GENERALIZED KINETIC THEORY OF ELECTRONS AND PHONONS

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Abstract. A Generalized Kinetic Theory [1] was proposed in order to have the possibility to treat particles which obey a very general statistics. By adopting the same approach, we generalize here the Kinetic Theory of electrons and phonons. Equilibrium solutions and their stability are investigated.

1. Introduction
Very recently [1], a Generalized Kinetic Theory (GKT) has been proposed by Rossani and Kaniadakis, in order to have the possibility to treat, at a kinetic level, particles which obey a very general statistics.

The quasi–classical Boltzmann equation introduced in ref. [1] is a generalization of the Uehling–Uhlenbeck equation [2], which is intended for bosons and fermions only. In ref. [1] we have shown that our generalized Uehling–Uhlenbeck equation (GUUE) assures particle, momentum and energy conservation. Equilibrium, its uniqueness and stability (via an H–theorem) have been investigated.

In ref. [3] Koponen points out that fractal or inverse power law distributions of phonon excitations are of interest in modeling various meaningful situations in solid state physics. Moreover, he feels that until recently there has been little guidance on how to generalize the kinetic theory of electrons and phonons obeying non Gibbsian statistics.

Here we propose a Generalized Kinetic Theory for Electrons and Phonons (GKTEP), by following the same ideas which lead to the GUUE. In order to keep our GKTEP as general as possible, we introduce modified collision terms not only for phonons, but also for electrons, so that an application is allowed not only to electrons, but also to other particles (obeying a general statistics) which interact with a crystal lattice.

The paper is organized as follows. In section 2 the Bloch–Boltzmann–Peierls [4] equations are briefly recalled, and our generalization is introduced.

In section 3 and 4 we study the equilibrium solutions to the GKTEP equations and their stability is investigated, via an H theorem.

2. Generalized kinetic equations for electrons and phonons
The most complete description, at a mesoscopic level, of a system of electrons and phonons, is based on the Bloch–Boltzmann–Peierls (BBP) equations [4].

Consider two populations: electrons (e), whose number is conserved, obey Fermi–Dirac statistics; phonons (p), whose number is not conserved, obey Bose–Einstein statistics. Of course, one should deal, in principle, with p–p, p–e, and e–e interactions. A first important assumption is the following: electrons (distribution function $n$) are considered as a rarefied gas in a ”sea” of phonons (distribution function $N$). This means that e–e interactions can be neglected. In e–p interactions only electrons and energy are conserved. In p–p interactions only energy is conserved.
By adopting the notation of ref. [5], let $N_g = N_g(k, x, t)$ be the distribution function of phonons (quasi–momentum $k$, energy $\omega_g(k)$) of type $g$ (i.e. branch $g$ of the phonon spectrum) and $n = n(p, x, t)$ the distribution function of electrons (quasi–momentum $p$, energy $\epsilon(p)$). The distribution functions $N_g$ and $n$ are normalized so that the thermal energy density $E_p$ of the crystal is given by

$$E_p(x, t) = \frac{1}{8\pi^3} \sum_g \int \omega_g N_g(k, x, t) dk,$$

while the concentration $N$ and the energy density $E_e$ of the electron gas are given, respectively by

$$N(x, t) = \frac{1}{8\pi^3} \int n(p, x, t) 2dp, \quad E_e(x, t) = \frac{1}{8\pi^3} \int \epsilon(p)n(p, x, t) 2dp,$$

where the factor 2 inside these integrals accounts for degeneracy.

The BBP equation for phonons reads

$$\frac{\partial N_g}{\partial t} + u_g \cdot \frac{\partial N_g}{\partial x} = \left( \frac{\partial N_g}{\partial t} \right)_{coll} = \left( \frac{\partial N_g}{\partial t} \right)_{pp} + \left( \frac{\partial N_g}{\partial t} \right)_{pe}$$

(1)

$$\left( \frac{\partial N_g}{\partial t} \right)_{pp} = \int \left\{ -\frac{1}{2} \sum_{g_1, g_2} w_{pp}(k_1, k_2 \rightarrow k) \delta(\omega_g - \omega_{g_1} - \omega_{g_2})[N_g(N_{g_1} + 1)(N_{g_2} + 1)$$

$$- (N_g + 1)N_{g_1}N_{g_2} + \sum_{g_1, g_3} w_{pp}(k, k_1 \rightarrow k_3) \delta(\omega_{g_3} - \omega_g - \omega_{g_1})[(N_g + 1)(N_{g_1} + 1)N_{g_3}$$

$$- N_g N_{g_1}(N_{g_3} + 1))] \right\} \frac{dk_1}{8\pi^3},$$

and

$$\left( \frac{\partial N_g}{\partial t} \right)_{pe} = \int 8w_{pe}(p \rightarrow p', k)[n_p(1 - n_{p'}) (1 + N_g) - n_{p'}(1 - n_p)N_g] \delta(\epsilon_{p'} + \omega_g - \epsilon_p) \frac{dp}{8\pi^3},$$

where $n_p = n(p)$, $\epsilon_p = \epsilon(p)$, $w_{pp}$ and $w_{pe}$ are transition probabilities.

The first term in the braces corresponds to the direct and reverse processes

$$(g, k) \rightleftharpoons (g_1, k_1) + (g_2, k_2),$$

where

$$k_2 = k - k_1 - b$$

(2)
and \( b \) is a vector of the reciprocal lattice.

The second term in braces correspond to the processes (direct and reverse)

\[
(g_3, k_3) \Leftrightarrow (g, k) + (g_1, k_1),
\]

where

\[
k_3 = k + k_1 + b.
\]  

(3)

The BBP equation for electrons reads

\[
\frac{\partial n_p}{\partial t} + v \cdot \frac{\partial n_p}{\partial x} - eE \cdot \frac{\partial n_p}{\partial p} = \left( \frac{\partial n_p}{\partial t} \right)_{ep}
\]  

where

\[
\frac{\partial n_p}{\partial t} = \sum_g \int \left\{ w_{ep}(p', k \rightarrow p)[n_{p'}(1 - n_p)N_g
\]

\[
- n_p(1 - n_{p'})(1 + N_g)]\delta(\epsilon_p + \epsilon_{p'} - \omega_g)
\]

\[
+ w_{ep}(p' \rightarrow p, k)[n_{p'}(1 - n_p)(1 + N_g) - n_p(1 - n_{p'})N_g]\delta(\epsilon_p + \omega_g - \epsilon_{p'}) \right\} \frac{dk}{8\pi^3},
\]

(4)

The first term corresponds to processes with emission of a phonon having quasi–momentum \( k \) by an electron having a given quasi–momentum \( p \), and reverse processes with absorption of a phonon \( k \) by electrons \( p' \) with return to the quasi–momentum \( p \):

\[
p = p' + k + b.
\]  

(5)

The second term corresponds to processes with absorption of a phonon by an electron \( p \) and the reverse processes of its emission by electrons \( p' \):

\[
p + k = p' + b.
\]  

(6)

We shall generalize [1] the expressions of

\[
\left( \frac{\partial N_g}{\partial t} \right)_{pp}, \left( \frac{\partial N_g}{\partial t} \right)_{pe}, \left( \frac{\partial n_p}{\partial t} \right)_{ep},
\]

by introducing the following substitutions:

\[
1 + N_g \rightarrow \Psi(N_g), \quad N_g \rightarrow \Phi(N_g)
\]

\[
1 - n_p \rightarrow \psi(n_p), \quad n_p \rightarrow \varphi(n_p),
\]
where $\Psi$, $\Phi$, and $\psi$, $\varphi$, are, respectively, non negative functions of $N_g$ and $n_p$, obeying the conditions

$$\Psi(0) = \psi(0) = 1, \quad \Phi(0) = \varphi(0) = 0.$$  

We assume that $\Phi(N_g)/\Psi(N_g)$ and $\varphi(n_p)/\psi(n_p)$ are monotonically increasing functions, respectively, of $N_g$ and $n_p$. This is trivially true for bosons and fermions. In general, this assumption is justified \textit{a posteriori}, since it assures uniqueness and stability of equilibrium.

The functionals $\psi$, $\varphi$ and $\Psi$, $\Phi$ replace the Pauli blocking and boson enhancement factors in the phase space, respectively. Alternatively, one could say that generalized statistics, defined by means of the couples $\Psi$, $\Phi$ and $\psi$, $\varphi$, are introduced for phonons and electrons, respectively.

We have then

$$\left( \frac{\partial N_g}{\partial t} \right)_{pp} = -(1/2) \int \sum_{g_1 g_2} w_{pp}(k_1, k_2 \rightarrow k) \delta(\omega_g - \omega_{g_1} - \omega_{g_2})[\Phi(N_g)\Psi(N_{g_1})\Psi(N_{g_2}) - \Psi(N_g)\Phi(N_{g_1})\Phi(N_{g_2}) + \sum_{g_1 g_3} w_{pp}(k, k_1 \rightarrow k_3) \delta(\omega_{g_3} - \omega_g - \omega_{g_1})[\Psi(N_g)\Psi(N_{g_1})\Phi(N_{g_3}) - \Phi(N_g)\Phi(N_{g_1})\Psi(N_{g_3})]] \frac{dk_1}{8\pi^3},$$

$$\left( \frac{\partial N_g}{\partial t} \right)_{pe} = -\int 2w_{pe}(p, p' \rightarrow k)[\varphi(n_p)\psi(n_{p'})\Psi(N_g) - \varphi(n_{p'})\psi(n_p)\Phi(N_g)]\delta(\epsilon_{p'} + \omega_g - \epsilon_p) \frac{dp}{8\pi^3},$$

$$\left( \frac{\partial n_p}{\partial t} \right)_{ep} = \sum_{g} \int \{w_{ep}(p', k \rightarrow p)[\varphi(n_{p'})\psi(n_p)\Phi(N_g) - \varphi(n_p)\psi(n_{p'})\Psi(N_g)]\delta(\epsilon_p + \epsilon_{p'} - \omega_g) + w_{ep}(p' \rightarrow p, k)[\varphi(n_{p'})\psi(n_p)\Psi(N_g) - \varphi(n_p)\psi(n_{p'})\Phi(N_g)]\delta(\epsilon_p + \omega_g - \epsilon_{p'}) \frac{dk}{8\pi^3}.$$  

### 3. Equilibrium

Even though the generalized equations are certainly more complicated than the original ones, many of the usual techniques of kinetic theory are still applicable in the study of equilibria and their stability. In particular, we will prove an $H$ theorem for the present problem, whose connections with the entropy law are easily established.

In the space homogeneous and forceless case, equilibrium is defined by

$$\left( \frac{\partial N_g}{\partial t} \right)_{coll} = \left( \frac{\partial n_p}{\partial t} \right)_{ep} = 0. \quad (7)$$

In order to study equilibrium and its stability, it is useful to introduce the following functional:

$$\mathcal{D} = \sum_g \int \left( \frac{\partial N_g}{\partial t} \right)_{coll} \ln \frac{\Phi(N_g)}{\Psi(N_g)} dk + 2 \int \left( \frac{\partial n_p}{\partial t} \right)_{ep} \ln \frac{\varphi(n_p)}{\psi(n_p)} dp, \quad (8)$$

4
which can be put in the following form:

\[
D = \frac{1}{2} \sum_{g, g_2 g_3} \int \int w_{pp}(k_2, k_3 \rightarrow k_1) \delta(\omega_{g_1} - \omega_{g_2} - \omega_{g_3}) (-\Phi_{g_1} \Psi_{g_2} \Psi_{g_3} + \Psi_{g_1} \Phi_{g_2} \Psi_{g_3}) \ln \frac{\Phi_{g_1} \Psi_{g_2} \Psi_{g_3}}{\Psi_{g_1} \Phi_{g_2} \Psi_{g_3}}\]

\[+ 2 \sum_{g} \int \int w_{ep}(p \rightarrow p', k) \times \]

\[\times (-\varphi' \psi \Phi_{g} + \varphi \psi' \Psi_{g}) \delta(\epsilon_{p'} + \omega_{g} - \epsilon_{p}) \ln \frac{\varphi' \psi \Phi_{g}}{\varphi \psi' \Psi_{g}} dkd\]

where \(\Phi_{g_i} = \Phi(N_{g_i}(k_i)), \Psi_{g_i} = \Psi(N_{g_i}(k_i)), \]

\(\varphi' = \varphi(n_{p'}), \psi' = \psi(n_{p'}).\)

**Proposition 1.**

Condition (7) is equivalent to the following couple of equations:

\[
\Psi(N_g)\Phi(N_{g_1})\Phi(N_{g_2}) = \Phi(N_g)\Psi(N_{g_1})\Phi(N_{g_2}) \quad \forall \ k, \ k_1 \]

(10)

\[
\varphi(n_{p})\psi(n_{p'})\Psi(N_g) = \varphi(n_{p'})\psi(n_{p})\Phi(N_g) \quad \forall \ p, \ k. \]

(11)

**Proof.** First of all we observe that (10), (11) \(\implies\) (7). On the other hand, from (8) we have (7) \(\implies\) \(D = 0\). Now, since in eq. (9) both the integrands are never positive, one has \(D = 0 \implies\) (10), (11).

Condition (10) shows that \(\ln(\Phi^*/\Psi^*)\) is a collisional invariant for phonons, that is

\[
\ln \frac{\Phi(N_g^*)}{\Psi(N_g^*)} = -\omega_g / T
\]

(12)

(hereinafter * means ”at equilibrium”), where \(T\) is the absolute temperature of the whole system (electrons plus phonons).

From (11) and (12), taking into account that \(\epsilon_p = \epsilon_{p'} + \omega_g\), we find that, at equilibrium, \(\ln[\varphi(n_{p})/\psi(n_{p})] + \epsilon_p / T\) is a collisional invariant for electrons, that is

\[
\ln \frac{\varphi(n_{p})}{\psi(n_{p})} = (\mu - \epsilon_{p}) / T,
\]

(13)

where \(\mu\) is the chemical potential of the electron gas.

Observe that, due to the monotonicity of both \(\Phi/\Psi\) and \(\varphi/\psi\), equations (12) and (13) give unique solutions for \(N_g^*\) and \(n_{p}^*\), respectively.

We would like to stress that, with a proper choice of the ratios \(\Phi/\Psi\) and \(\varphi/\psi\), it is possible to reproduce the non-standard quantum statistics proposed in the last years and compare them from the point of view of the GKTEP, but this will be matter of a separate future paper [6].
4. Stability

In order to study the stability of such equilibrium solutions, let us introduce the following functional:

\[ H = H_p + H_e = \sum_g \int \mathcal{H}_p(N_g) d\mathbf{k} + \int \mathcal{H}_e(n_p) d\mathbf{p}, \]

where

\[ \frac{\partial H_p(N_g)}{\partial N_g} = \ln \frac{\Phi(N_g)}{\Psi(N_g)}, \quad \frac{\partial H_e(n_p)}{\partial n_p} = 2 \ln \frac{\varphi(n_p)}{\psi(n_p)}. \]

Observe that, since \( \Phi/\Psi \) and \( \varphi/\psi \) have been assumed to be monotonically increasing, \( H_p \) and \( H_e \) are convex functions of \( N_g \) and \( n_p \), respectively.

We can now prove the following H theorem:

**Proposition 2.**

\( H \) is a Lyapounov functional for the present problem.

**Proof.** First of all, it is easily verified that \( \dot{H} = \mathcal{D} \leq 0 \). Then we observe that

\[ \sum_g \int \left( \frac{\partial H_{pg}}{\partial N_g} \right)^* (N_g - N_g^*) d\mathbf{k} + \int \left( \frac{\partial H_{ep}}{\partial n_p} \right)^* (n_p - n_p^*) d\mathbf{p} = 0, \]

where \( H_{pg} = \mathcal{H}_p(N_g) \) and \( H_{ep} = \mathcal{H}_e(n_p) \), due to electron and energy conservation.

Now we can write

\[ H - H^* = \sum_g \int \hat{\mathcal{H}}_{pg} d\mathbf{k} + \int \hat{\mathcal{H}}_{ep} d\mathbf{p}, \]

where

\[ \hat{\mathcal{H}}_\alpha = \mathcal{H}_\alpha - \left[ \mathcal{H}_\alpha^* + \left( \frac{\partial \mathcal{H}_\alpha}{\partial \phi_\alpha} \right)^* (\phi_\alpha - \phi_\alpha^*) \right], \]

where \( \phi_\alpha = N_g \) for \( \alpha = pg \) and \( \phi_\alpha = n_p \) for \( \alpha = ep \).

Due to the convexity of \( \mathcal{H}_\alpha \), we have \( \hat{\mathcal{H}}_\alpha \geq 0 \) and finally \( H - H^* \geq 0 \).

By defining entropy as

\[ S = S_p + S_e = -\frac{H_p + H_e}{8\pi^3}, \]

these results are easily interpreted on a physical ground. In fact, \( \dot{H} \leq 0 \) and \( H - H^* \geq 0 \) simply mean that entropy is always non decreasing and it attains a maximum at equilibrium.

Observe that this definition of \( S \) is consistent with the definitions of \( T \) and \( \mu \) we already gave. In fact, at equilibrium, the following thermodynamical relationships are recovered:

\[ \left( \frac{\partial S}{\partial N} \right)_E = -\frac{\mu}{T}, \quad \left( \frac{\partial S}{\partial E} \right)_N = \frac{1}{T}, \]

where \( E = E_p + E_e \).

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References
[1] A. Rossani, G. Kaniadakis, ”A generalized quasi–classical Boltzmann equation”, Physica A, 277 (2000) 349
[2] R. L. Liboff, Kinetic Theory, Prentice Hall, London (1990)
[3] I. Koponen, ”Thermalization of an electron–phonon system in a nonequilibrium state characterized by fractal distribution of phonon excitations”, Phys. Rev. E, Vol. 55, No. 6, 7759 (1997)
[4] J. M. Ziman, Electrons and Phonons, Claredon Press, Oxford (1967)
[5] E. M. Lifshitz, L. P. Pitaevskii, Physical Kinetics, Pergamon Press, Oxford (1981)
[6] A. Rossani, A.M. Scarfone, submitted to Physica A, 2001