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LETTER TO THE EDITOR

Ground states of one-dimensional systems and fixed points of 2*n*-dimensional maps

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Abstract. The ground-state problem for discrete one-dimensional systems with interactions between n-nearest neighbours is connected with $2n$-dimensional maps. Fixed points of these maps correspond to periodic system configurations. For a general class of systems it is explicitly shown for the first time that fixed points with some elliptic character cannot represent ground states.

Among the discrete invertible maps, those which are of special physical importance arise by minimising the potential energy or the Ginzburg–Landau free energy F of an infinite, discrete one-dimensional system. The trajectories generated by such maps, however, represent *all* energy extrema and not only the ground states or the states of thermodynamic equilibrium. Thus it is for theoretical reasons as well as of practical interest (e.g. for numerical investigations) to exclude as many sets of trajectories as possible from being ground-state candidates.

Up to now this was done for a class of systems with a one-'particle' potential and with nearest-neighbour interaction only (Aubry and Le Daeron 1983, Eilenberger 1983, MacKay 1982); the corresponding maps are two-dimensional. The best known member of this class is the Frenkel–Kontorova model

$$F\{\phi\} = \sum_i W(\phi_i, \phi_{i+1}) = \sum_i \tfrac{1}{2}(\phi_{i+1} - \phi_i - \Delta)^2 + \rho(1 - \cos\phi_i)$$

and its dynamic analogue, the Chirikov standard map. One of the results for systems like this is that periodic ground-state configurations—whose map counterparts have to consist of fixed points of the iterated map—can only be represented by hyperbolic fixed points, i.e. while owing to area preservation of the investigated two-dimensional maps the generic types of fixed points are either elliptic (both eigenvalues λ, $1/\lambda$ of the linearised iterated map complex, $|\lambda| \neq 1$) or hyperbolic (both eigenvalues λ, $1/\lambda \neq 1$ real), only the mapping-unstable hyperbolic points are possible ground states. Regarding the inevitable round-off errors of computers, this is of course of special significance for all attempts to calculate numerically ground states of higher periodicity.

The crucial point in proving this hyperbolicity of periodic ground states is the 'convexity' of the nearest-neighbour interaction

$$-\partial^2 F/\partial\phi_i \partial\phi_{i+1} > 0.$$

In this letter I shall prove the generalisation of the hyperbolicity of periodic ground states to a class of systems not restricted to nearest-neighbour interactions.

I consider systems characterised by an energy density

$$f\{\boldsymbol{\phi}\}=\frac{1}{N}\sum_{i=-N/2}^{N/2} W(\phi_i,\phi_{i+1},\phi_{i+2},\ldots,\phi_{i+n}),$$

$N\to\infty$, where W stands for one-particle energies and interactions between two or more particles up to n lattice sites apart. In these general considerations I confine myself to systems where the off-diagonal matrix elements $\partial^2 f/\partial\phi_i\partial\phi_j$ of the investigated ground state satisfy

$$-\partial^2 f\{\boldsymbol{\phi}\}/\partial\phi_i\partial\phi_{j\neq i}\geqslant 0. \tag{1}$$

A possible ground-state configuration necessarily has to obey the extremum condition $\partial f\{\boldsymbol{\phi}\}/\partial\phi_i=0$ at all lattice sites i; this condition produces the relation

$$(\partial/\partial\phi_i)(W(\phi_i,\ldots,\phi_{i+n})+W(\phi_{i-1},\ldots,\phi_{i+n-1})+\ldots+W(\phi_{i-n},\ldots,\phi_i))=0. \tag{2}$$

Equation (2) has to be singularly resolvable for ϕ_{i+n} as a function of $\phi_{i+n-1},\ldots,\phi_{i-n}$:

$$\phi_{i+n}=g(\phi_{i+n-1},\ldots,\phi_{i-n}), \tag{3}$$

or similarly for ϕ_{i-n} as a function of $\phi_{i-n+1},\ldots,\phi_{i+n}$ to guarantee the existence of an invertible map. This map is $2n$-dimensional because the variables of $2n$-neighboured particles have to be known to generate, via (3), step by step, all the other variables.

Let us now start from any configuration $\{\boldsymbol{\phi}^0\}$ of periodicity p, which means that for each j, particle j and particle $j+p$ have the same or some modulo positions. Introducing small perturbations ε_i of the periodic particle positions,

$$\phi_i=\phi_i^0+\varepsilon_i,$$

an expansion of the energy up to second order in the perturbations yields

$$f=f_0+\frac{1}{N}\sum_i\frac{\partial f_0}{\partial\phi_i^0}\varepsilon_i+\frac{1}{2}\frac{1}{N}\sum_{i,j}\frac{\partial^2 f_0}{\partial\phi_i^0\partial\phi_j^0}\varepsilon_i\varepsilon_j \tag{4}$$

with $f_0\{\boldsymbol{\phi}^0\}$ as the energy density of the periodic configuration. If the configuration $\{\boldsymbol{\phi}^0\}$ is a ground state, and this is assumed in the following, the contribution linear in ε has to vanish, while the contribution quadratic in ε has to be in any case non-negative. Because of the range of the interactions the second derivative $\partial^2 f_0/\partial\phi_i^0\partial\phi_j^0$ can be non-zero only for $|j-i|\leqslant n$; but as no confusion can arise from this point, no explicit marking is required. For practical reasons I introduce different abbreviations for the second-order f_0 derivatives:

$$\frac{1}{2}\frac{\partial^2 f_0}{\partial\phi_i^0\partial\phi_j^0}=\begin{cases}a_i & \text{for } i=j\\ -b_{i,j}=-b_{j,i} & \text{for } i\neq j\end{cases}$$

so that (4) reads

$$\Delta f=f-f_0=+\frac{1}{N}\Big(\sum_i a_i\varepsilon_i^2-\sum_{i\neq j} b_{i,j}\varepsilon_i\varepsilon_j\Big). \tag{5}$$

The real quantities a, b are of course functions of the variables $\{\boldsymbol{\phi}^0\}$ describing the p-periodic configurations and hence are invariant to a translation of p lattice sites:

$$a_{k+p}=a_k \qquad b_{k+p,l+p}=b_{k,l}. \tag{6}$$

While the periodic ground state is represented by fixed points of the p-fold iterated $2n$-dimensional map, the perturbed configurations considered so far do not have to be described by trajectories of the map, i.e. do not have to be configurations of extremal energy. For the investigation of the *mapping* stability of the fixed points, however, one has to consider mapping trajectories that are—at least in a certain region of the chain—infinitely close to the fixed-point trajectory. In the linearised approximation, these trajectories obey

$$0 = \partial\Delta f/\partial\varepsilon_i = 2a_i\varepsilon_i - 2\sum_{j\neq i} b_{ij}\varepsilon_j. \tag{7}$$

Fixed-point analysis now means that one looks for the $2n$ eigenvectors and eigenvalues of the linearised p-fold iterated map, i.e. one looks for—now generally complex—solutions $\{x\}$ of (7) reproducing themselves after p lattice sites, despite a factor of λ:

$$X_{lp+r} = X_r \cdot \lambda^l$$

with $l = 0, \pm 1, \pm 2 \ldots$ and $r = 1, 2 \ldots p$. Writing $j = mp + t$ with $m = 0, \pm 1, \pm 2 \ldots$ and $t = 1, \ldots p$, (7) yields

$$a_r X_r - \sum_{m,t}{}' b_{r,mp+t}\lambda^m X_t = 0 \tag{8}$$

where the prime indicates $mp + t \neq r$.

The solubility condition for the set of p equations like (8) reads

$$\det \mathbf{M}(\lambda) = 0 \tag{9}$$

with the $p \times p$ matrix

$$M_{r,t}(\lambda) = -\sum_m b_{r,mp+t}\lambda^m (1 - \delta_{r,t}) + \delta_{r,t}\Big(a_r \sum_{m\neq 0} b_{r,mp+r}\lambda^m\Big). \tag{10}$$

(Taking into account the symmetry and periodicity of $b_{i,j}$ one can see $M_{r,t}(\lambda) = M_{t,r}(1/\lambda)$, and with (9) this shows explicitly that the eigenvalues appear in $(\lambda, 1/\lambda)$ pairs.)

The same matrix $\mathbf{M}$, but for $\lambda = 1$, characterises the change in the energy density if the perturbation itself is made periodic with period p: i.e. $\varepsilon_{lp+r} = \varepsilon_r$ results, with equation (5), in

$$\begin{aligned}\Delta f_p &= \frac{1}{p}\sum_{r=1}^{p}\Big(a_r\varepsilon_r^2 - \varepsilon_r \sum_{m,t}{}' b_{r,mp+t}\varepsilon_t\Big) \\ &= p^{-1}\boldsymbol{\varepsilon}^{\mathrm{T}}\mathbf{M}(\lambda = 1)\boldsymbol{\varepsilon}.\end{aligned} \tag{11}$$

As it is assumed that our periodic configuration is a ground state, the eigenvalues of this real-symmetric matrix $\mathbf{M}(\lambda = 1)$ have to be non-negative and thus $\det \mathbf{M}(\lambda = 1)$ has to be non-negative too. In the case of one-particle potentials and convex nearest-neighbour interactions only—or for *two-dimensional maps*—only $|m| \leq 1$-terms appear in (10) and the property of $\det \mathbf{M}(\lambda = 1)$ together with (9) is sufficient already to exclude elliptic fixed points (and even alternating hyperbolic points, i.e. hyperbolic points with negative eigenvalues) from being possible ground states (Eilenberger 1983). Expansion of $\det \mathbf{M}(\lambda)$ yields in this case

$$0 = \det \mathbf{M}(\lambda) = \det \mathbf{M}(\lambda = 1) - \Big(\lambda + \frac{1}{\lambda} - 2\Big)\prod_{r=1}^{p} 2b_{r,r+1}. \tag{12}$$

For convex systems, the product on the right-hand side is positive and hence (12) cannot be realised for elliptic or alternating hyperbolic fixed points.

In the case of longer-ranged interactions—or *higher-dimensional maps*—the situation is more complicated: $|m|$-values greater than one appear in (10) and hence the expansion of det $\mathbf{M}(\lambda)$ gives contributions of higher λ, λ^{-1} powers. In order to exclude for this case certain sets of fixed points from being possible ground states, I consider special periodic perturbations in order to demonstrate a contradiction to the ground-state assumption. Take $\varepsilon_{lp+r} = \varepsilon|X_r|$, where $X_1, \ldots, X_p$ belong to one of the eigenvector solutions fulfilling (8) with an eigenvalue λ, and ε is any (small) real constant. Then one has from (11)

$$\Delta f_p = \frac{\varepsilon^2}{p} \sum_{r=1}^{p} \Big(a_r |X_r|^2 - |X_r| {\sum_{m,t}}' b_{r,mp+t} |X_t| \Big).$$

With (8) one can express

$$a_r |X_r|^2 = X_r^* {\sum_{m,t}}' b_{r,mp+t} \lambda^m X_t$$

and the last relations give

$$\Delta f_p = -\frac{\varepsilon^2}{p} \sum_r {\sum_{m,t}}' b_{r,mp+t} (|X_r||X_t| - \lambda^m X_r^* X_t).$$

Using the symmetry and periodicity of $b_{i,j}$ (see definition and equation (6)), one finally arrives at

$$\Delta f_p = -\frac{\varepsilon^2}{p} \Big(\sum_{r,t<r} 2b_{r,t} (|X_r||X_t| - \mathrm{Re}(X_r^* X_t)) + \sum_{r,t} \sum_{m>0} 2b_{r,mp+t} \Big(|X_r||X_t| - \frac{\lambda^m}{2} X_r^* X_t - \frac{\lambda^{-m}}{2} X_r X_t^* \Big) \Big). \tag{13}$$

Now $\{\phi^0\}$ was assumed to be a ground state, i.e. e.g. Δf, equation (5), has to be non-negative. Perturbations of the particle positions with $\Delta f = 0$—if they exist—have to be extremal configurations of the second-order expansion and hence solutions of the linearised map equation (7). If now (and this generic situation will be considered in the following) the ε part of the modified periodic configuration

$$\phi_{r+lp} = \phi_r^0 + \varepsilon|X_r| \tag{14}$$

itself is no solution of the linearised map (for this it is for example sufficient that none of the eigenvalues of the considered fixed points is exactly equal to one) then necessarily $\Delta f_p > 0$ for this perturbation. Regarding equation (13) with $b_{i,j} \geq 0$, from equation (1), the following is obvious. If *at least* one of the $2n$ eigenvalues (and this implies, as shown, a pair of eigenvalues) is complex and on the unit circle, $\lambda = e^{i\gamma} \neq 1$, then $\lambda^m X_r^* X_t + \lambda^{-m} X_r X_t^* = 2\,\mathrm{Re}(\lambda^m X_r^* X_t) \leq 2|X_r||X_t|$ and the periodic configuration (14) related to this eigenvalue does not increase the energy, $\Delta f_p \leq 0$, and thus the configuration $\{\phi^0\}$ cannot be a ground state, i.e. if the fixed points corresponding to a periodic configuration have in an obvious meaning some elliptic character, they cannot be possible minima of the energy.

At this point the following should be mentioned. In the classes of systems for which these results are valid, those of Aubry and Le Daeron (1983) are included. From their results—explicitly shown only for nearest-neighbour interactions—one can conclude that the fixed points should have at least one pair of eigenvalues not on the complex unit circle to describe periodic ground states. The calculations presented here—being much more direct and more easily understood—show that *no* complex eigenvalue may be on the unit circle.

One example of a system class for which these calculations hold true is

$$F_A\{\boldsymbol{\phi}\} = \sum_i \left(V_1(\phi_i) + \sum_{k=1}^{n-1} |C_k|(\phi_{i+k} - \phi_i)^{2\tau_k} + \tfrac{1}{2}(\phi_{i+n} - \phi_i)^2 \right)$$

with $\tau_k = 0, 1, 2 \ldots$. A subclass of this is the mean-field free energy of a ferromagnetic Ising model on a d-dimensional hypercubic lattice with one-dimensional inhomogeneity (Pandit and Wortis 1982)

$$F_I\{\boldsymbol{M}\} = -\sum_i \left(H_i M_i + T \int_0^{M_i} \mathrm{d}y \tanh^{-1} y \right) - \sum_{i,j} |k_{i,j}| M_i M_j .$$

The generalisation of these considerations to more complicated systems—e.g. with attracting and repulsing two-particle interactions—requires the confinement to less general systems and more subtle perturbations ε. This will be the topic of a subsequent paper.

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