Journal of Statistical Physics, Vol. 124, No. 5, September 2006 (© 2006)
DOI: 10.1007/s10955-006-9180-1

Collisional Invariants for the Phonon Boltzmann Equation

Herbert Spohn[1]

Received May 22, 2006; accepted July 9, 2006
Published Online: August 1, 2006

For the phonon Boltzmann equation with only pair collisions we characterize the set of all collisional invariants under some mild conditions on the dispersion relation.

KEY WORDS: collisional invariants.

In the study of the Boltzmann equation, collisional invariants play an important role: for the spatially homogeneous equation they are in one-to-one correspondence with its stationary solutions and for the linearized Boltzmann equation they yield the eigenvectors spanning the zero subspace. In the kinetic theory of gases, under rather general conditions, a collisional invariant is necessarily of the form $\psi(v) = a\frac{1}{2}v^2 + b \cdot v + c$ with arbitrary coefficients $a, b, c^{(1)}$. In case the particles are relativistic, the kinetic energy, $\frac{1}{2}v^2$, will be replaced by its relativistic cousin $(1 + p^2)^{1/2}$, see Ref. 2 for the characterization of the collisional invariants.

In this note we discuss collisional invariants for the phonon Boltzmann equation with 4-phonon processes only. The essential difference to the kinetic theory of gases lies in the fact that the role of the kinetic energy is taken by the dispersion relation $\omega(k)$ which is a fairly arbitrary, non-negative function on $\mathbb{T}^d$, the d-dimensional torus of wave numbers.

To keep notation simple we discuss a single band model with the hypercubic lattice $\mathbb{Z}^d$ as crystal lattice. Amongst the allowed 4-phonon processes we study first only the number-conserving ones. For them, under conditions to be specified, a collisional invariant is necessarily of the form $\psi(k) = a\omega(k) + c$, $a, c \in \mathbb{R}$. It is then a simple substitution to check whether the set of collisional invariants

[1] Zentrum Mathematik and Physik Department, TU München, D-85747 Garching, Boltzmannstr. 3, Germany; e-mail: spohn@ma.tum.de

is further reduced by $c = 0$ when taking the remaining 4-phonon collisions into account.

We will work in the extended zone scheme. The dispersion relation $\omega : \mathbb{R}^d \to \mathbb{R}$ then satisfies $\omega \geq 0$ and is $\mathbb{Z}^d$-periodic, i.e. $\omega(k+n) = \omega(k)$ for all $n \in \mathbb{Z}^d$. Physically

$$\omega(k)^2 = \sum_{n \in \mathbb{Z}^d} \gamma(n) e^{i2\pi k \cdot n} \tag{1}$$

with γ of exponential decay. Thus ω is real analytic except at points where $\omega(k) = 0$. For multiband models further points of non-analyticity may occur because of bund crossings. Therefore we are led to the following.

Assumption 1. Let $\omega : \mathbb{R}^d \to \mathbb{R}$ be continuous and $\mathbb{Z}^d$-periodic. There exists a manifold $\Lambda_0 \subset \mathbb{R}^d$ of codimension at least 1 such that $\omega \in C^2$ on $\mathbb{R}^d \setminus \Lambda_0$. ω has bounded second derivatives which may diverge as Λ_0 is approached.

Definition. A measurable, $\mathbb{Z}^d$-periodic function $\psi : \mathbb{R}^d \to \mathbb{R}$ is called a *collisional invariant* if

$$\psi(k_1) + \psi(k_2) = \psi(k_3) + \psi(k_4) \tag{2}$$

for almost every $(k_1, k_2, k_3, k_4) \in \mathbb{R}^{4d}$ under the constraint that

$$k_1 + k_2 = k_3 + k_4\,, \tag{3}$$

$$\omega(k_1) + \omega(k_2) = \omega(k_3) + \omega(k_4)\,. \tag{4}$$

Assumption 2. Let $\Lambda_{\text{Hess}} = \{k \in \mathbb{R}^d \setminus \Lambda_0, \det \text{Hess}\, \omega(k) = 0\}$. $\overline{\Lambda}_{\text{Hess}}$ is a set of codimension at least 1.

Proposition. Let $d \geq 2$ and let ω satisfy Assumptions 1 and 2. Furthermore

$$\int_{M^*} |\psi(k)| dk < \infty \tag{5}$$

with $M^* = \{k = (k^1, \ldots, k^d) \in \mathbb{R}^d \mid |k^j| \leq 1/2\,,\ j = 1, \ldots, d\}$. Then a collisional invariant is necessarily of the form

$$\psi = a\omega + c \qquad \text{a.s.} \tag{6}$$

for some constants $a, c \in \mathbb{R}$.

Remark. The L^1-norm in (5) can be replaced by any L^p norm, $1 \leq p \leq \infty$.

For the proof we partition $\mathbb{R}^{2d}$ into the sets $\Lambda_{\eta,\varepsilon} = \{(k_1, k_2) \in \mathbb{R}^{2d} | k_1 + k_2 = \eta\,,\ \omega(k_1) + \omega(k_2) = \varepsilon\}$ with $\Lambda_{\eta,\varepsilon} = \emptyset$ allowed. Let $\widetilde{\phi}(k_1, k_2) = \psi(k_1) + \psi(k_2)$.

Then by assumption

$$\int_{(M^*)^2} |\widetilde{\phi}(k_1, k_2)| dk_1 dk_2 < \infty \tag{7}$$

and by definition, except for a set of measure zero, $\widetilde{\phi}$ is constant on each set $\Lambda_{\eta,\varepsilon}$.

Let $\phi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ be smooth and $\mathbb{Z}^d$-periodic in its first argument. We use the shorthands $\omega_j = \omega(k_j)$, $\psi_j = \psi(k_j)$, $\partial_\alpha^j = \partial/\partial k_j^\alpha$, $\partial_\omega = \partial/\partial\omega$. Then for any test function $f \in \mathcal{S}(\mathbb{R}^{2d})$ with support away from $(\Lambda_0 \times \mathbb{R}^d) \cup (\mathbb{R}^d \times \Lambda_0)$ one has

$$\begin{aligned}
&\int \phi(k_1 + k_2, \omega_1 + \omega_2)\big(\partial_\alpha^1 - \partial_\alpha^2\big)\big(f\big(\partial_\beta^1 - \partial_\beta^2\big)(\omega_1 + \omega_2)\big) dk_1 dk_2 \\
&= -\int \big(\big(\partial_\alpha^1 - \partial_\alpha^2\big)\phi\big(k_1 + k_2, \omega_1 + \omega_2\big)\big) f\big(\partial_\beta^1 - \partial_\beta^2\big)(\omega_1 + \omega_2) dk_1 dk_2 \\
&= -\int \partial_\omega \phi\big(k_1 + k_2, \omega_1 + \omega_2\big)\big(\big(\partial_\alpha^1 - \partial_\alpha^2\big)(\omega_1 + \omega_2)\big) \\
&\quad \times f\big(\partial_\beta^1 - \partial_\beta^2\big)(\omega_1 + \omega_2) dk_1 dk_2 \qquad (8)\\
&= -\int \big(\big(\partial_\beta^1 - \partial_\beta^2\big)\phi(k_1 + k_2, \omega_1 + \omega_2)\big) f\big(\partial_\alpha^1 - \partial_\alpha^2\big)(\omega_1 + \omega_2) dk_1 dk_2 \\
&= \int \phi(k_1 + k_2, \omega_1 + \omega_2)\big(\partial_\beta^1 - \partial_\beta^2\big)\big(f(\partial_\alpha^1 - \partial_\alpha^2)(\omega_1 + \omega_2)\big) dk_1 dk_2 \,,
\end{aligned}$$

integration over $\mathbb{R}^{2d}$. Taking limits the identity (8) holds for all ϕ's such that $\int_{(M^*)^2} |\phi(k_1 + k_2, \omega_1 + \omega_2)| dk_1 dk_2 < \infty$. Since, by the argument above, $\widetilde{\phi}$ is in this class, we conclude

$$\begin{aligned}
&\int (\psi_1 + \psi_2)\big(\big(\partial_\alpha^1 - \partial_\alpha^2\big)(\omega_1 + \omega_2)\big)\big(\partial_\beta^1 - \partial_\beta^2\big) f dk_1 dk_2 \\
&\quad = \int (\psi_1 + \psi_2)\big(\big(\partial_\beta^1 - \partial_\beta^2\big)(\omega_1 + \omega_2)\big)\big(\partial_\alpha^1 - \partial_\alpha^2\big) f dk_1 dk_2. \qquad (9)
\end{aligned}$$

We choose now the particular test function

$$f(k_1, k_2) = \partial_\gamma^1 f_1(k_1)\partial_\delta^2 f_2(k_2) \tag{10}$$

with f_1 and f_2 supported away from Λ_0 and set

$$\begin{aligned}
&A_{\alpha\beta}(f) = \int \psi(k_1)\partial_\alpha\partial_\beta f(k_1) dk_1 \,, \\
&B_{\alpha\beta}(f) = \int \omega(k_1)\partial_\alpha\partial_\beta f(k_1) dk_1 \,, \\
&A(f_1) = A \,,\ A(f_2) = \widetilde{A} \,,\ B(f_1) = B \,,\ B(f_2) = \widetilde{B} \,. \qquad (11)
\end{aligned}$$

Then, see Ref. 3, Section 12, for more details,

$$A_{\alpha\gamma}\widetilde{B}_{\beta\delta} + \widetilde{A}_{\alpha\delta}B_{\beta\gamma} = A_{\beta\gamma}\widetilde{B}_{\alpha\delta} + \widetilde{A}_{\beta\delta}B_{\alpha\gamma}\,. \tag{12}$$

Let us choose f_1, f_2 such that B and $\widetilde{B}$ are invertible and set

$$C = AB^{-1}\,,\ \widetilde{C} = \widetilde{A}\widetilde{B}^{-1}\,. \tag{13}$$

Then, see Ref. 3 Appendix 18.4,

$$C_{\alpha\gamma}\delta_{\beta\delta} + \widetilde{C}_{\alpha\delta}\delta_{\beta\gamma} = C_{\beta\gamma}\delta_{\alpha\delta} + \widetilde{C}_{\beta\delta}\delta_{\alpha\gamma}\,. \tag{14}$$

Setting $\alpha = 1$, $\beta = 2$ and $\gamma = 1, 2$, $\delta = 1, 2$, yields

$$C_{21} + \widetilde{C}_{21} = 0\,, \quad C_{12} + \widetilde{C}_{12} = 0\,, \tag{15}$$

$$C_{11} = \widetilde{C}_{22}\,, \quad \widetilde{C}_{11} = C_{22}\,. \tag{16}$$

In (15) we choose $f_1 = f_2$ to infer that $C_{12} = 0$, $C_{21} = 0$. From (16) we deduce that there is a constant a such that $C_{11} = a$, $C_{22} = a$, independent of the admissable test function. Repeating for further pairs of indices one concludes that

$$C(f) = a\mathbb{1} \tag{17}$$

and hence

$$A(f) = aB(f) \tag{18}$$

for all test functions f supported away from Λ_0 and such that $B(f)$ is invertible. Since the matrix $\{\partial_\alpha\partial_\beta\omega(k)\}_{\alpha,\beta=1,\ldots,d}$ is invertible for k away from $\Lambda_{\mathrm{Hess}} \cup \Lambda_0$ and since both sets have a codimension larger than 1, by taking limits, (18) holds for all $f \in \mathcal{S}(\mathbb{R}^d)$, to say the collisional invariant ψ has to satisfy

$$\int \psi\,\partial_\alpha\partial_\beta f dk = a\int \omega\partial_\alpha\partial_\beta f dk \tag{19}$$

for all $f \in \mathcal{S}(\mathbb{R}^d)$. Integrating yields

$$\psi(k) = a\omega(k) + b\cdot k + c \qquad \text{a.s.}\,. \tag{20}$$

To have ψ periodic forces $b = 0$, which is the assertion of the Proposition.

ACKNOWLEDGEMENT

I thank Jani Lukkarinen for helpful discussions.

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