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Soliton, Non-Recurrent Minimum Energy Configuration, and Extended Numbers

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We show that the non-recurrent minimum energy configurations such as the solitons and the incommensurate defects are naturally associated with suitably defined extended numbers. The physics behind such associations are elaborated in detail. In particular, we point out how to construct and classify the incommensurate defects and explain why they are chiral and carry no particle number.

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I. Introduction

Extended numbers such as $0^{\pm}$, meaning infinitesimally positive or negative, are employed quite often in physics to indicate certain limiting procedures. In nonlinear dynamics, when mode locking to commensurate ratios of parameters is a common phenomenon, they can be more precisely defined and are closely related to solitons or non-recurrent minimum energy configurations in general.

As we shall demonstrate below, a recurrent configuration is usually associated with parameters which take values locked in a dense subset of a certain interval. In this case, a non-recurrent configuration can be obtained by allowing the parameters to become extended numbers defined with respect to that dense subset. The fact that the parameters associated with them differ by an *infinitesimal* amount suggests that a non-recurrent configuration can be produced from a recurrent one by a simple operation. In the examples discussed below, the operations amount to moving a single particle in an *infinite* system. The non-recurrent configurations manifest themselves as defects in a physical system.

In this note, we shall consider specifically two kinds of extended numbers, both of which are defined with respect to a dense subset in the interval $[0,1]$. Let Q be the rational numbers in $[0, 1]$ and let $\bar{Q}$ denote all equivalent classes of strictly monotonic sequences of numbers in Q with a limiting point. If the limiting point is not in Q, the sequence can be identified with an irrational number. If the limiting point is p/q, an irreducible representation of an element in Q, then we shall call $(p/q)^-$ the (equivalent class of) strictly increasing sequence and $(p/q)^+$ the (equivalent class of) strictly decreasing sequence in $\bar{Q}$

with this limiting point. This type of extended numbers has already been employed in the literature [1], and is related to soliton configurations. To be specific, let us consider a one-dimensional chain of particles moving in a periodic potential, i.e., the Frenkel-Kontorova (FK) model [2, 3]. Physically a soliton, in a background of a periodic configuration with winding number p/q, is produced by adding a particle to the system and allowing the system to relax to an equilibrium configuration [4]. Since $1/\omega$ is the average number of particles per period and only a single particle is added to an infinite system, the resulting non-recurrent configuration should have winding number w = $(p/q)^-$ intuitively. Similarly, an anti-soliton, produced by removing a particle from a periodic configuration, is a non-recurrent configuration with w = $(p/q)+$. We shall return to the soliton configurations shortly.

The other kind of extended numbers is defined with respect to the dense subset $\mathcal{S}_\omega \equiv \{\mathrm{Frac}[n\omega]|n \in 2)$ of $[0, 1]$, with w being an irrationalnumber in [0, 1] and $\mathrm{Frac}[x] = x - \mathrm{Int}[x]$ being the fractional part of x. Again we denote $\bar{\mathcal{S}}_\omega$ the set of equivalent classes of strictly monotonic sequences of elements in $\mathcal{S}_\omega$ with a limiting point in [0, 1]. In case the limiting point β is in $\mathcal{S}_\omega$, we shall call β^- the (equivalent class of) strictly increasing sequence and β^+ the (equivalent class of) strictly decreasing sequence in $\bar{\mathcal{S}}_\omega$ with this limiting point. This type of extended numbers is closely related to the non-recurrent minimum energy configurations *with irrational winding number w,* the existence of such was first pointed out by R. B. Griffiths *et al.* [5] in a class of FK models with d(d > 1) subwells in a given period of the potential (See Fig. 1 for an example). In this case, the recurrent minimum energy configuration is specified by the winding number w and the filling fractions ν_i for each type of subwell, where $1 \leq i \leq$ d labels each type of subwells from left to right in a given period of the potential. For our purposes, it is more convenient to use the variables $\beta_i \equiv \nu_1 + \nu_2 + \cdots + \nu_i$. When w is irrational and certain resonance conditions, to be specified later, are met, a new type of defect can be produced by moving the particle in the (i + 1)-th type subwells, which is closest to one of the i-th type tips (thought of as the potential maxima) among all the particles, over the corresponding i-th type tip into its neighboring well [6]. Since a single particle is removed from the (i + l)-th type subwell and added to the neighboring i-th type subwell over the entire infinite system, ν_i increases by an infinitesimal amount while ν_{i+1} decreases by the same amount and the resulting configuration should be specified by β_i^+ intuitively. Similarly, if we move the particle in the i-th type subwells, which is closest to one of the (i + l)-th type tips among all particles, over the corresponding $(i+$ l)-th type tip, the resulting non-recurrent configuration will be specified by β_i^-. Contrary to the case of soliton and anti-soliton, it is obvious that this new type of defect does not carry " charge ", i.e., particle number. The orbit corresponding to the non-recurrent configuration is homoclinic to the orbit corresponding to its recurrent background.

It is clear that in any finite region of an infinite system, one cannot distinguish a given non-recurrent configuration from a certain recurrent one. Our assertion that a non-recurrent minimum energy configuration can be obtained from a recurrent one by replacing the values of some parameters with the corresponding extended numbers indicates that a non-recurrent configuration can be constructed as the limit of a sequence of recurrent configurations of which the characteristic scales increase to infinity. In the following, we shall illustrate our points by a class of solvable FK models.

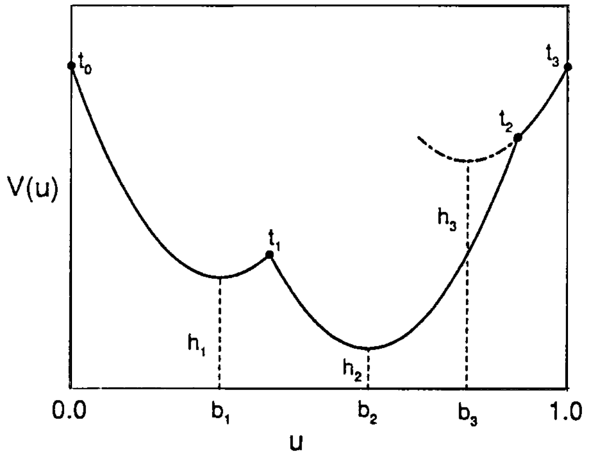

FIG. 1. Periodic potential V in Eq. (11) for d = 3.

In FK models, a recurrent minimum energy configuration can be described by [2]

$$u_n = f_\omega(n\omega + \alpha), \tag{1}$$

where u_n gives the coordinate of the n-th particle and the hull function f_ω is increasing and satisfies

$$f_\omega(x+1) = f_\omega(x) + \ \cdot \tag{2}$$

Because of this property, the arguments of f_ω are referred to as phase variables generically. When w = p/q, f_ω is a step function with q steps [7]. When w is irrational, f_ω is smooth for sufficiently weak potential and becomes discontinuous as the strength of the potential increases over a critical value [2]. It is clear that whenever f_ω is discontinuous, $\omega^\pm$ defined as a strictly monotonic sequence (equivalent class of sequences) with limiting value w, need not describe the same configuration as w. Indeed w = $(p/q)^-$ describes the soliton configuration as we shall illustrate with the solvable FK models [8,9] whose potential is

$$XV(u) = \frac{\lambda}{2}\left(\mathrm{Frac}[u] - \frac{1}{2}\right)^2 . \tag{3}$$

In this model, the soliton in the background of the recurrent minimum energy configuration with winding number p/q can be described by [10]

$$u'_n = \begin{cases} f_{p/q}\left(\frac{np}{q} + \frac{1}{2q}\right) - \delta_- e^{n\chi}, & n \le q; \\ f_{p/q}\left(\frac{np}{q} - \frac{1}{2q}\right) + \delta_+ e^{-n\chi}, & n \ge 0, \end{cases} \tag{4}$$

where

$$\delta_+ = \frac{1}{2}(d_q + d_0), \quad \delta_- = \frac{1}{2}(d_q - d_0) \tag{5}$$

and

$$e^{-\chi} = \frac{2 + \lambda - \sqrt{\lambda^2 + 4\lambda}}{2}, \quad d_0 = \sqrt{\lambda/(\lambda+4)}, \quad d_q = d_0 \coth \frac{q}{2}\chi. \tag{6}$$

The hull function in Eq. (1) is given by

$$f_\omega(x) = d_0 \sum_{n=-\infty}^{\infty} e^{-|n|\chi} \tilde{b}(x + n\omega), \tag{7}$$

where $\tilde{b}(x) = \mathrm{Int}[x] + 1/2$ gives the coordinate of the bottom of the potential well where a particle with phase x would lie in.

For w = (p/q)-, it is straightforward to check that for n ≥ 0

$$f_\omega(n\omega) - f_{p/q}\left(\frac{np}{q} - \frac{1}{2q}\right) = \delta_+ e^{-n\chi} \tag{8}$$

and for $n \leq q$

$$f_\omega(n\omega) - f_{p/q}\left(\frac{np}{q} \mathrm{t} \frac{1}{2q}\right) = -\delta_- e^{n\chi}, \tag{9}$$

so that $u'_n = f_\omega(n\omega)$, confirming our assertion and the intuitive physical picture that w $=(p/q)^-$ in $\bar{\mathcal{Q}}$ should describe that soliton configuration.

We may construct a representative sequence of $(p/q)^-$ explicitly in the following way. Let $\mathcal{Q}_\Lambda$ denote the set of rational numbers T/s (an irreducible fraction) in $[0,1]$, whose denominator s is no larger than the cutoff $s_\Lambda \gg q$. We may arrange elements of $\mathcal{Q}_\Lambda$ in an ascending order. Let w ' $= p'/q'$ be the rational number in $\mathcal{Q}_\Lambda$ which is closest to w $= p/q$ from below. Then we have [11]

$$pq' - p'q = 1. \tag{11}$$

As s_Λ is sent to infinity step by step, the collection of p'/q' at each stage will give us a representative sequence of (p/q)-.

Equation (10) implies that p ' w-molecules (each consisting of q particles in p wells) [12] and p w '-molecules (each consisting of q' particles in p' wells) differ by a single particle in a total of *pp ' wells.* Hence the recurrent minimum energy configuration with winding number w ' can be considered as an approximate soliton lattice over the background of the recurrent minimum energy configuration with winding number w and the lattice spacing is $l = p'$ [4]. As the cutoff s_Λ is removed, the lattice spacing l approaches infinity and the configuration of a single soliton is recovered.

It is useful to introduce the tensile force σ, which is dual to the variable w and keeps the particles at an equilibrium separation of σ in the limit of vanishing external potential XV. As σ is varied, the system is locked at rational values of w = p/q. When σ is decreased, a critical value is reached when the enthalpy of the soliton configuration is equal to that of its recurrent background [3]. Similar phenomenon occurs for the anti-soliton configuration as σ is increased. As we shall see, the case of incommensurate non-recurrent minimum energy configurations is exactly the same but with more control parameters.

Now we turn to the second type of extended numbers. We shall focus on FK models with multiple subwells in a period of the external potential which support the new kind of incommensurate defects mentioned above. More specifically, we consider the solvable FK model [13-16] with the following periodic potential of period 1,

$$V(u) = \min_{1 \leq i \leq d} \{V_i(u)\} \tag{11}$$

for $0 \leq u < 1$, with

$$V_i(u) = \frac{1}{2}(u - b_i)^2 + h_i. \tag{12}$$

An example is shown in Fig. 1. It is clear that h_i will not appear in the force balance equation. It plays the role of chemical potential for the i-th species of particles, i.e., particles in the i-th type subwells, and is conjugate to the variable ν_i, the filling fraction of the i-th type subwells (cf. σ and w in the previous case). We assulme that b_i's are arranged in the order $b_1 < b_2 < \cdots < b_d < 1 + b_1$. It is convenient to define $h_{d+i} = h_i$, $b_{d+i} = 1 + b_i$, $\nu_{d+i} = \nu_i$, and $\beta_{d+i} = 1 + \beta_i$ so that the indices of these variables are not restricted to the range of $\{1, 2, \ldots, d\}$. For our purpose, it is also convenient to use the variables t_i, given by

$$t_i = \frac{b_i + b_{i+1}}{2} + \frac{\Delta h_i}{\Delta b_i}, \quad \text{with } h_i = h_{i+1} - h_i \text{ and } \Delta b_i = b_{i+1} - b_i, \tag{13}$$

which gives position of the i-th tip of the potential and is sort of conjugate to the phase variable β_i. Clearly $t_{d+i} = 1 + t_i$. We choose $t_0 = 0$ and require that $t_0 = 0 < t_1 < \cdots < t_d = 1$.

The hull function $f_\omega(x)$ is still given by Eq. (7) except that the function $\tilde{b}(x)$ should be modified to [16]

$$\tilde{b}(x) = b_i \text{ for } \beta_{i-1} \leq x < \beta_i, \tag{14}$$

where $\tilde{b}(x + 1) = 1 + \tilde{b}(x)$ and w now becomes $\omega \equiv (\text{w}, \beta_0 = 0, \beta_1, \ldots, \beta_{d-1})$. The function *b(s)* can be expressed explicitly in terms of the integer function $\text{Int}[x]$ and we have [16]

$$f_\omega(x) = 1 + b_j + d_0 \sum_{i=j}^{j+d-1} \Delta b_i \sum_{n=-\infty}^{\infty} e^{-|n|\chi} \, \text{Int}[x + n\omega - \beta_i], \tag{15}$$

valid for any integer j.

The variables *hi*'s, or equivalently t_i's, do not appear in Eq. (15) but for $u_n = f_\omega(n\omega + \alpha)$ to be a stationary configuration, they must satisfy the consistency condition

$$f_\omega(\beta_i + 0^-) < t_i < f_\omega(\beta_i + 0^+), \forall i. \tag{16}$$

It is clear from the hull function that there is a principal gap of width $d_0\Delta b_i$ associated with each β_i, or the tip t_i, for $0 \leq i < d$. For each principal gap, say the i-th one, there is a tower of secondary gaps occuring at $\mathrm{Frac}[\beta_i + n\omega]$ with width $d_0\Delta b_i e^{-|n|\chi}$ for all non-zero integer n. The principal gap together with its associated secondary gaps is called a hole [17].

We note that the total width of the i-th hole, i.e., the sum of the widths of all its gaps, is Δb_i and $\sum_{i=1}^{d} \Delta b_i = 1$. Hence the gaps in a period almost fill the interval [0, 1] and the allowed positions of the particles form a Cantor set called the Cantori.

When $\beta_i - \beta_j \in S_\omega$ for some $0 \leq j < i <$ d, we say that they are in resonance. The corresponding holes join each other to become a single hole. If $\beta_i = \beta_j + \mathrm{Frac}[n_{ij}\omega]$, the principal gap width around t_i becomes $d_0\Delta b_i + d_0\Delta b_j e^{-|n_{ij}|\chi}$ and the widths of the secondary gaps become $d_0\Delta b_i e^{-|n|\chi} + d_0\Delta b_j e^{-|n+n_{ij}|\chi}$ for all n. The resonance condition is an equivalent relation which could divide $\{\beta_0, \beta_1, \ldots, \beta_{d-1}\}$ into several subsets of equivalent β_i's.

Given an irrational winding number w, when the variables t_i'sare varied, the ground state configuration of the system is locked to the case where all the β_i's are in resonance, i.e., $\beta_i = \mathrm{Frac}[n_i\omega] \in S_\omega$ for i = **0, 1,** . . . , d − 1 [16]. There is only a single hole and particles will be located at either the upper ends of all the gaps or at the lower ends for a recurrent minimum energy configuration when the phase variable α in Eq. (1) belongs to S_ω. In the former (latter) case, the configuration can be specified as $u_n = f_\omega(n\omega)[u_n = f_\omega(n\omega + 0^-)]$ and there exists a particle closest from above (below) to the i-th type tips and has the coordinate u_{n_i} for each $0 \leq$ i < d. A defect can be produced by moving the particle closest to the i-th type tips for some i over the tip to its neighboring well. Assuming we are moving the n_i-th particle from above the tips to below, the resulting defect configuration is

$$u'_n = u_n - d_0\Delta b_i e^{-|n-n_i|\chi}. \tag{17}$$

As in the case of solitons, it is straightforward to show that [16]

$$u'_n = f_{\omega'}(n\omega), \quad \omega' = \langle \omega, \beta_0, \ldots, \beta_{i-1}, \beta_i^+, \beta_{i+1}, \beta_{d-1} \rangle. \tag{18}$$

The particles are now located inside the gaps. There no longer exists a particle closest (from above) to the i-th type tips although there are still particles closest to the j-th type tips for all $j \neq$ i. We can construct a representative sequence of β_i^+ by choosing a sequence of integers $\{m_{ik} | k = 1, 2, \ldots\}$ such that $\mathrm{Frac}[m_{ik}\omega] > \mathrm{Frac}[m_{i,k+1}\omega]$ and $\lim_{k\to\infty} \mathrm{Frac}[m_{ik}\omega] = \mathrm{Frac}[n_i\omega]$. Clearly $\lim_{k\to\infty} |m_{ik}| = \infty$ and at any cutoff N, the particle closest to the i-th type tips, from above, is the m_{iN}-th one. As the cutoff is removed, the particle closest to the i-th type tip "moves off" to spatial infinity.

In the defect configuration, the particle originally at $u_{n_j}, j \neq i$, moves from the upper end of the gap around t_j to u'_{n_j} which is inside the gap. It is clear that $|\mathrm{Frac}[u'_n] - \mathrm{Frac}[u'_{n_j}]| > \min(\Delta u_{n_j}, \Delta_j - \Delta u_{n_j})$ with $\Delta u_{n_j} \equiv u_{n_j} - u'_{n_j}$ and Δ_j being the width of the gap around t_j, for any n other than n_j showing that the defect configuration is non-recurrent.

We can also move both the n_i-th and the n_j-th particles, closest to the i-th type and the j-th type tips respectively, over the corresponding tips to their neighboring wells resulting in a new defect configuration with

$$u''_n = u_n - d_0\Delta b_i e^{-|n-n_i|\chi} - d_0\Delta b_j e^{-|n-n_j|\chi} = f_{\omega''}(n\omega) \tag{19}$$

with $\omega'' = \langle\omega, \beta_0, \ldots, \beta_{i-1}, \beta_i^+, \beta_{i+1}, \ldots, \beta_{j-1}, \beta_j^+, \beta_{j+1}, \ldots, \beta_{d-1}\rangle$. It should be obvious how to generalize this construction of the incommensurate defects.

As t_i's are varied in the region in $t = \langle t_1, \ldots, t_{d-1}\rangle$ space, where the ground state configuration is locked to $\beta_i = \mathrm{Frac}[n_i\omega]$ for $i = 1, \ldots, d-1$, boundaries consist of pieces of hypersurfaces of dimensions lower than $d-1$ will be reached (compared with the case of solitons whell σ is varied). These boundaries are determined by the conditions that the energy of a certain defect configuration as constructed above equals the energy of its recurrent background minimum energy configuration. The types of boundaries are classified according to the types of defect configurations [16]. At the boundaries, the single hole is just about to break into two or more holes.

For irrational ω, the $\mathbf{t}$-space is filled with $(d-1)$-dimensional domains which are stability regions of given $\boldsymbol{\beta}$'s with all $\beta_i \in S_\omega$. Boundaries of such regions are hypersurfaces of $(d-l)$-dimensions with $1 < l \leq d$. These $(d-l)$-domains are stability regions of the corresponding $\boldsymbol{\beta}$ where $l-1$ of its components β_i's become extended numbers β_{ji}^+ (or β_{ji}^-) for $\beta_{ji} \equiv \beta_j - \beta_i$ and some $0 \leq i < j < d$. There, however, exist $(d-l)$-domains in the $\mathbf{t}$-space which are not boundaries of any $(d-1)$-domains. In particular, there are $(d-2)$-dimensional hypersurfaces which are not the boundary of any $(d-1)$-domains of finite measure. Instead, there are $(d-1)$-domains of arbitrarily small dimension in a particular direction, arbitrarily close to such a $(d-2)$-hypersurfaces. These $(d-2)$-domains in $\mathbf{t}$-space are stability regions of corresponding $\boldsymbol{\beta}$'s whose components form two resonance subsets.

In general, for a given $\boldsymbol{\beta}$, the resonance conditions divide $\{\beta_0, \beta_1, \ldots, \beta_{d-1}\}$ into l subsets of equivalent β_i's. There are l distinct holes in the Cantori. Correspondingly, there exist l distinct types of orbits. The stability region of such $\boldsymbol{\beta}$ in $\mathbf{t}$-space is a $(d-l)$-dimensional domain which is not the boundary of a higher-dimensional domain. The boundaries of such a $(d-l)$-domain are again determined by the conditions that it costs no energy (enthalpy) to create incommensurate defects. The incommensurate defects can be constructed for each of the l subsets of equivalent β_i's. Let $\{\beta_{i_1}, \ldots, \beta_{i_k}\}$ be such a subset. An incommensurate defect configuration can be constructed by allowing one or more of the differences $(\beta_{i_j} - \beta_{i_1}) \in S_\omega$ to become extended numbers in $\bar{S}_\omega$. In practice, this is achieved by choosing the phase parameter α in Eq. (1) to equal β_{i_1} first. The defect configurations are then obtained as described for the case of $m = 1$.

In this note, we have elaborated on the relations between extended numbers and non-recurrent minimum energy configurations as well as the physics behind such relations. We demonstrate that the soliton and anti-soliton can be understood as resulting from adding or removing a single particle from the recurrent background thus changing the average particle number per period by an infinitesimal amount. They can also be understood as a soliton or anti-soliton lattice in the limit of infinite lattice spacing. Extended number fits naturally both descriptions. We also explained in detail the physics and the constructin of the incommensurate defects first discussed by R. B. Griffiths *et al.* [5]. The defects result from moving one or more particles closest to a certain type of potential tips over the tip to its neighboring well thus changing the filling fractions of the neighboring type of potential wells by an infinitesimal amount. This immediately reveals that the defects are chiral and carrying no particle number [16]. It is obvious from our discussion that this new type of defect is generic in nonlinear dynamical systems and could appear in quasi-crystals or other physical systems with quasi-periodic ordering.

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References

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[1] J. N. Mather and G. Forni, in Transition *to Chaos in* Classical and Quantum Mechanics, eds. J. Bellissard and S. Graffi, *Lecture Notes in* Mathematics 1589 (Springer, Berlin, 1994).

[2] (a) S. Aubry, Physica **D7**, 240 (1983); (b) S. Aubry and P. Le Daeron, Physica D8, 381 (1983).

[3] R. B. Griffiths, in Fundamental *Problems* in *Statistical Mechanics VII,* ed. H. van Beijeren (Elsevier Science Publisher, New York, 1990).

[4] More precisely, the configurations correspond to solitons in the usual sense only when $\omega = 1/q$. For w = p/q with $p > 1$, the discommensurations are defects with &fractional charge" $1/p$.

[5] R. B. Griffiths, H. J. Schellnhuber, and H. Urbschat, Phys. Rev. Lett. 65, 2551 (1990).

[6] The existence of a particle closest to a given type of tips *at finite region of the system* is guaranteed by the resonance condition. See [10] for details.

[7] S. Aubry and P. Quemerais, in *Low-Dimensional Electronic Properties of Molybdenum Bronzes* and *Oxides*, ed. C. Schlenker, (Kluwer Academic Publisher, the Netherlands, 1989).

[8] S. Aubry, in *Solitons and Condensed Matter Physics,* eds. Bishop and T. Schneider, Solid *State* Sciences (Springer, Berlin, 1978), Vol. 8.

[9] S. Aubry, J. Phys. **C6**, 2497 (1983).

[10] S.-C. Lee and W.-J. Tzeng, *Eur. Phys. J. B3, 563 (1999).*

[11] See, for example, I. Niven, H. S. Zuckerman, and H. L. Montgomery, in An *Introduction to the Theory of Nambers* (Wiley, New York, 1991), Chap. 6.

[12] S.-C. Lee and W.-J. Tzeng, Chin. J. Phys. 35, 56 (1997); H.-C. Kao, S.-C. Lee, and W.-J. Tzeng, Physica D107, 30 (1997).

[13] R. B. Griffiths, H. J, Schellnhuber, and H. Urbschat, Phys. Rev. B56, 8623 (1997); T. Scheidsteger *et al.*, Phys. Rev. **B56**, 8631 (1997).

[14] P. Delaly, Ph.D. thesis, Carnegie Mellon University, 1995.

[15] H. C. Kao, S.-C. Lee, and W.-J. Tzeng, unpublished (solv-int/9607001).

[16] S.-C. Lee and W.-J. Tzeng, unpublished.

[17] C. Baesens and R. S. MacKay, Physica **D69**, 59 (1993); C. Baesens and R. S. MacKay, Physica **D71**, 372 (1994); J. Ketoja and R. S. MacKay, Physica **D73**, 388 (1994).