

Nonlinear Peierls-Boltzmann Equation for Phonons: Structure and Stability of Solutions

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Phonon transport in locally disturbed media is considered. The steady state solutions of the Peierls-Boltzmann type equations are studied. In particular, the flux-dependence of local excitations is investigated. It is proven that for a large class of scattering processes only two types of steady states are possible: a hysteresis type and a threshold one. 4 different types of factorization procedures are applied and it is shown that for these cases the steady states remain nearly unchanged. The stability conditions are reformulated in such a way that one can give a geometrical interpretation. The only stable solutions are nodes. The necessary modification of our model system to allow for limit cycles is indicated. Also, a more complicated situation, where the interaction Hamiltonian H_I is a superposition of terms of different order, is investigated. The resulting steady state solution is again a hysteresis.

1. Introduction

In two recently published papers ^{1, 2} (henceforth referred to as I, II) it was shown that a kind of transport phase transition may occur in a simple non-translationally invariant model system. In particular a phonon system has been considered which is coupled to some additional local degrees of freedom. The presuppositions for such a process are 1) nonlinearities in the kinetic equations, i. e. in our case in the Peierls-Boltzmann equations; 2) that the systems are open (external stimulation); 3) that stable states far away from thermal equilibrium exist. These three conditions are necessary, but not sufficient for the existence of transport phase transitions ³. In our previous work it has turned out as a rule that there are only two types of steady state solutions: Threshold and hysteretic behaviour. No other types appear, although a great variety of different models (different orders of perturbation expansions, different coupling structures) has been considered. Both the hysteresis and the threshold solution show analogies to the phase transitions in thermal equilibrium. The first one may be viewed as a first order phase transition, the other one as a second order type ⁴. In this study we will show that the stated rule can be proven for arbitrary processes and for arbitrary interactions. The only assumption is that the interaction energy is much smaller than the total energy of the local system. Then on the one hand one can expand the interaction itself and on

the other hand apply perturbation theoretical expansions. This was done in some detail in paper I.

It is further shown that the steady state solutions remain nearly unchanged for different choices of factorization procedures which are used to close a subhierarchy. Finally we reformulate the stability conditions for the steady state solutions in such a way that they are applicable to a broad class of processes.

Our starting point is the modified Peierls-Boltzmann equations for phonons which were derived in I and extended in II. We discuss in some detail the allowed forms of the function $F(x, y)$ which represents the nonlinearity in our kinetic equations and the characteristic polynomial for the steady state solutions. We then apply different factorization procedures. Stability is studied by means of Ljapunov's first method ⁶. It turns out that only nonoscillating stable steady state solutions are possible.

Finally we investigate a more complicated situation, where the interaction Hamiltonian H_I is a superposition of terms of different order. In this case the above statements remain valid, and, moreover, a special type of hysteresis solution appears which one may view as an "envelope hysteresis".

2. Structure of the Nonlinearity in the Peierls-Boltzmann Equation for Phonons and Factorization Procedures

We start with a set of kinetic equations which is restricted to the two variable form [vid. Eqs. (II, 9, 10)]:

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$$\partial_t y - \Phi = -\frac{y}{\tau_k} - \beta F(x, y), \quad (1)$$

$$\partial_t x = -\frac{x}{\tau_s} + \alpha F(x, y); \quad (2)$$

y and x represent the averaged excitation of the phonon mode in the transporting system S_1 and the local mode in the nontransporting system S_2 , respectively. Φ stands for the averaged phonon flux. This flux describes the coupling of the system S_1 to the external heat baths of different temperature in a rather simplified way (vid. I). It has to be kept in mind that this external stimulation must be consistent with the steady state solutions of Eqs. (1) and (2). The coupling strength, the result of the summations over the different modes and all factors and parameters are contained in α and β of Equations (1), (2).

The nonlinear function $F(x, y)$ is determined both by the order of perturbation theoretical expansions of the transition probability $W_{\mu\nu}(t)$ and by the coupling strength between S_1 and S_2 .

In II we have defined an arbitrary process $P(\mu, \nu; n, m)$ which is given by the following set of operators

$$(a_k^+ a_k)^\nu (b_s^+ b_s)^\mu a_{k_1} \dots a_{k_n} (b_s^+)^m + \text{h.c.} \quad (3)$$

The underlying overall process is one where m local modes are created by n phonon modes, i.e. a process with $n \omega_k \approx m \omega_s$, $m < n$. Here a_k^+ and a_k are the phonon creation and annihilation operators, whereas b_s^+ and b_s represent the local mode. The operator combination (3) is either directly contained in the interaction Hamiltonian $H_I = \lambda V$, and then describes energy conserving processes via the Fermi Golden Rule, or it is an indirect combination of parts of H_I and becomes effective in Higher Golden Rules in a cumulative manner. For both cases the resulting nonlinear function $F(x, y)$ in the Boltzmann equation of the collision term reads

$$F(x, y) = \langle (x+m)^{2\mu} \cdot y^{2\nu} \cdot y^n \cdot (x+1)(x+2) \dots (x+m) - (x-m+1)^{2\mu} \cdot (y=1)^{2\nu} (y+1)^n x(x-1) \dots (x-m+1) \rangle. \quad (4)$$

We want to study the function $F(x, y)$ without specifically performing the averaging and factorization procedure at this place. We apply a certain type of adiabatic elimination of the stable variable y . The steady state solution for Eq. (1) reads

$$y_s = \Phi \tau_k - \beta \tau_k F(x, y_s). \quad (5)$$

Now, in II it has been stressed that the only physical relevant case is that one for which $0 \leq S < 1$, with S given by

$$S = \beta \tau_k \cdot (\alpha \tau_s)^{-1}. \quad (6)$$

The difference in the steady state excitation $\langle x_s \rangle$ between $S = 0$ and $S = 1$ is less than 1% in the whole region where the transition occurs.

Therefore the second part on the r.h.s. of Eq. (6) may be neglected without any appreciable changes in the steady state behaviour of our system:

$$y_s \approx \varphi; \quad \varphi = \Phi \cdot \tau_k. \quad (5a)$$

Restricting ourselves to the steady state solutions, from Eqs. (2), (4) and (5) we have

$$\begin{aligned} \alpha G(x_s, y_s \approx \varphi) &\equiv \alpha F(x_s, \varphi) - \tau_s^{-1} \cdot x_s \\ &= 0 = \alpha (-A \langle x_s^{2\mu+m} \rangle + B \langle x_s^{2\mu+m-1} \rangle \\ &\quad + C \langle x_s^{2\mu+m-2} \rangle + \dots + \left(R - \frac{1}{\alpha \tau_s} \right) \\ &\quad \cdot \langle x_s \rangle + m! m^{2\mu} \cdot \varphi^{2\nu+n}); \end{aligned} \quad (7)$$

with

$$\begin{aligned} A &= (\varphi+1)^{2\nu+n} - \varphi^{2\nu+n} + 0(\varphi^{2\nu+n-1}) + \dots, \\ B, C, D \dots &= f_B(\varphi), f_C(\varphi), f_D(\varphi), \dots, \\ R &= [m! m^{2\mu-1} \cdot 2\mu + a_{m-m+1}(m) \cdot m^{2\mu} \\ &\quad - (m-1)! (m-1)^{2\mu}] \varphi^{2\nu+n}. \end{aligned} \quad (8)$$

The coefficients $a_{m-m+1}(m)$ are evaluated in the appendix. There, we also show that $A, B, C, D, \dots, R > 0$.

Equation (8) is only solvable if we perform the averaging and factorization procedure, symbolically abbreviated by $\langle x_s^{2\mu+m} \rangle$. This means that one should factorize the powers in a way which has to be specified and then take the steady state value.

Nearly nothing is known about the appropriate choice of a factorization procedure. However, the thermal equilibrium must remain the solution for vanishing flux. We have applied four different types:

a direct factorization, i. e. $\langle x^n \rangle = \langle x \rangle^n$, (DF);

a method which makes use of the formal introduction of an eigentemperature T_s for the local system, (ETF), i. e.

$$\langle x^n \rangle = \sum_x x^n e^{-\beta_s w x} (1 - e^{-\beta_s w x}), \beta_s = (k_B T_s)^{-1};$$

an averaging with the aid of a Poisson distribution, (PDF);

a cumulant expansion, (CE).

Quite generally, for any of the four methods one will find

$$\langle x^n \rangle = a_n \langle x \rangle^n + a_{n-1} \langle x \rangle^{n-1} + a_{n-2} \langle x \rangle^{n-2} + \dots + a_1 \langle x \rangle + a_0 \quad (9)$$

where the a_n depend on the specific factorization procedure. From Eqs. (8), (9) we get

$$\begin{aligned} 0 = & \langle x_s \rangle^{2\mu+m} (-A a_{2\mu+m}) \\ & + \langle x_s \rangle^{2\mu+m-1} (-A a_{2\mu+m-1} + B b_{2\mu+m-1}) \\ & + \langle x_s \rangle^{2\mu+m-2} (-A a_{2\mu+m-2} + B b_{2\mu+m-2} \\ & + C c_{2\mu+m-2}) + \dots \\ & \vdots \\ & + \langle x_s \rangle \left(-A a_1 + B b_1 + C c_1 + \dots + R - \frac{1}{\alpha \tau_s} \right) \\ & + (m! m^{2\mu} \varphi^{2\mu+n} - A a_0 + B b_0 + C c_0 \\ & + \dots + Q q_0) . \end{aligned} \quad (10)$$

The sequences $\{a_i\}$, $\{b_i\}$, etc. are respectively determined by the factorization used [vid. Equation (9)]. In principle, a term of power n (i. e. $\langle x_s \rangle^n$) gets contributions from all higher powers, i. e. from terms $\langle x_s^m \rangle$ with $m \geq n$. The order of the polynomial $G(x_s, \varphi) = 0$ is the same for all four stated factorization procedures. However, the magnitude of the coefficients a_i , b_i etc. is not the same for the different procedures. But one can show that they are all positive or zero. We will point out this fact. In appendix B we will demonstrate this fact for one of the four procedures, but it can be similarly done for the others. It is also shown there that the negative contribution from the highest power cannot change the sign of the coefficients in any of the lower terms. This again is true for all factorization procedures considered.

If we restrict ourselves to the DF, there are no contributions from higher terms of Equation (8). We replace $\langle x_s^n \rangle$ by $\langle x_s \rangle^n$ in Equation (8). Although the order of the polynomial $G(x_s, \varphi)$ is [vid. Equation (II. 21)]

$$\tilde{r} = 2\mu + m \quad (11)$$

which would allow $2\mu + m$ real solutions, we can prove that only two or three positive and real roots can appear. This follows from Eq. (8) by means of the scheme (Cardani's rule):

$$- + + \dots + \pm + \quad (12)$$

i. e. only one or three changes of sign are possible. For $\tilde{r} \geq 3$ we always will find this situation, i. e. the hysteresis type of solution with one or three

positive steady states. The special case $\tilde{r} = 2$ yields the scheme

$$- \pm + \quad (12a)$$

and corresponds to the threshold behaviour, i. e. one positive and one negative root.

The upper and lower signs in the last but one term of Eqs. (12), (12a) belong to $R > (\alpha \tau_s)^{-1}$ and $R < (\alpha \tau_s)^{-1}$, respectively; R strongly depends on Φ . If $R > (\alpha \tau_s)^{-1}$, which is true in the upper flux region, the external stimulation in S_1 overcompensates the damping in system S_2 . In this case there only exists the highly excited branch.

We also have calculated the slope of the steady state solutions, i. e. $\partial_\varphi \langle x_s \rangle$. It exhibits the precise characteristics either for the threshold or the hysteresis type of solution. The same behaviour remains valid for the other types of factorization, which can be seen if an analogous study is performed. There again one has scheme (12), but R must be placed by \tilde{R} , with

$$\tilde{R} = R - A a_1 + B b_1 + C c_1 + \dots \quad (13)$$

which follows from Equation (10).

These considerations then prove that only the hysteresis and the threshold type of solutions are inherent in Eq. (8), if we remain within the restrictions of the four indicated factorization techniques, i. e. DF, ETF, PDF and CE.

A more detailed analysis further shows that the width of the hysteresis (i. e. $\Delta = \Phi_{cu} - \Phi_{ci}$) differs in the four cases. This is shown in Figure 1. The changes in the marginal points of the hysteresis follow from Eq. (13); i. e. $R > (\alpha \tau_s)^{-1}$ must be replaced by $\tilde{R} > (\alpha \tau_s)^{-1}$. Yet in the threshold case the position of Φ_c nearly remains unchanged. It turns out that DF has the largest width parameter Δ .

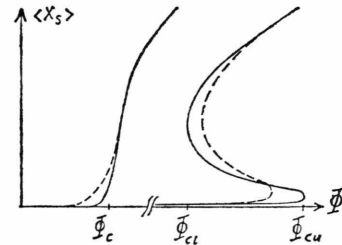


Fig. 1. Excitation of a local mode coupled to a one-dimensional phonon system. Hysteresis and threshold case. $\langle X_s \rangle$ is the occupation deviation from thermal equilibrium, Φ the average phonon flux. $\alpha \tau_s$ is fixed. Two different factorization procedures are applied: — direct factorization procedure; --- factorization via the introduction of an eigen-temperature for the local system.

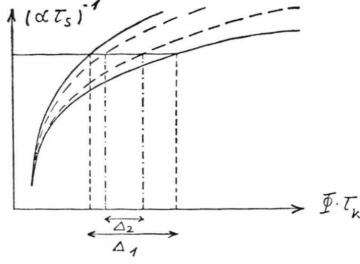


Fig. 2. Steady state solution $\langle X_s \rangle$ as a function of the parameters of the system and of the flux (hysteresis case). $\Delta_i = \Phi_{cu,i} - \Phi_{cl,i}$ is the width parameter. $\alpha \tau_s$ is given. The solid lines belong to total factorization, whereas the dashed lines are the results for the ETF-procedure.

In Fig. 2 we have drawn the width of the hysteresis (i. e. $\Delta = \Phi_{cu} - \Phi_{cl}$) and its position as a function of the parameter $\alpha \tau_s$ for two different types of factorization procedures. It is interesting to note also the asymptotical behaviour of the upper branch of the steady state curve. From Eq. (8) we find

$$\langle x_s \rangle = \frac{2 \sum_{\alpha=0}^{m-1} \alpha + 4 \mu m + m - 2 \mu}{(2 \nu + n)(2 \mu + m)} \varphi \quad (14)$$

for the ETF and similar expressions for the DF, PDF and CE.

3. Stability of Steady States

With the transformation

$$y = y_s + v, \quad x = x_s + w, \quad (15)$$

Eqs. (1) and (2) read

$$\begin{aligned} \partial_t v = & -\frac{y_s}{\tau_k} + \Phi - \beta F(x_s, y_s) - \beta \partial_x F \cdot w \\ & - \beta \partial_y F \cdot v - \frac{v}{\tau_k} + \text{NL} \end{aligned} \quad (16)$$

$$\begin{aligned} \partial_t w = & -\frac{x_s}{\tau_s} + \alpha F(x_s, y_s) + \alpha \partial_x F \cdot w \\ & + \alpha \partial_y F \cdot v - \frac{w}{\tau_s} + \text{NL} \end{aligned} \quad (17)$$

where we have expanded the nonlinear function $F(x, y)$ around its steady state value. We restrict ourselves again to the physically relevant situation $S \rightarrow 0$, i. e. $y_s = \Phi \tau_k$. x_s is calculated from Eq. (7),

$$G(x_s, \varphi) \equiv F(x_s, \varphi) - (\alpha \tau_s)^{-1} x_s = 0. \quad (18)$$

A linear stability analysis of Eqs. (16) and (17) is necessary and sufficient to produce global stability

of the steady state solution. This was illustrated in paper I. The stability conditions read⁶

$$\begin{aligned} a d - b c = & \left(-\frac{1}{\tau_s} + \alpha F_1 \right) \left(-\frac{1}{\tau_k} - \beta F_2 \right) + \alpha \beta F_1 F_2 \\ \approx & (\tau_s \tau_k)^{-1} - \alpha F_1 (\tau_k)^{-1}, \end{aligned} \quad (19)$$

$$a + d = -\frac{1}{\tau_s} - \frac{1}{\tau_k} + \alpha F_1 - \beta F_2 \quad (20)$$

with the abbreviations

$$\begin{aligned} F_1 = & \partial_x F|_{x=x_s}, \\ F_2 = & \partial_y F|_{y=y_s}. \end{aligned}$$

We want to trace back these conditions to a geometrical interpretation in the $\langle x_s \rangle$ - φ -diagram. From Eq. (16) we get

$$\begin{aligned} \partial_\varphi \langle x_s \rangle = & -\frac{\partial_\varphi G(x_s, \varphi)}{\partial_{\langle x_s \rangle} G(x_s, \varphi)} \\ = & -\frac{\partial_\varphi G(x_s, \varphi)}{\partial_{\langle x_s \rangle} F(x_s, \varphi) - (\alpha \tau_s)^{-1}}. \end{aligned} \quad (21)$$

With the aid of Eq. (19) the denominator of Eq. (21) can be replaced by

$$\partial_{\langle x_s \rangle} F(x_s, \varphi) - (\alpha \tau_s)^{-1} = -\tau_k \alpha^{-1} (a d - b c). \quad (22)$$

From Eqs. (8) and (18) we have

$$\begin{aligned} \partial_\varphi F = & -\partial_\varphi A \langle x_s^{2\mu+m} \rangle + \partial_\varphi B \langle x_s^{2\mu+m-1} \rangle \\ & + \dots + \partial_\varphi R \langle x_s \rangle + \partial_\varphi \tilde{S} \end{aligned} \quad (23)$$

with

$$\partial_\varphi \tilde{S} = \partial_\varphi (m! m^{2\mu} \varphi^{2\nu+n}) \quad (24)$$

which yields

$$\partial_\varphi \tilde{S} = (2\nu+n) \varphi^{-1} \tilde{S}. \quad (25)$$

The function \tilde{S} on the r.h.s. of Eq. (25) is replaced by the expression for \tilde{S} from Equation (8). Equation (23) then can be written in the form

$$\begin{aligned} \partial_\varphi F(x_s, \varphi) = & [(2\nu+n) A \varphi^{-1} - \partial_\varphi A] \langle x_s^{2\mu+m} \rangle \\ & - (2\nu+n) B \varphi^{-1} - \partial_\varphi B \langle x_s^{2\mu+m-1} \rangle \\ & - \left((2\nu+n) \left(R - \frac{1}{\alpha \tau_s} \right) \varphi^{-1} - \partial_\varphi R \right) \langle x_s \rangle. \end{aligned} \quad (26)$$

The general structure of the coefficients $B, C, D \dots M - R$ is

$$\begin{aligned} M = & a \varphi^{2\nu+n} - b \varphi^{2\nu+n-1} - c \varphi^{2\nu+n-2} - \dots \\ & a, b, c \dots > 0 \end{aligned} \quad (27)$$

[vid. Eq. (A 5) of the appendix].

From this we readily obtain

$$(2\nu+n)M\varphi^{-1}-\partial_{\varphi}M \\ = (2\nu+n)(a\varphi^{2\nu+n-1}-b\varphi^{2\nu+n-2} \\ -c\varphi^{2\nu+n-3}\dots)-(2\nu+n)a\varphi^{2\nu+n-1} \\ + (2\nu+n-1)b\varphi^{2\nu+n-2}+\dots \quad (28)$$

The first term on the r.h.s. of Eq. (26) yields

$$(2\nu+n)(\varphi+1)^{2\nu+n}-\varphi^{2\nu+n}+0(\varphi^{2\nu+n-1})\varphi^{-1} \\ - (2\nu+n)(\varphi+1)^{2\nu+n-1} \\ + (2\nu+n)\varphi^{2\nu+n-1} > 0. \quad (29)$$

From Eqs. (27), (28) and (29) we find

$$\partial_{\varphi}F > 0. \quad (30)$$

Rewriting now Eq. (21) by means of Eq. (22)

$$\partial_{\varphi}\langle x_s \rangle = a\tau_k^{-1}\partial_{\varphi}F \cdot (ad-bc)^{-1} \quad (31)$$

we are able to discuss the behaviour of $\langle x_s \rangle$. For $ad-bc < 0$, the steady state solution $\langle x_s \rangle$ is a saddle point, $ad-bc > 0$ implies both $a+d < 0$ [vid. Eqs. (19) and (20)] and

$$(a+d)^2 > 4(ad-bc),$$

which has the unique consequence of a stable node.

For an arbitrary process $P(\mu, \nu; n, m)$ we end up with the stability conditions

$$\partial_{\varphi}\langle x_s \rangle < 0 \rightarrow \langle x_s \rangle \text{ is a saddle point,} \\ \partial_{\varphi}\langle x_s \rangle > 0 \rightarrow \langle x_s \rangle \text{ is a stable node.} \quad (32)$$

Thus, a positive slope in the $\langle x_s \rangle\varphi$ -diagram corresponds to an asymptotically stable steady state, whereas a negative slope displays an absolutely unstable behaviour (vid. Figure 3).

No bifurcation to an oscillating solution is possible, since the necessary conditions for the existence of a limit cycle are not fulfilled^{5,6}. The only situation, where a limit cycle type of oscillation might

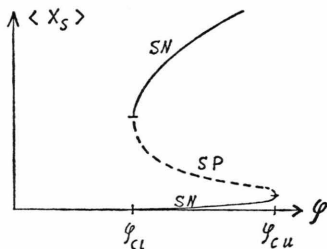


Fig. 3. Stability of the steady states $\langle x_s \rangle$. Stationary excitation of a local mode as a function of the external stimulation $\varphi \equiv \Phi \tau_k$ for the hysteresis type of solution. The dashed part of the hysteresis is unstable. The solid lines (positive slope) are stable (SN = stable node, SP = saddle point; $\varphi_{cl} = \Phi_{cl} \tau_k$, $\varphi_{cu} = \Phi_{cu} \tau_k$).

occur is shown in Figure 4. Here the phonon flux Φ is restricted to

$$\Phi_{cl} \leq \Phi \leq \Phi_{cu} \quad (33)$$

and the system may “oscillate” as shown in the figure. Condition (33) requires the inclusion of a feedback type of mechanism in our kinetic equations in such a way that the external flux Φ is no longer a free parameter, but is controlled by the internal excitation. For a more quantitative consideration of this point a detailed analysis of the time scales for the transitions $B \rightarrow C$ and $D \rightarrow A$ in relation to those of $A \rightarrow B$ and $C \rightarrow D$ is necessary. Details of these calculations are beyond the scope of the above studies.

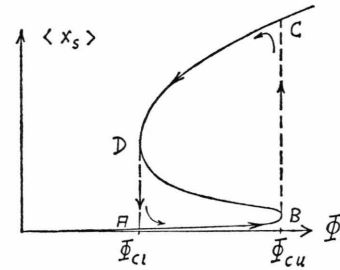


Fig. 4. Steady state excitation $\langle x_s \rangle$ of a local mode as a function of the phonon flux Φ . Under certain conditions (see text) the closed curve ABCDA may be viewed as a discontinuous limit cycle behaviour of the system.

4. “Mixed” Interaction Hamiltonian

A rather interesting situation arises if we take a more complicated interaction Hamiltonian of the form

$$H_I = \sum_{i,j} (H_I)_{ij} = \sum_{i,j} A(k_i, s_j) \hat{A}_{k_i} \dots \hat{A}_{k_i} (\hat{B}_s)^j \quad (34)$$

e. g.

$$H_I^{(1)} = \sum_k \lambda(k, s) \hat{A}_k \hat{B}_s + \sum_k \delta(k, s) \hat{A}_k \hat{B}_s^2 \\ + \sum_{k,k'} \gamma(k, k', s) \hat{A}_k \hat{A}_{k'} \hat{B}_s \\ \equiv (H_I)_{11} + (H_I)_{12} + (H_I)_{21} \quad (35)$$

where

$$\hat{A}_k = a_k + a_k^\dagger; \quad \hat{B}_s = b_s + b_s^\dagger.$$

We have studied $H_I^{(1)}$ rather exhaustively.

If we restrict ourselves to a special process, i. e. $w_s \approx w_k + w_{k'} + w_{k''}$ and if we apply the same kind of approximations as in our previous cases, each part $(H_I)_{ij}$ of $H_I^{(1)}$ leads to a hysteresis type of steady state solutions. The combined interactions

exhibit a behaviour that may be viewed as an “envelope hysteresis” (vid. Figure 5). Details of these calculations are omitted since they are quite long but very simple.

It is astonishing that the lengthy investigation of H_I leads to the result that the qualitative results of Chapter 2 and 3 remain valid. Again there are only two types of solutions, the threshold and the hysteresis type.

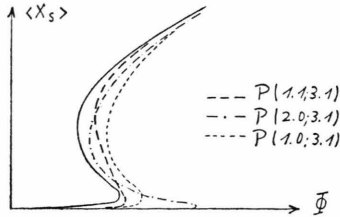


Fig. 5. Steady state behaviour for a combination of three interactions, each of which is restricted to a 3-phonon process. The dashed curves show the excitation of the local mode for three separated processes, the solid line corresponds to the combination $H_I = (H_I)_{11} + (H_I)_{12} + (H_I)_{21}$, [vid. Eq. (35)].

5. Summary

In this paper and two previous ones^{1,2} we have applied a re-formulated and modified Peierls-Boltzmann transport equation for phonons to a simple model system, i. e. a linear chain coupled to some local degrees of freedom. In the present study we have proved that only two types of steady state solutions can exist, a threshold and a hysteresis type. This property holds irrespective of the order of the interaction Hamiltonian H_I and of the order of the perturbation theoretical expansion. In addition, we have shown that the above two steady state solutions remain nearly unchanged for different factorization procedures.

The dependence of the steady state solutions from the parameters of the system, above all the damping constants κ_k and κ_s and the coupling strength, exhibits a similar behaviour for all types of processes and interactions.

From these results one may conclude that our modified Peierls-Boltzmann transport equations show a remarkable structural stability. We have made the following presuppositions:

a) the coupling of a nontransporting system to a transporting one, i. e. an open system,

b) the inclusion of nonlinearities in the collision term and
c) the validity of a perturbation theoretical expansion for both the interaction Hamiltonian and the transition probabilities.

In addition we have restricted ourselves to energy conserving overall transitions via energy non conserving intermediate states. From our result we thus conclude that neither small changes of the parameters nor changes in the nonlinearities lead to any other steady state solutions than hysteresis or threshold. The same conclusions hold with respect to the stability of the solutions.

The stated threshold and hysteresis type of steady state solutions seem to be the dominating types of transport phase transitions not only in physics, but also in chemistry, engineering, biology and related topics. This is valid as far as no time and/or space periodic solutions can occur. If these solutions are also possible, limit cycles, pattern formation and traveling waves must be taken into account.

Appendix A

We start from Equation (4). For simplicity and for physical reasons we restrict ourselves to $S \rightarrow 0$. The general case $0 \leq S < 1$ can be handled in the same way and does not lead to any relevant changes. Equation (4) reads

$$F(x, \varphi) = \langle (x+m)^{2\mu} y^{2\nu+n} X_m^+ - (x-m+1)^{2\mu} (y+1)^{2\nu+n} X_m^- \rangle \quad (\text{A } 1)$$

with

$$X_m^+ = (x+1)(x+2) \dots (x+m-1)$$

and

$$X_m^- = x(x-1)(x-2) \dots (x-m+1).$$

The functions X_m^+ , X_m^- can be evaluated due to the scheme:

$$X_m^+ = a_m(m)x^m + a_{m-1}(m)x^{m-1} + \dots + a_{m-(m+1)}(m)x + a_0(m)$$

with

$$a_{m-n}(m) = \sum_{j_1 \dots j_n} k_{j_1} \cdot k_{j_2} \cdot \dots \cdot k_{j_n}; \quad k_j = 1, 2, 3, \dots \quad (\text{A } 2)$$

$$X_m^- = b_m(m)x^m + b_{m-1}(m)x^{m-1} + b_{m-(m+1)}(m)x$$

with

$$b_{m-n}(m) = \sum_{j_1 \dots j_n} k_{j_1} k_{j_2} \cdot \dots \cdot k_{j_n}; \quad k_j = 1, 2, 3, \dots \quad (\text{A } 3)$$

and

$$\text{sign } b_{m-n}(m) = (-1)^{m-n}.$$

We can rewrite Eq. (A 1) with Eqs. (A 2), (A 3)

$$\begin{aligned}
 F(x, \varphi) = & \left\langle \sum_{j=0}^{2\mu} \binom{2\mu}{j} x^{2\mu-j} \{m^j \varphi^{2\nu+n} X_m^+ - (1-m)^j (\varphi+1)^{2\nu+n} X_m^-\} \right\rangle \\
 = & \left\langle \left[x^{2\mu+m} \varphi^{2\nu+n} - (\varphi+1)^{2\nu+n} + \sum_{j=1}^{2\mu} \binom{2\mu}{j} x^{2\mu+m-j} (\gamma - \delta) + \right. \right. \\
 & + \sum_{j=0}^{2\mu} \binom{2\mu}{j} x^{2\mu-j} \{x^{m-1} (a_{m-1}(m)\gamma - a_{m-2}(m-1)\delta) + x^{m-2} (m_{m-2}(m)\gamma - a_{m-3}(m-1)\delta) + \dots \\
 & \left. \left. + x^{m-m+1} (a_{m-m+1}(m)\gamma - a_{m-m}(m-1)\delta) + x^0 \cdot a_0(m)\gamma \right\} \right] \right\rangle \quad (\text{A } 4)
 \end{aligned}$$

with the abbreviations

$$\begin{aligned}
 \gamma &= \gamma(j, \nu, n) = m^j \varphi^{2\nu+n} \\
 \delta &= \delta(j, \nu, n) = (1-m)^j (\varphi+1)^{2\nu+n}
 \end{aligned} \quad (\text{A } 5)$$

and the relation

$$a_{m-n}(m) = |b_{m+1-n}(m+1)|. \quad (\text{A } 6)$$

By inspection, we find from Eq. (A 2)

$$a_{m-n}(m) > a_{m-(n+1)}(m-1) \quad (\text{A } 7)$$

and

$$\gamma > \delta, \quad \gamma > 0, \quad \delta \geq 0, \quad (\text{A } 8)$$

where we have excluded the unimportant case $m=0$, $\varphi=0$. The case $j=0$ must be checked separately, but it turns out that this situation does not lead to relevant changes. From Eqs. (A 1) – (A 4) we find

$$\begin{aligned}
 F(x, \varphi) = & -A \langle x^{2\mu+m} \rangle + B \langle x^{2\mu+m-1} \rangle \\
 & + \dots + R \langle x \rangle; + m! m^{2\mu} \varphi^{2\nu+n}
 \end{aligned} \quad (\text{A } 9)$$

B, C, \dots, R are sums of terms of the form

$$a_{m-n}(m)\gamma - a_{m-(n+1)}(m-1)\delta \quad (\text{A } 10)$$

and therefore all these coefficients are positive. It should be noted that the coefficient A is of the order $\varphi^{2\nu+n-1}$, whereas all the other parameters (i. e. $B, C, \dots, R, \tilde{S}$) are of the order

$$\varphi^{2\nu+n}; \quad (\tilde{S} = m! m^{2\mu} \varphi^{2\nu+n}). \quad (\text{A } 11)$$

If we restrict ourselves to steady state solutions, we have from Eq. (2)

$$\begin{aligned}
 \alpha F(x_s, y_s = \varphi) - (\tau_s)^{-1} x_s \\
 \equiv \alpha G(x_s, \varphi) = 0.
 \end{aligned} \quad (\text{A } 12)$$

A combination of Eqs. (A 1) and (6) yields Equation (8).

Appendix B

We will give here a brief scheme from which one can derive the contributions in each order if one factorizes a term of power n . As an example we

choose the ETF-procedure (ETF = eigentemperature factorization).

The n -th moment is given by

$$\langle x^n \rangle = \sum_x x^n e^{-\beta_s w x} \left(\sum_x e^{-\beta_s w x} \right)^{-1}. \quad (\text{B } 1)$$

With

$$\sum_x e^{-\beta_s w x} = (1 - e^{-\beta_s w})^{-1} \quad (\text{B } 2)$$

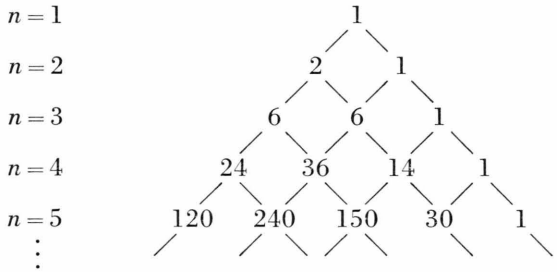
and

$$\beta_s = (k_B T_s)^{-1}.$$

Equation (B 1) can be written:

$$\langle x^n \rangle = (-1)^n (1 - e^{-\beta_s w}) \partial_{\beta_s w}^n (1 - e^{-\beta_s w})^{-1}. \quad (\text{B } 3)$$

From this equation we deduce the following scheme for the coefficients a_i, b_i etc. of Equation (10):



A term of the order n leads to contributions in all orders m (with $m < n$), e. g.

$$\langle x^4 \rangle = 24 \langle x \rangle^4 + 36 \langle x \rangle^3 + 14 \langle x \rangle^2 + 1 \langle x \rangle. \quad (\text{B } 4)$$

The coefficients a_i, b_i , etc. are all positive, the same is valid for B, C, \dots, R [vid. Eq. (10) and appendix A]. Since the coefficient A is of order $\varphi^{2\nu+n-1}$ and all the other coefficients start with $\varphi^{2\nu+n}$, the negative contribution from the highest power (i. e. $\langle x_s^{2\mu+m} \rangle$) cannot change the sign of the total coefficients in Equation (10). We want to show this fact at a simple example. We choose the process $P(1, 0; 3, 1)$. From Eqs. (4), (5 a) we have

$$F(x, y_s) = \langle (x+1)^3 y_s^3 - x^3 (y_s+1)^3 \rangle. \quad (\text{B } 5)$$

Equation (10) then reads ($y_s \approx \varphi$)

$$0 = - (3 \varphi^2 + 3 \varphi + 1) \langle x_s^3 \rangle + 3 \varphi^3 \langle x_s^2 \rangle + \left(3 \varphi^3 - \frac{1}{\alpha \tau_s} \right) \langle x_s \rangle + \varphi^3. \quad (\text{B } 6)$$

Performing the ETF-procedure we get

$$0 = - \langle x_s \rangle^3 6 (3 \varphi^2 + 3 \varphi + 1) + \langle x_s \rangle^2 [6 \varphi^3 - 6 (3 \varphi^2 + 3 \varphi + 1)] + \langle x_s \rangle \left(3 \varphi^3 - \frac{1}{\alpha \tau_s} - (3 \varphi^2 + 3 \varphi + 1) + 3 \varphi^3 \right) + \varphi^3. \quad (\text{B } 7)$$

The negative contribution from the term $\langle X_s^3 \rangle$ is not significant, since the highest power of the flux (i. e. φ^3) dominates for $\varphi \gg 1$. The latter situation is always valid in the marginal region. This can be shown quite generally for DF, ETF, PDF and CE.

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¹ Fr. Kaiser and M. Wagner, Z. Naturforsch. **32a**, 375 [1977].

² Fr. Kaiser, Z. Naturforsch. **32a**, 697 [1977].

³ P. Glanzdorff and I. Prigogine, Thermodynamic Theory of Structure, Stability and Fluctuations, Wiley-Interscience, New York 1977.

⁴ H. Haken, Rev. Mod. Phys. **47**, 67–121 [1975].

⁵ A. A. Andronov, E. A. Leontovich, I. I. Gordon, and A. G. Maier, a) Theory of Bifurcations of Dynamic Systems on a Plane; b) Qualitative Theory of Second-Order Dynamic Systems. J. Wiley, New York 1973.

⁶ A. A. Andronov, A. A. Witt, and S. E. Khaikin, Theory of Oscillators, Pergamon Press, Oxford 1966.