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Directed transport of modulated structures in the Frenkel–Kontorova model with a pulsating coupling

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Abstract

We study the directed transport of commensurate and incommensurate modulated phases of the Frenkel–Kontorova model by (parametric driving) periodic pulsed variation of the nearest-neighbor coupling in the dissipative limit of the dynamics. We obtain that a directed current flow appears as the amplitude of the pulsating coupling C increases above a threshold coupling C_{th}. This threshold coupling depends on the average interspacing ω between the oscillators displaying singularities as the system becomes commensurable with the underlying lattice. By making use of the discommensuration theory of modulated phases we obtain that the dependence of the directed current on ω is a piecewise linear function with integer slope. Numerical results confirm these predictions.
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1. Introduction

The various ratchet effects have attracted a lot of interest [1] as they appear in diverse biological systems (molecular motors) [2], superlattices [3], Josephson coupled systems [4–6] just to name a few. In particular such systems display a *directed current* in the presence of deterministic and/or random ac force having a zero mean value and in the absence of the directed force. In order to quantitatively analyze the appearance of directed current, the dissipative dynamics of a single particle moving in a potential $U(x,t)$ has been used [1]. Here, the force $-\partial U(x,t)/\partial x$ is a periodic function of both the particle coordinate x and time t. In the case of a large dissipation the equation of particle motion is given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial U(x,t)}{\partial x} + \xi(t), \tag{1}$$

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where the Langevin force $\xi(t)$ characterizes the equilibrium thermal fluctuations. The appearance of a directed current is the direct consequence of a broken symmetry of the potential $U(x, t)$ in space and/or time [1,7]. Moreover, the time dependence of the external potential $U(x, t)$ can be of a parametric type, as $U(x, t) = C(t)U(x)$ (flashing ratchet), or of an additive type, as $U(x, t) = U(x) + C(t)x$ (rocked ratchet). A crucial difference between these two types of ratchet systems is that the parametrically driven single particle *does not* display directed motion in the absence of thermal fluctuations, i.e. in the limit of zero temperature. This is so because a single particle has to overcome a potential barrier, and it is just impossible in the absence of thermal fluctuations. At variance with the flashing ratchets, the directed current may persist even in the absence of thermal fluctuations for large enough values of the ac driving force $C(t)$ in rocked ratchet systems.

There is also a great interest in the problem of directed transport in systems of interacting many-particles [8–10]. It was shown that the directed current may indeed occur when the ac driving force is additive (rocked many-particle ratchet) [8,10]. In the case of a nonlinear discrete lattice such a directed current is realized in the form of a directed motion of soliton chain. Thus, the question naturally arises: is it possible to observe a directed current in *parametrically driven many-particle systems* when equilibrium thermal fluctuations are absent?

We present here a well supported answer to this question by analyzing a discrete nonlinear lattice of interacting particles (the generalized Frenkel–Kontorova model) subject to parametric time-periodic driving. In Section 2 we formulate the model along with the specific conditions of the driven dynamics that we have considered. Some technical advantages coming from the model symmetries, which play a central role in the subsequent analysis, are emphasized.

In Section 3 we argue the existence of a threshold value of the parametric driving strength for generic values of the inverse density of particles ω. We present also specific numerical computations of the this threshold as a function of ω, showing a complex structure of singularities. In Section 4 we show that the discommensuration theory of modulated phases of the Frenkel–Kontorova model provides not only a satisfactory understanding of the threshold singularities, but also sharp predictions on the flow, which are afterwards confirmed by numerics. Finally, we conclude with a summary of the main results and some concluding remarks in the last section.

2. The model

The Frenkel–Kontorova model, first introduced more than 60 years ago [11] to study crystal dislocations, has been since then successfully used for the description of a vast number of different condensed matter physical systems and phenomena: commensurate–incommensurate phase transitions [12,13], ionic conductors [14], adsorbates [15,16], charge density waves [17,18], Josephson junction arrays [18,19], dry friction [20–22] and anomalous heat conduction [23]. It is also a model of central interest in nonlinear physics, often under the name of discrete sine-Gordon equation [24,25]. The characterization of the equilibrium configurations of the model and its physical properties (still a subject of ongoing research [26]) were much clarified after the works of Aubry [27], via its connection to the Aubry–Mather theory for the break-up of Kolmogorov–Arnold–Moser tori.

In the Frenkel–Kontorova (FK) model a real variable u_n is defined at each site n of a one-dimensional macroscopic lattice. One can, as well, visualize u_n as the position of a nonlinear oscillator. There are two competing interactions: a periodic (period 1) potential $V(u) = V(u + 1)$ and a nearest-neighbour interaction $W(\Delta u)$ which will be assumed to be a convex function of the intersite increment (oscillator interspacing) Δu. Formally, the energy of the FK model is

$$H = \sum_n [V(u_n) + CW(u_{n+1} - u_n)], \tag{2}$$

where the parameter C controls the relative strength of both interactions, V and W, which are here the analytic functions. We restrict consideration to potentials V possessing a single minimum per period at $u = a \pmod 1$, and maxima at integer values of u, and harmonic interactions $W(\Delta u) = (1/2)(\Delta u)^2$. The competition between the two interactions translates into *length scales* competition, because V favors integer values of Δu, while W favors a constant value ω of Δu, fixed by boundary conditions. We are interested in the thermodynamic (infinite size) limit, and choose to work at fixed (arbitrary) $\omega = \langle u_{n+1} - u_n \rangle = \lim_{N\to\infty} N^{-1} \sum_n (u_{n+1} - u_n)$. Commensurate and incommensurate structures correspond, respectively, to rational and irrational values of ω, the modulating wavevector (or oscillator average interspacing) of the structure.

We study the directed transport of modulated (commensurate and incommensurate) structures of the FK model, in the dissipative limit of the dynamics:

$$\dot{u}_n = -\frac{\partial H}{\partial u_n}, \tag{3}$$

where the parameter C in Eq. (2) varies on time $C(t)$, as a squared-wave of period $T = \tau_0 + \tau_C$ taking alternatively the values 0 and C. A convenient further simplification is to consider semicycle times, τ_0 and τ_C, which are large compared to the characteristic relaxation times to equilibrium (for zero and C values of coupling, respectively). Thus during each semicycle the configuration relaxes to the corresponding equilibrium structure, and the system performs a two-(equilibrium) states cycle.

The dissipative dynamics of the FK model with convex interparticle interactions has the property that the asymptotic velocity of all trajectories is unique [18,28] for fixed model parameters. This allows us to restrict consideration to the simplest kind of structures (u_n) of the model, technically known as rotationally ordered. These are characterized by the following *cross-avoiding* property: (u_n) does not cross any of its own translates $(u'_n) = (u_{n+r} - s)$ (r, s arbitrary integers). Non-crossing means that there are not $n \neq m$ with $u'_n < u_n$ and $u'_m > u_m$. Rotationally ordered configurations form an invariant subset under dynamics (3), i.e. any rotationally ordered configuration remains so at any time.

It can be easily seen [18] that a rotationally ordered configuration (u_n) satisfy the following inequality, for all n:

$$|u_{n+1} - u_n - \omega| < 1. \tag{4}$$

In the next section we will make use of this simple bound on the interparticle distance to discuss the existence of a threshold coupling.

3. Existence of threshold coupling

The current is determined by

$$J = T^{-1} \int_0^T \langle \dot{u}_n \rangle \, \mathrm{d}t. \tag{5}$$

To compute this quantity, one can think of an observer measuring the density of sites (or oscillators) for which u_n (mod 1) crosses the value $u = 0$ during each semicycle, say J_0^0 and J_C^0. Thus the flow (5) will be the sum of both local flows $J = J_0^0 + J_C^0$.

It is easy to realize that $J_0^0 = 0$: in the absence of coupling and thermal fluctuations, no oscillator can cross a potential maximum. The oscillator positions in the equilibrium configuration after this semicycle will be located at potential minima, and the condition of rotational order fixes this configuration to be of the form:

$$u_n = \mathrm{Int}(n\omega + \alpha) + a, \tag{6}$$

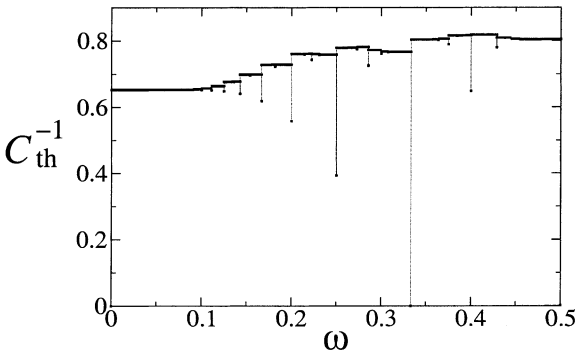

Fig. 1. Inverse (C_{th}^{-1}) of the threshold coupling parameter as function of ω. Drop lines are guides for the eyes.

where $\mathrm{Int}(x)$ is the integer part of x, a the position of the minimum of $V(u)$, and α an arbitrary phase (whose value can be brought to zero by relabeling the oscillators). This configuration (6) is the initial condition for the evolution when the coupling parameter is switched on to the value C and the next semicycle starts.

When C is very small compared to the absolute value of the maximal slope of the substrate potential ($C \ll K^* = \max_u |V'(u)|$) no oscillator will cross a potential maximum. Indeed, the interspacing Δu which would be needed for the elastic force, $C\Delta u$, to overcome K^* would be so large as to violate the bound (4) imposed on Δu by rotational order. Thus, the coupling C must exceed some threshold value $C_{th} > 0$ in order to have directed current $J \neq 0$.

Note that the argument above allows the threshold coupling to be infinite (and then no directed current), but we now provide some arguments supporting that it is generically finite. Detailed arithmetics [29,30] for the limit $C \to \infty$ shows that the flow for commensurate, $\omega = p/q$ (p, q coprime integers), and incommensurate (irrational ω) in that limit is given by

$$J\left(C \to \infty, \omega = \frac{p}{q}\right) = q^{-1}\mathrm{Int}\left[q\left(a - \frac{1}{2}\left(1 - \frac{1}{q}\right)\right)\right], \tag{7}$$

$$J\left(C \to \infty, \omega \neq \frac{p}{q}\right) = a - \frac{1}{2}. \tag{8}$$

For $a \neq 1/2$ this expression vanishes only for a finite number of rational values of ω ($0 \leq \omega \leq 1$), and thus the threshold is non-infinite for all except a finite number of rational ω values. Whenever the (single) minimum per period of $V(u)$ is not located at 1/2, *the threshold is finite for all incommensurate structures*. Note that only potential functions $V(u)$ lacking mirror symmetry could possibly satisfy $a \neq 1/2$, in agreement with the necessary breaking of this symmetry in order to have directed transport. The argument above will be adequately formalized elsewhere [30].

While a single-particle in a “flashing ratchet” potential does not show directed current in the absence of thermal fluctuations, we have just proved that the existence of directed current with no thermal fluctuations is generic for a many-particle system. In physical terms, the interparticle interaction provides the diffusive mechanism needed for the transport, so that thermal fluctuations are not anymore necessary.

We have numerically computed $C_{th}(\omega)$ for the particular (but arbitrary) potential function $V(u) = (2\pi)^{-2} \times [\sin(2\pi(u + b)) + 0.22\sin(4\pi(u + b))]$ (where $b = 0.194969\ldots$), with maxima at $u = 0$ (mod 1) and minima at $u = a = 0.610061\ldots$ (mod 1). In Fig. 1 we show the computed $C_{th}(\omega)$ for a fine grid of ω values in the interval [0, 1/2]. No other values have to be considered, for it can be proved that $C_{th}(1 + \omega) = C_{th}(1 - \omega) = C_{th}(\omega)$. For the threshold computation we have used a simple bisection scheme, and the integration of the equations of motion was made with a Runge–Kutta method.

The computed threshold function shown in Fig. 1 exhibits singularities at rational values of $\omega = p/q$, in the sense that the three values

$$C_{\text{th}}\left(\frac{p^+}{q}\right), C_{\text{th}}\left(\frac{p^-}{q}\right), C_{\text{th}}\left(\frac{p}{q}\right)$$

are different, i.e. there are both point and jump discontinuities at all rationals. However, the size of the discontinuities quickly decreases for increasing values of q. Note also that no jump discontinuity exist at $\omega = 0$ and $\omega = 1/2$ due to the symmetry $C_{\text{th}}(1+\omega) = C_{\text{th}}(1-\omega) = C_{\text{th}}(\omega)$ stated above.

As we will see below, this complex singular behavior admits a natural explanation and physical interpretation from the perspective of the theory of discommensurations. It is therefore convenient to remind briefly some known ideas and basic notions on the *emergent* [24] concept of discommensuration (DC); this will allow not only a correct understanding of the singular behavior of the threshold function, but also will enable us to make precise predictions on the flow $J(C, \omega)$ as a function of the model parameters, which we will check against detailed numerical results presented below.

4. Discommensuration theory

One of the most relevant physical properties of rotationally ordered commensurate ($\omega = p/q$) stable equilibria, (u_n), of the FK model is that they have a finite decay range or *coherence length* ξ, defined as follows: if the position of some arbitrary oscillator n is fixed at $u_n + \delta_n$, with δ_n small, and the rest of oscillators are left to relax subject to this restriction, their displacements δ_j behave as $\delta_j = \exp[-|j-n|/\xi]$. The physical consequence of this property is that commensurates admit localized defects [18,30,31]. If (u'_n) is the contiguous translate of the commensurate (u_n), such that, for all n, $u'_n > u_n$, an *advanced* DC is a rotationally ordered configuration (w_n^+) satisfying $w_n^+ \to u'_n$ as $n \to +\infty$, and $w_n^+ \to u_n$ as $n \to -\infty$. For the definition of a delayed or *retarded* DC (w_n^-), one has to interchange u'_n and u_n in the limits above.

The *excess length* Δ of a DC is the average amount by which $w_N - w_M$ $(M < N)$ exceeds the corresponding quantity $u_N - u_M$ in the commensurate, and it is $1/q$ $(-1/q)$ for an advanced (retarded) DC. The number of oscillators in the DC whose positions are appreciably distinct from the commensurate (the DC *width*) is of the order of the decay range ξ of the commensurate. The *center* of the DC can be defined as the oscillator index where the deviation from commensurate is maximum.

The discommensuration theory of modulated phases is based on the fact that any (commensurate or incommensurate) structure of ω close to the rational $\omega_0 = p/q$ is correctly described as an array of nearly equispaced DC's with a density $c = (\omega - \omega_0)/\Delta = q|\omega - \omega_0|$, which is the inverse average DC's interspacing in the array. In an equivalent way, one can say that a DC configuration is the one-sided limit of a sequence of (commensurate or incommensurate) structures of average interspacings ω_m approaching the rational p/q from left (retarded DC) or right (advanced DC) side.

From this perspective, the interpretation of the singularities of the threshold function $C_{\text{th}}(\omega)$ become crystal-clear: the threshold couplings of commensurate $C_{\text{th}}(p/q)$, advanced DC $C_{\text{th}}((p/q)^+)$ and retarded DC $C_{\text{th}}((p/q)^-)$, are generally different because the structures are indeed different. However, as $q \to \infty$ (incommensurate limit) the three thresholds converge to the corresponding incommensurate threshold. Moreover, these features are clearly generic, in the sense that they have to be expected for arbitrary $V(u)$ potential functions.

Now think of a DC configuration at time 0, $(w_n^{\pm}(0))$, that evolves to $(w_n^{\pm}(T))$ after a time interval T, and assume that both configurations are related by a symmetry translation, i.e. $(w_n^{\pm}(T)) = (w_{n+r}^{\pm}(0) - s)$, where the superscript $\pm$ refers to advanced/retarded. In this case the net number of oscillator positions which have crossed $u = 0$ (mod 1)

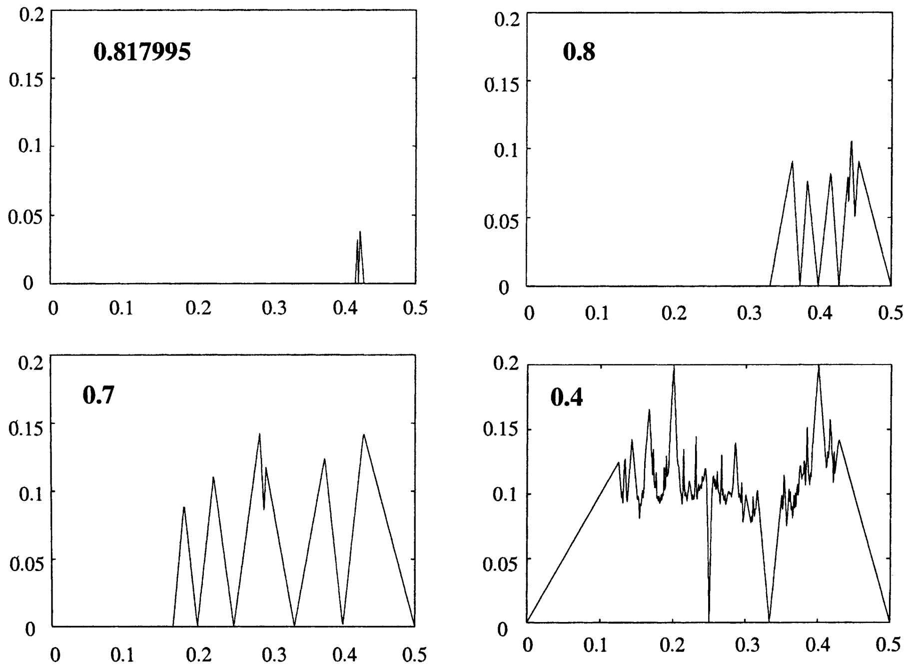

Fig. 2. Flow J vs. ω at four different C^{-1} values printed inside figures.

is the integer $\tilde{v} = j^{\pm}_{\mathrm{DC}}(T) - j^{\pm}_{\mathrm{DC}}(0)$, that is the difference between DC centers $j^{\pm}_{\mathrm{DC}}$ at both times. Whenever the DC center advance $\tilde{v}$ is finite, the macroscopic flow produced by the motion of the DC relative to commensurate is zero; however, for a density c of identical DC's the macroscopic flow associated to the relative DC's motion is $-\tilde{v}c\Delta$, and thus one can write the macroscopic flow of that structure as

$$J(\omega) = J(\omega_0) - \tilde{v}(\omega - \omega_0), \tag{9}$$

where $J(\omega_0)$ is the flow of the commensurate substrate where the DC's array lays upon. Note that (9) is a linear function with integer slope. The improvement of (9) through the inclusion of DC's overlap effects introduces corrections which are exponentially small in the ratio (DC width)/(DC interspacing); in other words, the power expansion of $J(\omega)$ around any rational has no terms higher than linear.

An immediate consequence of (9) is the following: whenever the retarded and advanced DC's on the rational ω_0 move at the same velocity (i.e. $\tilde{v}^+ = \tilde{v}^-$), the flow is differentiable at ω_0 with *integer* slope; if it is the case that retarded and advanced DC's move at different velocities, the flow shows an *integer* jump in first derivative. We have to emphasize that these predictions of the discommensuration theory on the flow are remarkably sharp.

In Fig. 2 we show the computed values of the flow $J(C, \omega)$ as a function of ω for different values of the coupling C. The sharp predictions of the DC theory are dramatically confirmed by our numerical results on the flow: at fixed value of C, the computed flow is a piecewise linear function of ω with exactly integer slopes.

5. Summary and concluding remarks

We have presented here some results on the directed transport of modulated structures of the Frenkel–Kontorova model with mirror-asymmetric potentials. Our results correspond to the dissipative regime of the dynamics and on–off pulsating coupling.

Under these conditions, and provided the pulse strength is large enough, the existence of directed transport is generic. Contrary to the single-particle "flashing ratchet", no thermal fluctuations are needed to induce a directed current in a many-particle system, the mutual interactions providing the diffusion mechanism for it.

We have provided heuristic arguments supporting that there exists a threshold function $C_{\text{th}}(\omega)$ whose complex structures of singularities is satisfactorily explained by the discommensuration theory of modulated phases. This also predicts a piecewise linear variation of the current flow with the commensurability ω of the modulated structure. These predictions are confirmed by the numerical computations that we have shown here.

Our results are based on the property of order preservation, which in turn relies on the dissipative character of the dynamics. When inertial terms are included in the equations of motion, but still the dissipation is high enough, certain extension of the property of order preservation has been recently proved by C. Baesens. Thus we expect that our results will also hold qualitatively for the regime of high dissipation for inertial dynamics. Indeed, preliminary numerical work seems to indicate that directed transport can be significantly enhanced by the inertial terms.

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References

[1] P. Reimann, Phys. Rep. 361 (2002) 57.
[2] F. Jülicher, A. Ajdari, J. Prost. Rev. Mod. Phys. 69 (1997) 1269.
[3] K. Seeger, W. Maurer, Solid State Commun. 27 (1978) 603.
[4] E. Trias, J.J. Mazo, F. Falo, T.P. Orlando, Phys. Rev. E 61 (2000) 2257.
[5] S. Weiss, D. Koelle, J. Mller, R. Gross, K. Barthel, Europhys. Lett. 51 (2000) 499.
[6] G. Carapella, G. Costabile, Phys. Rev. Lett. 87 (2001) 077002.
[7] O. Yevtushenko, S. Flach, Y. Zolotaryuk, Phys. Rev. Lett. 84 (2000) 2358.
[8] S. Flach, Y. Zolotaryuk, A.E. Miroshnichenko, M.V. Fistul, Phys. Rev. Lett. 88 (2002) 184101.
[9] M. Salerno, N.R. Quintero, Phys. Rev. E 65 (2002) 025602.
[10] M. Salerno, Ya. Zolotaryuk, Phys. Rev. E 65 (2002) 056603.
[11] T.A. Kontorova, Ya.I. Frenkel, Zh. Eksp. Teor. Fiz. 8 (1938) 1340.
[12] V.L. Pokrovsky, A.L. Talapov, Theory of Incommensurate Crystals, Soviet Scientific Reviews Supplement Series, Physics, vol. 1, Harwood, New York, 1984.
[13] R.B. Griffiths, in: H. van Beijeren (Ed.), Fundamental Problems in Statistical Mechanics, vol. VII, North-Holland, Amsterdam, 1990, pp. 69–110.
[14] L. Pietronero, W.R. Schneider, S. Strassler, Phys. Rev. B 24 (1981) 2187.
[15] S.C. Ying, Phys. Rev. B 3 (1971) 4160.
[16] S.C. Erwin, et al., Phys. Rev. Lett. 83 (1999) 1818.
[17] S.N. Coppersmith, D.S. Fisher, Phys. Rev. A 38 (1988) 6338.
[18] L.M. Floría, J.J. Mazo, Adv. Phys. 45 (1996) 505.
[19] S. Watanabe, et al., Physica D 97 (1996) 429.
[20] M.G. Rozman, M. Urbakh, J. Klafter, Phys. Rev. Lett. 77 (1996) 683.
[21] O.M. Braun, et al., Phys. Rev. Lett. 78 (1997) 1295.
[22] M. Weiss, F.J. Elmer, Phys. Rev. B 53 (1996) 7539.
[23] B. Hu, B. Li, H. Zhao, Phys. Rev. E 57 (1998) 2992;
B. Hu, B. Li, H. Zhao, Phys. Rev. E 61 (2000) 3828.

[24] A. Scott, Nonlinear Science, Emergence and Dynamics of Coherent Structures, Clarendon Press, Oxford, 1999.
[25] O.M. Braun, Y.S. Kivshar, Phys. Rep. 306 (1998) 1.
[26] O.V. Zhirov, G. Casati, D.L. Shepelyansky, Phys. Rev. E 65 (2002) 026220.
[27] S. Aubry, in: A.R. Bishop, T. Schneider (Eds.), Solitons in Condensed Matter Systems, Springer, New York, 1978;
S. Aubry, Physica D 7 (1983) 240;
S. Aubry, in: C. Godreche (Ed.), Structures et Instabilités, Editions de Physique, Les Ulis, 1985.
[28] C. Baesens, R. Mackay, Nonlinearity 11 (1998) 949.
[29] L.M. Floría, F. Falo, P.J. Martínez, J.J. Mazo, Europhys. Lett. 60 (2) (2002) 174.
[30] L.M. Floría, C. Baesens, in preparation.
[31] L.H. Tang, R.B. Griffiths, J. Stat. Phys. 53 (1989) 853.