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Electron transport in non-parabolic Kane bands

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Abstract. Linear and non-linear transport properties of carriers in non-parabolic Kane bands are investigated using the two extended balance equations introduced by Magnus, Sala and De Meyer (MSD) and by Lei. Formally, the MSD equations describe the motion of a single particle with fixed charge and fixed mass, while the Lei equations describe the motion of a single particle having fixed charge but variable effective mass. In the parabolic limit these two sets of equations are identical and reduce to the original Lei–Ting balance equations. In the non-parabolic case, although the linear resistivities predicted by the Lei and MSD equations are nearly the same for weakly to medially non-parabolic systems, non-linear drift-velocity–field behaviour obtained from these two sets of equations shows marked differences for medial and strong non-parabolicity. The reasons for these differences are discussed.

1. Introduction

Band non-parabolicity of electrons has been observed to influence many features of narrow-gap semiconductors where the energy bands are non-parabolic, resulting in special transport behaviour of these materials [1]. In the extremely non-parabolic band case, such as in a miniband of a semiconductor superlattice, electron conduction exhibits negative differential mobility [2]. A tight-binding model is widely used for describing superlattice minibands and the Kane $k \cdot p$ model [3] is believed to be suitable for describing most of the energy bands in narrow-gap semiconductors. The transport properties related to energy band non-parabolicity have been extensively studied using the Boltzmann equation [4] and Monte Carlo simulations [5–7].

A few years ago, Lei and Ting [8] proposed a balance equation theory for high-field electronic transport in semiconductors. The original equations were derived for parabolic bands or for systems that can be described by effective-mass approximations. In an attempt to extend the Lei–Ting theory to non-parabolic bands, Magnus, Sala and De Meyer [9] (MSD) suggested that the exact set of original Lei–Ting balance equations given in [8] can still be used to describe non-parabolic band structures, as long as the non-parabolic energy dispersion relation is taken into account in the electron density–density correlation function. They observed marked differences in the behaviour of this quantity in a parabolic and a non-parabolic band structure [9] and investigated electronic transport in $Al_xGa_{1-x}As/GaAs$ heterojunctions [10] with non-parabolicity included. However, it fails to produce a negative differential mobility in superlattice miniband transport [11]. On the other hand, one of the present authors proposed another extension of the Lei–Ting balance equations to an arbitrary energy band [12], in which two parameters (centre-of-mass momentum and electron

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temperature) are used to describe the hot carrier transport, and an ensemble-averaged inverse effective-mass tensor is introduced, which carries the non-parabolicity together with the velocity function and density–density correlation function. Lei's equations have been applied to superlattice miniband transport, obtaining the Esaki–Tsu negative differential velocity in good agreement with experiment [13, 14]. However, they have not yet been applied to non-parabolic band structures other than those of the tight-binding type.

The purpose of this paper is to compare the balance equations introduced by Lei and MSD through their application to hot electron transport in the same non-parabolic Kane band structure with varying degrees of non-parabolicity.

2. The MSD and Lei equations

We consider an interacting electron system that consists of N electrons moving within a GaAs background under the influence of a uniform electric field $\boldsymbol{E}$, the direction of which is taken as the z axis. The electron conduction band spectrum $\varepsilon(k)$ is taken as the Kane $k \cdot p$ model ($\hbar = 1 = k_B$ throughout the paper):

$$\varepsilon(1 + \alpha\varepsilon) = \frac{k^2}{2m} \tag{1}$$

where $m = 0.067m_0$ is the electron band mass in GaAs, and m_0 is the free electron mass. The non-parabolic coefficient of the conduction band, α, is generally taken as $\alpha = 1/E_g$, E_g being the band gap between the conduction and valence bands. Here we treat α as a parameter to measure the non-parabolicity.

According to MSD [9, 10], the non-parabolicity of the band structure only enters the density–density correlation function through a modification of the expression for the electron energy. Force and energy balance equations for a non-parabolic band are the same as those in the original Lei–Ting balance equations for a parabolic band [8], in which the centre-of-mass velocity v_d, i.e. the drift velocity of the electron system, and the electron temperature T_e are used as fundamental parameters, and may be written as follows:

$$\frac{e\boldsymbol{E}}{m} + \frac{\boldsymbol{F}_i}{m} + \frac{\boldsymbol{F}_p}{m} = 0 \tag{2}$$

and

$$e\boldsymbol{E} \cdot \boldsymbol{v}_d - W = 0. \tag{3}$$

The frictional forces due to impurity and phonon scatterings, $\boldsymbol{F}_i$ and $\boldsymbol{F}_p$, are given by

$$\boldsymbol{F}_i/m = \frac{2\pi n_i}{N} \sum_{k,q} |u(q)|^2 |g(k,q)|^2 \frac{q}{m} \frac{f\big(\varepsilon(k), T_e\big) - f\big(\varepsilon(k+q), T_e\big)}{\big|\epsilon\big(q, \varepsilon(k) - \varepsilon(k+q)\big)\big|^2} \times \delta\big(\varepsilon(k+q) - \varepsilon(k) + q \cdot v_d\big) \tag{4}$$

$$\boldsymbol{F}_p/m = \frac{4\pi}{N} \sum_{k,q,\lambda} |M(q,\lambda)|^2 |g(k,q)|^2 \frac{q}{m} \frac{f\big(\varepsilon(k), T_e\big) - f\big(\varepsilon(K+q), T_e\big)}{\big|\epsilon\big(q, \varepsilon(k) - \varepsilon(k+q)\big)\big|^2} \times \left[n\left(\frac{\Omega_{q\lambda}}{T}\right) - n\left(\frac{\Omega_{q\lambda} + q \cdot v_d}{T_e}\right) \right] \delta\big(\varepsilon(k+q) - \varepsilon(k) + q \cdot v_d + \Omega_{q\lambda}\big) \tag{5}$$

and the power dissipation rate from the electron system to the phonon system is

$$W = \frac{4\pi}{N}\sum_{k,q,\lambda}|M(q,\lambda)|^2|g(k,q)|^2\Omega_{q\lambda}\frac{f\big(\varepsilon(k),T_e\big)-f\big(\varepsilon(k+q),T_e\big)}{\big|\epsilon\big(q,\varepsilon(k)-\varepsilon(k+q)\big)\big|^2}$$
$$\times\left[n\left(\frac{\Omega_{q\lambda}}{T}\right)-n\left(\frac{\Omega_{q\lambda}+q\cdot v_d}{T_e}\right)\right]\delta\big(\varepsilon(k+q)-\varepsilon(k)+q\cdot v_d+\Omega_{q\lambda}\big). \quad (6)$$

In these equations, n_i is the impurity density, $\Omega_{q\lambda}$ is the frequency of the phonon with wavevector q in branch λ; $u(q)$ and $M(q,\lambda)$ are the Fourier representations of the impurity potential and electron–phonon coupling matrix element. The symbol T denotes the lattice temperature, and $n(x)=(e^x-1)^{-1}$ is the Bose function; $g(k,q)$ is a form factor determined by the electron wavefunction, and (with $v_c(q)=e^2/\epsilon_0 q^2$)

$$|\epsilon(q,\omega)|^2=\left(1-v_c(q)\sum_k\Pi_1^0(k,q,\omega)\right)^2+\left(v_c(q)\sum_k\Pi_2^0(k,q,\omega)\right)^2 \quad (7)$$

is the RPA dielectric function of the electron system, with $\Pi_1^0(k,q,\omega)$ and $\Pi_2^0(k,q,\omega)$ being the real and imaginary parts of the density–density correlation function in the absence of the intercarrier Coulomb interaction, $\Pi^0(k,q,\omega)$:

$$\Pi^0(k,q,\omega)=2|g(k,q)|^2\frac{f\big(\varepsilon(k+q),T_e\big)-f\big(\varepsilon(k),T_e\big)}{\varepsilon(k+q)-\varepsilon(k)+\omega+i\delta}. \quad (8)$$

Here

$$f\big(\varepsilon(k),T_e\big)=\{\exp\big[(\varepsilon(k)-\mu)/T_e\big]+1\}^{-1} \quad (9)$$

is the Fermi function at electron temperature T_e and μ is the chemical potential, which is determined by the total number of electrons, N, according to

$$N=2\sum_k f\big(\varepsilon(k),T_e\big). \quad (10)$$

On the other hand, Lei's extended equations [12] use the centre-of-mass momentum $P_d=Np_d$ and the electron temperature T_e as fundamental parameters. The major part of the non-parabolic effect on transport shows up through the ensemble-averaged inverse effective-mass tensor $\mathcal{K}$, which is defined by

$$\mathcal{K}=\frac{2}{N}\sum_k\nabla\nabla\varepsilon(k)f(\bar{\varepsilon}(k),T_e) \quad (11)$$

where

$$\bar{\varepsilon}(k)\equiv\varepsilon(k-p_d) \quad (12)$$

is the relative electron energy. Non-parabolicity also shows up through the energy function $\varepsilon(k)$ and the velocity function $v(k)\equiv\nabla\varepsilon(k)$. The average drift velocity of the electron system is given by

$$v_d=\frac{2}{N}\sum_k\nabla\varepsilon(k)f\big(\bar{\varepsilon}(k),T_e\big). \quad (13)$$

The force and energy balance equations for a non-parabolic band take the form

$$eE\cdot\mathcal{K}+A_i+A_p=0 \quad (14)$$

and

$$eE \cdot v_d - W = 0. \tag{15}$$

The accelerations due to impurity and phonon scatterings, A_i and A_p, and the energy dissipation rate, W, are respectively

$$A_i = \frac{2\pi n_i}{N} \sum_{k,q} |u(q)|^2 |g(k,q)|^2 [v(k+q) - v(k)] \delta\big(\varepsilon(k+q) - \varepsilon(k)\big) \times \frac{f\big(\bar{\varepsilon}(k), T_e\big) - f\big(\bar{\varepsilon}(k+q), T_e\big)}{\big|\epsilon\big(q, \bar{\varepsilon}(k) - \bar{\varepsilon}(k+q)\big)\big|^2} \tag{16}$$

$$A_p = \frac{4\pi}{N} \sum_{k,q,\lambda} |M(q,\lambda)|^2 |g(k,q)|^2 [v(k+q) - v(k)] \delta\big(\varepsilon(k+q) - \varepsilon(k) + \Omega_{q\lambda}\big) \times \frac{f\big(\bar{\varepsilon}(k), T_e\big) - f\big(\bar{\varepsilon}(k+q), T_e\big)}{\big|\epsilon\big(q, \bar{\varepsilon}(k) - \bar{\varepsilon}(k+q)\big)\big|^2} \left[n\left(\frac{\Omega_{q\lambda}}{T}\right) - n\left(\frac{\bar{\varepsilon}(k) - \bar{\varepsilon}(k+q)}{T_e}\right) \right] \tag{17}$$

$$W = \frac{4\pi}{N} \sum_{k,q,\lambda} |M(q,\lambda)|^2 |g(k,q)|^2 \Omega_{q\lambda} \frac{f\big(\bar{\varepsilon}(k), T_e\big) - f\big(\bar{\varepsilon}(k+q), T_e\big)}{\big|\epsilon\big(q, \bar{\varepsilon}(k) - \bar{\varepsilon}(k+q)\big)\big|^2} \times \delta\big(\varepsilon(k+q) - \varepsilon(k) + \Omega_{q\lambda}\big) \left[n\left(\frac{\Omega_{q\lambda}}{T}\right) - n\left(\frac{\bar{\varepsilon}(k) - \bar{\varepsilon}(k+q)}{T_e}\right) \right]. \tag{18}$$

Although formally the energy balance equation in the MSD and Lei prescriptions is similar (the expressions for the energy transfer rate, W, however, are not equivalent), the force balance equations, i.e. the equation of motion of the centre of mass, are apparently different in the two cases. The force balance equation (2) in the MSD case describes the motion of a single particle having fixed charge and fixed mass, while the force balance equation (14) in Lei's case describes the motion of a single particle having fixed charge but variable (p_d- and T_e-dependent) inverse effective mass $\mathcal{K}$. Nevertheless, both sets of balance equations reduce to the original Lei–Ting balance equations in the parabolic limit ($\alpha = 0$). The MSD equations have been used to calculate superlattice miniband transport, but no negative differential mobility has been found in the wide ranges of structure and material parameters investigated [11]. On the other hand, Lei's equations are able to give Esaki–Tsu negative differential mobility in the superlattice vertical transport at high electric field with predictions in good agreement with experiment [13, 14].

3. Non-linear and linear transport

In order to quantitatively compare the two extended balance equations in an application to electron transport in narrow-gap semiconductors, we have numerically calculated the linear and non-linear transport properties using the MSD and Lei equations for Kane non-parabolic band systems. The dominant scatterings are assumed to be polar optic phonons and randomly distributed impurities. The material parameters are taken as the well known bulk values of GaAs: LO-phonon energy $\Omega_{q\lambda} = 35.4$ meV, low-frequency dielectric constant $\kappa = 12.9$ and

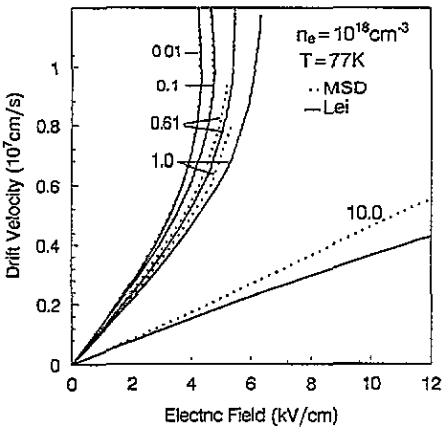

Figure 1. The drift velocity calculated from MSD equations (dotted curves) and Lei equations (full curves) is shown as a function of the electric field at $T = 77$ K. The systems are assumed to have a Kane non-parabolic band with a varying degree of non-parabolicity. The electron density $n_e = 10^{18}\,cm^{-3}$. The numbers near the curves are the values of the non-parabolic coefficient α (in units of eV^{-1}).

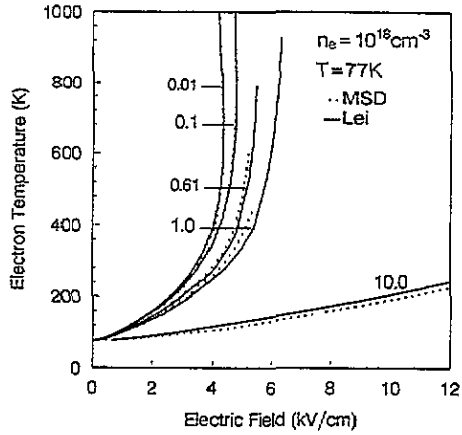

Figure 2. The electron temperatures against the external electric field are shown for the same system as in figure 1.

optical dielectric constant $\kappa_\infty = 10.8$. The system is assumed to be homogeneous and the impurity density is taken as the electron density.

First, we study the non-linear transport properties. In figure 1 we plot the non-linear drift velocity as a function of the electric field, calculated from MSD (dotted curves) and Lei (full curves) equations with varying degrees of non-parabolicity ($\alpha = 0.01$, 0.1, 0.61, 1.0 and $10.0\,eV^{-1}$) at electron density $n_e = 10^{18}\,cm^{-3}$. The lattice temperature is taken as 77 K. The drift-velocity–field behaviour obtained from these two sets of equations is similar and significantly depends on the energy dispersion relation: in the weakly non-parabolic band ($\alpha = 0.01$, $0.1\,eV^{-1}$), there exist positive, zero and negative differential resistivity regions. In the medially non-parabolic bands ($\alpha = 0.61$, $1.0\,eV^{-1}$), the negative differential resistivity region disappears. In the strongly non-parabolic case ($\alpha = 10.0\,eV^{-1}$), the curves become downward. The drift velocities in the medially to strongly non-parabolic bands obtained from the MSD equations are higher than those from the Lei equations within the whole range of the electric field. The electron temperature as a function of the electric field is shown in figure 2. The electron temperature in the MSD case is higher than that in the Lei case in medial non-parabolicity, while it is lower in strongly non-parabolic bands.

In the case that the electric field direction is taken as the z axis, for the Kane band, the inverse effective-mass tensor K introduced in the Lei equations, defined by (11), has only non-vanishing diagonal components, $K_{ij}=0$ ($i \neq j$), and only the diagonal component along the E direction, which we denote as $1/m^*$, plays a role in the force balance equation (14). To gain an idea of how the effective mass varies in the Lei equations, we plot in figure 3 the normalized inverse effective mass, m/m^*, as a function of the electric field. The dependence of m/m^* on the electric field is significant for the medially to strongly non-parabolic case. This inverse effective-mass tensor, which involves an average over the whole energy band, represents a major effect of the non-parabolicity on transport. This is different from that of the cyclotron resonance experiment at low temperature, where the electron effective mass represents the effect of an equal-energy surface in the non-parabolic

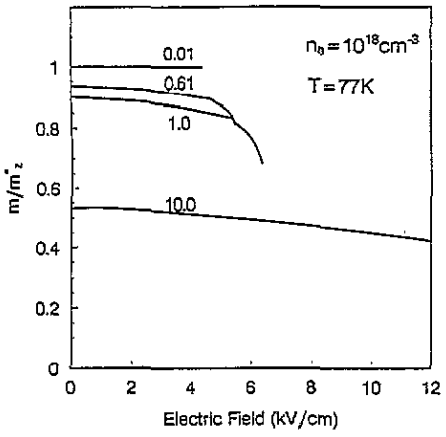

Figure 3. Normalized inverse effective mass m/m_z^* in the Lei equations plotted against the electric field for the same system as in figure 1. The numbers near the curves are the values of the non-parabolic coefficient α (in units of eV^{-1}).

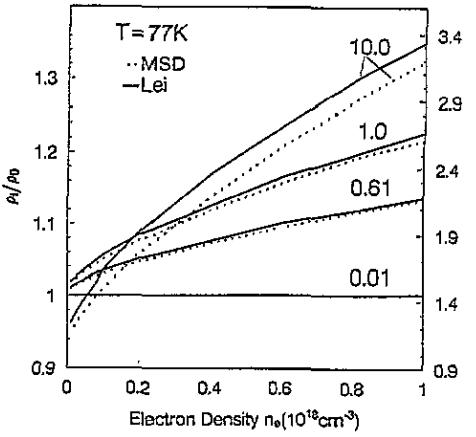

Figure 4. Normalized linear resistivities due to impurities, ρ_i/ρ_0, obtained from the MSD approach (dotted curves) and from the Lei approach (full curves) are shown as a function of the electron density at a lattice temperature $T = 77$ K with a varying degree of non-parabolicity; ρ_0 is the linear resistivity in the parabolic band. The scale of the vertical axis on the left-hand side refers to the curves of $\alpha = 0.01$, 0.61 and $1.0\,eV^{-1}$ and that on the right-hand side to the curves of $\alpha = 10.0\,eV^{-1}$. The numbers near the curves are the values of non-parabolic coefficient α (in units of eV^{-1}).

band [15].

From the force balance equations, (2) and (14), the linear resistivities due to impurity from the two methods, ρ_{i-MSD} and ρ_{i-Lei}, can be written as

$$\rho_{i-MSD} = C_i \int \sin\theta d\theta \int d\phi \int \sin\theta_1 \, d\theta_1 \int dq |\bar{u}(q)|^2 q^5 \frac{\cos^2\theta_1}{|\cos\xi|^3} \times [1 + 2\alpha\varepsilon(k)] \frac{e^{(\varepsilon(k)-\mu)/T}}{(e^{(\varepsilon(k)-\mu)/T}+1)^2}\bigg|_{k=-q/2\cos\xi} \tag{19}$$

and

$$\rho_{i-Lei} = \frac{C_i}{C^2(\alpha)} \int \sin\theta \, d\theta \int d\phi \int \sin\theta_1 \, d\theta_1 \int dq |\bar{u}(q)|^2 q^5 \frac{\cos^2\theta_1}{|\cos\xi|^3} \times [1 + 2\alpha\varepsilon(k)]^{-1} \frac{e^{(\varepsilon(k)-\mu)/T}}{(e^{(\varepsilon(k)-\mu)/T}+1)^2}\bigg|_{k=-q/2\cos\xi} \tag{20}$$

respectively. In these equations, $\cos\xi \equiv \cos\theta\cos\theta_1 + \sin\theta\sin\theta_1\cos\phi$, $\bar{u}(q)$ is the statically screened electron–impurity potential and $C(\alpha)$ and C_i are given by

$$C(\alpha) = \frac{2}{N}\sum_k \{[1 + 2\alpha\varepsilon(k)]^{-1} - 2\alpha k_z^2 [1 + 2\alpha\varepsilon(k)]^{-3}/m\} f(\varepsilon(k), T) \tag{21}$$

and

$$C_i = \frac{4n_i}{n^2 e^2 (2\pi)^4}. \tag{22}$$

The second term in (21) is small and can be neglected.

In figure 4, we show the normalized linear resistivities due to impurity scattering, ρ_i/ρ_0, as functions of the electron density (from 10^{16} to $10^{18}\,\mathrm{cm}^{-3}$) at a lattice temperature $T = 77\,\mathrm{K}$; ρ_0 is the linear resistivity of the parabolic band under the same conditions. The dotted and the full curves refer to the results of the non-parabolic band from the MSD and Lei equations respectively. The scale of the vertical axis on the left-hand side refers to the curves of $\alpha = 0.01,\ 0.61,\ 1.0\,\mathrm{eV}^{-1}$ and that on the right-hand side to the curves of $\alpha = 10.0\,\mathrm{eV}^{-1}$. The deviation of the linear impurity resistivities of the non-parabolic bands from those of the parabolic band increases with increasing electron density because of the high-energy states occupied by the electrons. The numerical results indicate that the linear resistivities from these two equations are almost equivalent for small to medial non-parabolicity (e.g. $\alpha \leqslant 1.0$) within the whole range of carrier density. For strongly non-parabolic bands, the difference of linear resistivities from these two equations appears. The coincidence of the linear resistivity predicted by both sets of equations for small and medial α can be understood by comparing (19) and (20). If, for dominant $\varepsilon(k)$, the non-parabolic coefficient α satisfies the condition $\alpha\varepsilon \ll 1$, we can expand ρ_{i-Lei} to first order in terms of $\alpha\varepsilon$ and get

$$\rho_{i-Lei} = C_i \int \sin\theta\,\mathrm{d}\theta \int \mathrm{d}\phi \int \sin\theta_1 \mathrm{d}\theta_1 \int \mathrm{d}q |\bar{u}(q)|^2 q^5 \frac{\cos^2\theta_1}{|\cos\xi|^3} \times \{1 + 2\alpha\varepsilon(k) + 4\alpha[\bar{E} - \varepsilon(k)]\} \frac{\mathrm{e}^{(\varepsilon(k)-\mu)/T}}{(\mathrm{e}^{(\varepsilon(k)-\mu)/T} + 1)^2}\bigg|_{k=-q/2\cos\xi} \tag{23}$$

with

$$\bar{E} \equiv \frac{2}{N}\sum_k \varepsilon(k) f\big(\varepsilon(k), T\big). \tag{24}$$

For these small to medial α, which satisfy the inequality $\alpha\varepsilon \ll 1$, we have

$$C_i \int \sin\theta \mathrm{d}\theta \int \mathrm{d}\phi \int \sin\theta_1\,\mathrm{d}\theta_1 \int \mathrm{d}q |\bar{u}(q)|^2 q^5 \frac{\cos^2\theta_1}{|\cos\xi|^3} \times \left(\frac{\bar{E} - \varepsilon(k)}{\varepsilon(k)}\right) \frac{\mathrm{e}^{(\varepsilon(k)-\mu)/T}}{(\mathrm{e}^{(\varepsilon(k)-\mu)/T} + 1)^2}\bigg|_{k=-q/2\cos\xi} \ll 1 \tag{25}$$

and the two expressions for impurity-induced linear resistivity, (19) and (23), are equivalent.

4. Conclusion

We have investigated the linear and non-linear electron transport from MSD and Lei balance equations for systems with Kane band structure. We find not only that qualitatively different results are predicted by MSD and Lei equations in the case of tight-binding miniband conduction, but also that in the case of the Kane band the non-linear drift velocity and the electron temperature obtained from these two sets of equations exhibit a marked difference for medially and strongly non-parabolic systems. In the linear region, however, we find that the two sets of equations predict almost the same resistivities due to impurities for weak to medial non-parabolicity.

To understand the physical reason for these markedly different predictions by MSD and Lei theories in the non-linear transport regime in strongly non-parabolic bands (both tight-binding-type and Kane-type bands), one should trace back to the physical foundation of the

original Lei–Ting theory [8]. The MSD equations for non-parabolic bands are, in fact, exactly the same as the balance equations of Lei and Ting [8], with the original parabolic energy $\varepsilon(k)$ in the electron density–density correlation function interpreted as the non-parabolic energy dispersion. However, the Lei–Ting equations were derived based on the separation of the centre of mass (with the electric field) from the relative electrons in the Hamiltonian. This separation is valid only for parabolic bands. When $\varepsilon(k)$ becomes non-parabolic the complete separation is impossible and one cannot derive the force and energy balance equations as in the original Lei–Ting theory. Using them for non-parabolic bands may result in the loss of important non-parabolic effects other than those involved in the electron density–density correlation functions, as is the case in the MSD prescription. Lei's method for non-parabolic bands is not a trivial extension of the Lei–Ting balance equations. It is not based on the separation of the centre of mass from relative electrons, and non-parabolic effects are included, in addition to those related to the energy dispersion in the electron density–density correlation function, in (i) the centre of mass treated as a mass variable particle, and (ii) the non-parabolic velocity function $v(k) = \nabla\varepsilon(k)$, rather than q/m, used in the force balance equation. It happens that in the case of linear transport these two non-parabolic effects almost cancel each other for a weakly to medially non-parabolic band. In the non-linear regime this cancellation disappears and quantitatively marked differences appear between the predictions of the MSD and Lei equations.

Acknowledgments

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