Scattering in a Fermi Kinetics Transport Model

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INTRODUCTION

Computational tools capturing essential hot electron physics efficiently enough for 3D component simulation could aide with high speed microelectronics development for civilian and military applications such as secure broadband wireless, standoff detection, and noninvasive sensing. Ensemble Monte Carlo (EMC) [1] and spherical harmonic expansion offer high accuracy but at much computational cost. Energy transport models such as hydrodynamics are more efficient but often invoke statistical fitting parameters for accuracy and stability. A robust alternative based on the kinetics of ideal Fermi gases has demonstrated considerable flexibility and may provide numerically efficient accuracy suitable for computer-aided engineering.

A salient feature of Fermi kinetics is its use of the thermodynamic identity instead of an electron thermal conductivity for electronic heat flow [2]. This provides stability and versatility allowing its application to realistic band structures such as Fig. 1, which shows GaAs energy isosurfaces sorted into conduction band valleys. Separate Fermi gases are assigned to different valleys and band structure properties required for their kinetics (e.g. density of states, scattering rates/lifetimes, group velocities, etc.) are integrated over the corresponding isosurfaces. For example, real space charge flux from the 1st moment of the Boltzmann equation,

$$\boldsymbol{J}_i = \int_{E_i} \left[\int_{\boldsymbol{k}_i} \frac{v^2 \tau \delta_{E,E_{\boldsymbol{k}}} d\boldsymbol{k}}{12\pi^3 |\nabla_{\boldsymbol{k}} E|} \right] \left(q\boldsymbol{E} \frac{df_i}{dE} - \nabla f_i \right) dE, \tag{1}$$

can be evaluated when the quantity in brackets is integrated over each isosurface and saved as a function of electron energy, as shown for the Γ valley in Fig. 2. Other isosurface integral spectra of scattering rates, as determined by Fermi's Golden Rule, are computed, saved, and then used to evaluate charge dynamics in momentum space. Transport simulation balances the exchange of particles and energy in real space between neighboring Fermi gases with scattering in momentum between gases in different valleys, as depicted schematically in Fig. 3. A prototype considering optical deformation potential and polar optical mode scattering in GaAs computed the electron drift velocities in Fig. 4 that compared favorably with those from EMC [1], [3].

INCORPORATING ADDITIONAL SCATTERING

Further work has produced techniques for including other processes such as acoustic phonon, ionized impurity, and electron-electron scattering. It has indicated that even though moderately heated electrons in GaAs dissipate energy mostly through optical phonons, the umklapp-assisted acoustic phonon scattering depicted in Fig. 5 can have non-negligible effects on momentum relaxation and device currents. It has also suggested that momentum and energy conservation may significantly limit the "short range" screened Coulombic electron-electron interaction for a nonlinear band dispersion but that the "long range" plasmon interaction may have an important impact on momentum relaxation. Methods for implementing these processes will be presented along with their effects on isosurface integrals Fig. 2, electron transport properties Fig. 4, and device I-V characteristics Fig. 6.

ACKNOWLEDGMENT

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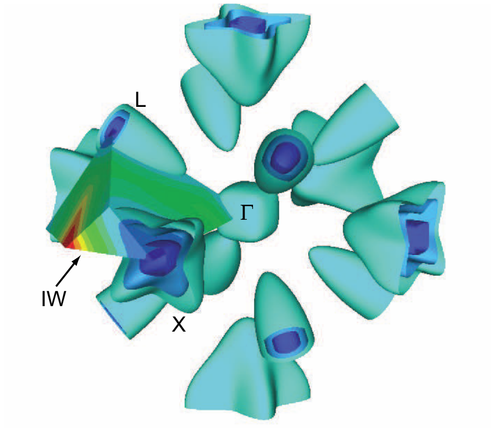

Fig. 1. Electron energy in the irreducible wedge (IW) and isosurfaces for Γ, L, and X valleys in the Brillouin zone of GaAs.

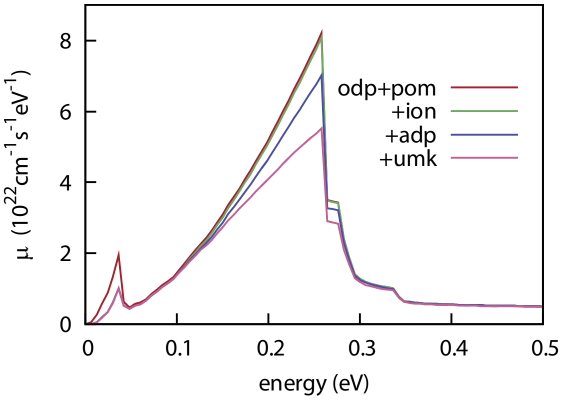

Fig. 2. Bracketed integrals in (1) for the Γ valley with optical deformation potential and polar optical mode scattering “odp+pom”, with additional ionized impurity scattering “+ion”, and including acoustic phonons both without “+adp” and with “+umk” umklapp assistance.

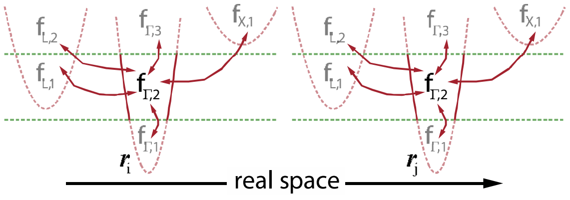

Fig. 3. Schematic of separate Fermi gases exchanging particles and energy in both real and momentum space. Real space exchanges occur between gases occupying the same regions of $\boldsymbol{k}$ space located at different $\boldsymbol{r}$. At each real space point $\boldsymbol{r}$, gases in different valleys interact by scattering in momentum space.

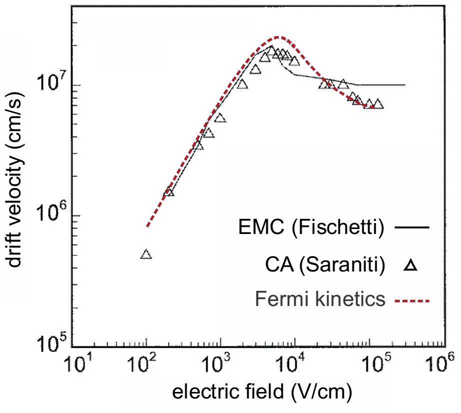

Fig. 4. Electron drift velocity in bulk GaAs with optical deformation potential and polar optical mode scattering “odp+pom” included in the Fermi kinetics model [1], [3].

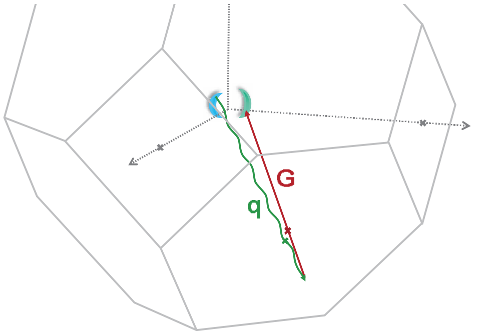

Fig. 5. Portion of the GaAs Brillouin zone showing low energy Γ states with anti-parallel $\boldsymbol{k}$ vectors interacting through umklapp-assisted acoustic phonon scattering $\boldsymbol{G} + \boldsymbol{q}$.

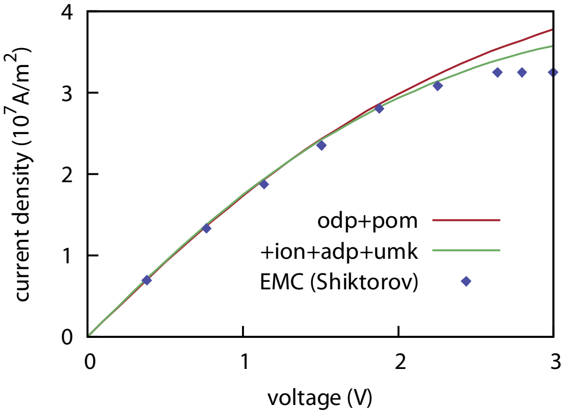

Fig. 6. Current vs. voltage computed for an n^+nn^+ device structure considering different scattering [3].