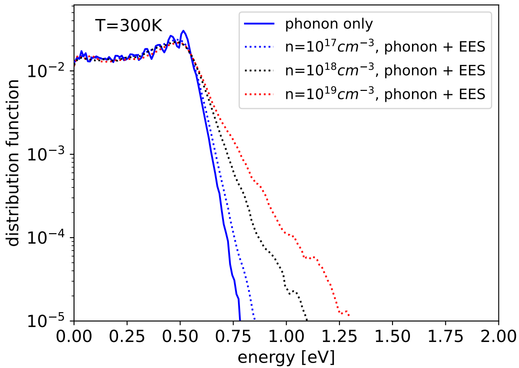


Phonon scattering only

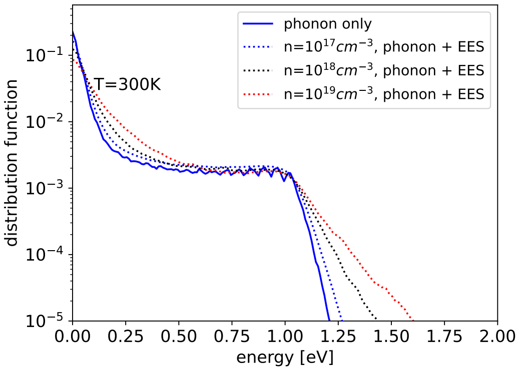


Phonon scattering + EES

Distribution Function in a FET Channel



Position A



Position B

Conclusion

- The stationary MC algorithm for the BTE is extended to the 6D momentum space

  The curse of high dimensionality does not apply to Monte Carlo

- Bulk semiconductors

  Negligible effect of EES on stationary averages and distribution function

- Devices

  EES enhances the high-energy tail in FET channels as predicted by P. Childs

  Enhancement scales with the electron density