Comparison of Non-Parabolic Hydrodynamic Models Based On Different Band Structure Models

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This paper presents two non-parabolic hydrodynamic model formulations suitable for the simulation of inhomogeneous semiconductor devices. The first formulation uses the Kane dispersion relationship, \( (\hbar k)^2/2m = W(1 + \alpha W) \). The second formulation makes use of a power law, \( (\hbar k)^2/2m = xW^y \), for the dispersion relation. The non-parabolicity and energy range of the hydrodynamic model based on the Kane dispersion relation is limited. The power law formulation produces closed form coefficients similar to those under the parabolic band approximation but the carrier concentration can deviate. An extended power law dispersion relation is proposed to account for band structure effects, \( (\hbar k)^2/2m = xW^{1+y} \). This dispersion relation closely matches the calculated band structure over a wide energy range and may lead to closed form coefficients for the hydrodynamic model.

1. INTRODUCTION

Current hydrodynamic models consist of a set of conservation equations derived by taking moments of the Boltzmann transport equation. During the derivation of the conservation equations the parabolic band approximation is used to obtain rather simple coefficients on the forcing terms in the flux equations. By relying on the parabolic band approximation higher order energy transport effects due to variations in the band structure are neglected. Accounting for band structure effects in hydrodynamic device simulation is important because parabolic models can not adequately account for high energy effects in semiconductors with non-parabolic band structures.

Non-parabolic hydrodynamic models have been reported for homogeneous material systems \([1-4]\) using the Kane dispersion relationship \([5]\). The general functional form obtained is similar to parabolic hydrodynamic models with first order corrections on the diffusion term. However, the non-parabolic coefficient in the field term and the forcing terms due to non-uniform band structure are neglected in the moment equations. Cassi and Riccio \([6]\) introduced an alternative to the Kane relation in the form of a power law for the dispersion relationship. Instead of using a classical Kane dispersion law relating the energy and momentum, the band was fit over a specified energy range using two adjustable parameters. The approximations and assumptions implied by assuming the power law formulation were absent. It was shown in \([7]\) that the power law dispersion relation leads to a more simplistic and compact formulation than the classical Kane expression. A third non-parabolic dispersion relation is also proposed. It is shown that this new relation more closely matches the \( k^*P \) or pseudo-potential band structure calculations over a very wide energy range in several material systems.

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2. DISPERSION RELATIONS, CONCENTRATIONS, FLUX EQUATIONS

The dispersion relations considered in the derivation of the hydrodynamic conservation equations are; parabolic, Kane dispersion, power law, and extended power law

\[
\frac{(hk)^2}{2m_e} = W \quad \frac{(hk)^2}{2m_e} = W(1 + \alpha W)
\]

\[
\frac{(hk)^2}{2m_e} = xW^y \quad \frac{(hk)^2}{2m_e} = xW^{1+yW}
\]

where \(\alpha\) is the non-parabolicity factor and \(x, y\) are fitting parameters over a specified energy range. If the power law is fit over the energy range \(1.5 < W < 3.0\text{ eV}\) as suggested in [6] the deviation in carrier concentration from the parabolic case and the Kane formulation is greater than 80% at most reduced energy values. However, when fit over the energy range \(0 \leq W \leq 0.2\text{ eV}\) the deviation is only 2% [7]. This is due to the distribution function weighing more heavily to the lower energy. Therefore, to accurately account for the carrier concentration the dispersion relation must match at lower energies and to simulate high energy effects it must match the band structure at higher energies.

3. EXTENDED POWER LAW DISPERSION

Current work focuses on the development of a hydrodynamic formulation which uses an extended power law dispersion relation, \((hk)^2/2m = xW^{1+yW}\). Figures 1, 2, and 3 display comparison of this new formulation to band structure calculations and to the other non-parabolic formulations for Si, GaAs and GaN.

The following values and fitting parameters were used in the comparison of the dispersion relations.

<table>
<thead>
<tr>
<th>Dispersion</th>
<th>Material</th>
<th>Si</th>
<th>GaAs</th>
<th>GaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kane formulation ((\alpha))</td>
<td>0.4039</td>
<td>0.607</td>
<td>0.336</td>
<td></td>
</tr>
<tr>
<td>Power Law</td>
<td>(0 &lt; x &lt; 0.2\text{ eV fit})</td>
<td>(x = 3.1604)</td>
<td>(x = 0.7249)</td>
<td>(x = 1.0121)</td>
</tr>
<tr>
<td></td>
<td>(y = 1.0339)</td>
<td>(y = 0.8101)</td>
<td>(y = 1.05758)</td>
<td></td>
</tr>
<tr>
<td>Extended Power Law</td>
<td>(0 &lt; x &lt; 2.0\text{ eV fit})</td>
<td>(x = 3.1969)</td>
<td>(x = 2.9816)</td>
<td>(x = 0.9273)</td>
</tr>
<tr>
<td></td>
<td>(y = 0.1062)</td>
<td>(y = 2.2151)</td>
<td>(y = 0.1935)</td>
<td></td>
</tr>
</tbody>
</table>

The insert in Figures 1-3 show the fit at lower energies and displays that the extended power law is a good fit. In all cases the extended power law relation also provides a very good fit up to very high energy ranges, note that both of the other non-parabolic formulations are poor fits at the higher energy ranges. Preliminary derivations indicate the extended power law relation may produce closed form coefficients for specific distribution functions. Note that there is a substantial difference in the definition of the \(y\) term in the power law case as compared to the extended power law formulation. In the power law case \(y\) approaches 1 as non-parabolicity is decreased, on the other hand \(y\) approaches 0 as non-parabolicity is decreased in the extended power law formulation.

4. FLUX CONSERVATION EQUATIONS

The derivation and comparison of models based on the Kane formulation and power law are given in references [7-8]. Similarly the electron energy flux equations using these dispersion relations can also be formulated [7]. In reference [7] it was shown that as \(y\) approaches 2 in the power law formulation the field contribution to current is diminished. If the field pref-
actor is not included, as in previous models, then the flux would be overestimated. The resulting flux equations for the dispersion relations in equation (1) are

\[
\frac{\partial}{\partial t} (\nabla f) + \frac{2}{3m_e} \nabla_f (fW) + \nabla_f f - \frac{m_e}{m_e^2} fW = \nabla_f (f - f_0) \quad (2)
\]

\[
\frac{\partial}{\partial t} (\nabla f) + \frac{2}{3m_e} \nabla_f \left( \frac{fW(1 + \alpha W)}{(1 + 2\alpha W)^2} \right)
- \left( \frac{W^2}{m_e(1 + 2\alpha W)^4} \right) \nabla_f = \nabla_f (f - f_0) \quad (3)
\]

\[
\frac{\partial}{\partial t} (\nabla f) + \frac{2}{3m_{exy}} V (fW^{2-\gamma}) 
+ \left[ \frac{\nabla m_e}{m_e} + \frac{\nabla x}{x} \right] \frac{W^{2-\gamma}(y-4)}{3m_{exy}} 
+ \left( \frac{fW^{1-\gamma}}{m_{exy}} \right) \left( \frac{2}{y-1} \right) \nabla_f + \left( \frac{fW^{2-\gamma}}{m_{exy}} \right) 
\left( -\frac{2}{3} (1 + 2\ln(W) + y\ln(W)) \right) \nabla_f = \nabla_f (f - f_0) \quad (4)
\]
\[
\frac{\partial}{\partial t} (\nabla_k f) + \frac{2}{3m_e x} \nabla \left( \frac{f W^{1-y}}{(1 + yW (1 + \ln(W)))^2} \right) \nabla x + \frac{\nabla m_e}{m_e} \frac{\nabla x}{x} f W^{1-y} \frac{3m_e x (1 + yW (1 + \ln(W)))^2}{1 - \frac{4(1 - yW)}{(1 + yW (1 + \ln(W)))^2}} \nabla \phi_e \]
\[
+ \left( \frac{f W^{2-y}}{m_e x (1 + yW (1 + \ln(W)))^3} \right) \left( \frac{2(1 - yW)}{(1 + yW (1 + \ln(W)))^2} - 1 \right) \nabla \phi_e \]
\[
+ \ln(W) (1 + yW (1 + \ln(W))) \right) + \frac{2}{3} (1 + \ln(W)) \right) \nabla \phi = \nabla_k \frac{f - f_0}{\tau} \tag{5}
\]

Each of these equations must be integrated over all \( k \) space or equivalently over energy after some form of the distribution function or a closing relation for the distribution function is assumed. In reference [8] the distribution function was assumed to be a heated Fermi-Dirac to provide a valid basis of comparison between the different models simulated.

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References
