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Equivalence of Certain Convex and Nonconvex Models of Spatially Modulated Structures

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The ground states of a certain class of one-dimensional models with a nonconvex interatomic interaction which exhibit spatially modulated structures are proved to be equivalent to those of the Frenkel–Kontorova-type models with a convex interatomic interaction. One of the nonconvex models numerically studied by Marchand *et al.* belongs to this class, and it turns out to be equivalent to the exactly solvable model with a complete devil's staircase studied by Aubry.

KEY WORDS. Frenkel–Kontorova models; convex interactions; nonconvex interactions; commensurate–incommensurate; ground states.

1. INTRODUCTION

Our understanding of commensurate–incommensurate phase transitions,[1] in which a complex phase diagram results from two (or more) competing length scales whose ratio can "lock" at a series of rational values as the temperature (pressure, etc.) varies, has been greatly aided by the study of simple one-dimensional models with nearest neighbor interaction,[2] whose properties can be worked out in considerable detail. In particular, a great deal is known (including a number of mathematically rigorous results)[3] about the ground states of the Frenkel–Kontorova[4] model and its extensions in cases in which the interparticle potential, W in Eq. (1) below, is a *convex* function.

Nonconvex interactions are equally (and sometimes more) reasonable from a physical point of view, even though they seem less easy to analyze mathematically. Numerical studies of several nonconvex models[5–8] have

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produced features in phase diagrams which seem not to be observed in the convex case (and are sometimes rules out by rigorous theorems). However, there are other instances[6,7,9] in which the ground-state phase diagrams resemble the convex case.

The purpose of this paper is to show that the ground state of a certain class of nonconvex models can be mapped onto those of corresponding convex models and vice versa. This result opens up the possibility of applying some of the rigorous results and the detailed analysis available for the convex case to a category of nonconvex models with nontrivial phase transitions. To be sure, this category is fairly special, but the equivalence which we shall demonstrate is nontrivial, and it may prove to be of some use in identifying which features of nonconvex interactions lead to phase transitions which are qualitatively different from the convex case.

2. EQUIVALENCE OF CONVEX AND NONCONVEX MODELS

We consider a one-dimensional system with energy

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

where the real number u_n denotes the position of the nth (classical) atom, $V(x)$ is an external potential, and $W(y)$ is the interaction between neighboring atoms a distance y apart. (One can think of V as arising from atoms other than those under consideration, whose positions remain fixed.) A *configuration* u is a collection $\{u_n\}$ of atomic positions.

The models of interest to us are constructed as follows. Let $V_0(x)$ be a continuous function which tends to $+\infty$ as x goes to $+\infty$ or $-\infty$, chosen so that it agrees with the function (see Fig. 1)

$$V^*(x) = \min_{m \in \mathbb{Z}} V_0(x+m) \tag{2}$$

for x inside an interval $[x_0, x_0+1]$ of unit length. The minimum is over all integers, and consequently V^* is periodic: $V^*(1+x) = V^*(x)$. Next let $W_0(y)$ be a strictly convex function with a minimum at $y = \gamma$,

$$0 \leqslant \gamma \leqslant 1 \tag{3}$$

and define (see Fig. 1)

$$W_1(y) = \min\{W_0(y), W_0(1+y)\} \tag{4}$$

$$W^*(y) = \min_{m \in \mathbb{Z}} W_0(y+m) \tag{5}$$

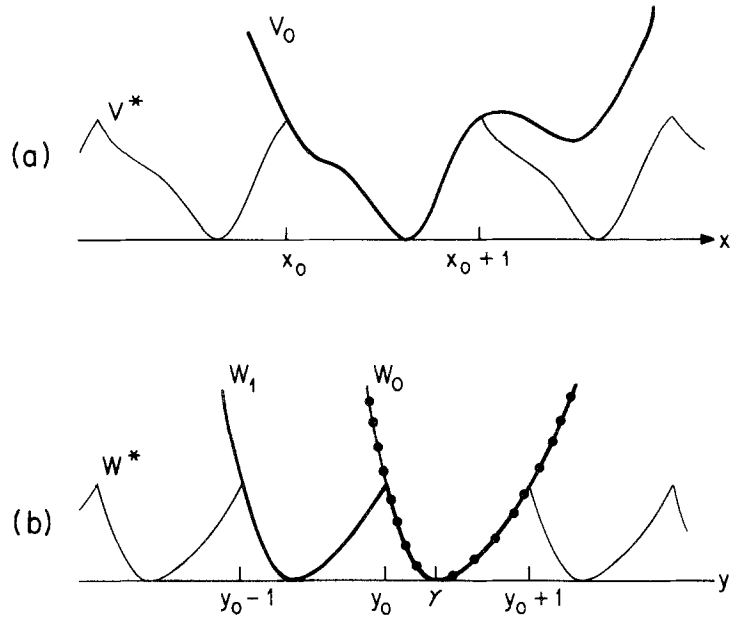

Fig. 1. (a) The potential V_0 indicated by the heavy curve coincides with V^*, the light curve, between x_0 and x_0+1. (b) The interaction W_0 is indicated by the line with dots, W_1 by the heavy curve, and W^* by the light curve (except where it coincides with W_1).

If y_0 is defined by the relation $W_0(y_0)=W_0(y_0+1)$, then W_0, W_1, and W^* coincide on the interval $[y_0, y_0+1]$ and W_1 and W^* on the interval $[y_0-1, y_0+1]$. Note that W^*, like V^*, is periodic with period 1.

We now define the models of interest to us by giving for each of them the pair of functions (V, W) which enter (1):

Model I: $V=V^*$, $W=W_0$

Model II: $V=V_0$, $W=W_1$

Model III: $V=V^*$, $W=W^*$

Model I is the type which has been studied extensively, especially by Aubry and his collaborators[3]: V is periodic and W is strictly convex. Indeed, any such model with continuous V is of this form, for if the period is different from 1, one simply rescales x and y, and given $V^*=V$, it is easy to construct a corresponding V_0 (in many different ways). Model II has a nonconvex W with a double well (Fig. 1). The particular case

$$V_0(x)=\tfrac{1}{2}Kx^2; \qquad W_0(y)=\tfrac{1}{2}(y-\gamma)^2 \tag{6}$$

was studied in refs. 6 and 7, using a slightly different notation. Note that we do not require that V_0 be convex.

Model III can be thought of as the "compact" version of model I: since both V and W are periodic, the energy remains invariant if the position of any atom is changed by a integer, and hence one need only study the case where all the u_n fall in the same unit interval, say [0, 1). It was employed by Chou and Griffiths[10] in numerical studies of model I.

We shall show that the ground states of all three models are equivalent by constructing maps (next paragraph) which carry one onto another with no change in energy. By "ground state" we shall mean a configuration of a *finite* number of atoms which minimizes (1), e.g., for n running from $-N+1$ to N. The results will then apply to infinite configurations obtained by letting N tend to infinity in a suitable way. This approach is not the one employed in either ref. 3 or 10, where only infinite configurations were considered. The resulting ground states for model I have a close affinity with those in ref. 10. They are, in particular, "minimal-enthalpy" states. However, we have not worked out the technical details.

The maps carrying configurations of one model onto another always consist in adding suitable integers to the atomic positions in order to obtain a new set of positions. For convenience we shall let u, v, and w stand for configurations of I, II, and III, respectively. For maps of I or II onto III, the added integer is zero: $w_j = u_j$ (or v_j). For maps of I or III onto II we demand that the image configuration v satisfy

$$x_0 \leqslant v_j < x_0 + 1 \tag{7}$$

Finally, for maps of II or III onto I, we demand that the position of some specific atom in the image configuration u, say u_0, lie in some specified unit interval, say [0, 1), and the remainder be chosen so that

$$y_0 \leqslant u_{j+1} - u_j < y_0 + 1 \tag{8}$$

for all j.

Let H_{I}, H_{II}, and H_{III} be the energies for models I, II, and III, respectively. As V^* is always less than or equal to V_0, and W^* is less than or equal to both W_0 and W_1, it follows that the energy $H_{\mathrm{III}}(w)$ for a configuration w obtained by mapping a configuration u or v of I or II onto III cannot exceed $H_{\mathrm{I}}(u)$ or $H_{\mathrm{II}}(v)$, as the case may be. This leads to an important conclusion:

If it can be shown that any ground state w of III maps onto a state u in I and a state v in II with the same energy, then the maps defined in the previous paragraph always map ground states onto ground states.

Suppose, for example, that w is a ground state and $H_{II}(v) = H_{III}(w)$, but v is not a ground state of II. Then there is a $\bar{v}$ in II with lower energy, whose image $\bar{w}$ in III cannot have larger energy:

$$H_{III}(\bar{w}) \leqslant H_{II}(\bar{v}) < H_{II}(v) = H_{III}(w) \tag{9}$$

contradicting the assumption that w is a ground state of III. Suppose, on the other hand, that $\bar{v}$ is a ground state of II, but its image $\bar{w}$ is not a ground state of III. Then there is (by continuity and compactness) a ground state w of III of lower energy which maps onto a v with equal energy:

$$H_{II}(v) = H_{III}(w) < H_{III}(\bar{w}) \leqslant H_{II}(\bar{v}) \tag{10}$$

contradicting the assumption that $\bar{v}$ is a ground state of II. The same argument works equally well for I in place of II. That ground states of I map onto II (and vice versa) is a consequence of first mapping I to III and then III to II (or the reverse).

What remains is to show that any ground state w of III maps onto states of I and II with the same energy. For I the argument is elementary: the map obviously preserves the value of $V = V^*$ for each atom, as V^* is periodic, while (8) guarantees that the interaction energy W_0 equals W^*. For II, (7) ensures that the V contributions to the energy are the same. However, one must in addition show that

$$y_0 - 1 \leqslant v_{j+1} - v_j \leqslant y_0 + 1 \tag{11}$$

in order that W_1 give the same result as W^*. To this end we first map w onto u and employ the result (see Appendix) that for any ground state u of I,

$$0 \leqslant u_{j+1} - u_j \leqslant 1 \tag{12}$$

The map from I onto II is given by the explicit formula

$$v_j = u_j - \mathrm{Int}(u_j - x_0) \tag{13}$$

where $\mathrm{Int}(x)$ is the largest integer not exceeding x. From (12) we see that $\mathrm{Int}(u_{j+1} - x_0) - \mathrm{Int}(u_j - x_0)$ is either 0 or 1, whence by (13) it follows that $(v_{j+1} - v_j) - (u_{j+1} - u_j)$ is either 0 or -1. Then (11) follows from (8).

3. REMARKS AND EXAMPLES

The equivalence of the ground states of models I and II depends on (3): the minimum of W_0 must lie between 0 and 1. If in addition to the con-

ditions given in Section 2 one assumes that $V_0(x)$ has a unique absolute minimum at $x=\bar{x}$, it can be shown (we shall not given the argument here) that the ground state of model II as N becomes infinite is

$$v_n = \bar{x} \tag{14}$$

for all n, for $\gamma < 0$ or $\gamma > 1$. But in general the ground state of I will not be the image of this v under the map discussed above.

For the specific case (6), model II has been studied numerically by Marchand *et al.*,[6,7] while Aubry[11] has obtained analytic expressions for the phase boundaries for the commensurate phase of model I. We have used the latter to compute phase boundaries to compare with the numerical results in Fig. 2 of ref. 6 or Fig. 6 of ref. 7. The agreement is excellent (confirming, incidentally, the general accuracy of the minimization eigenvalue approach used in refs. 6 and 7).

It is also worth remarking that there is an alternative way to demonstrate the equivalence of the two models in the present case, (6). This is done by mapping model II to a spin model. We define spin variables S_n, associated with a configuration v in model II, by

$$S_n = \begin{cases} 1 & \text{if} \quad v_n - v_{n-1} > y_0 \\ -1 & \text{if} \quad v_n - v_{n-1} \leqslant y_0 \end{cases} \tag{15}$$

Then, as long as stationary configurations (satisfying $\partial H/\partial v_n = 0$) are concerned, the energy of model II with (6) can be rewritten as

$$H_{\mathrm{II}} = \sum_n \sum_m J(n-m)\, S_n S_m + \frac{1}{2}\left(\gamma - \frac{1}{2}\right) \sum_n S_n \tag{16}$$

where the "exchange interaction" $J(n)$ between two spins n lattice sites apart is given by

$$J(n) = \frac{1-r}{8(1+r)}\, r^{|n|} \tag{17}$$

with r being defined by

$$r = 1 + \frac{K}{2} - \frac{1}{2}(K^2 + 4K)^{1/2} \tag{18}$$

Equation (16) is derived by using the technique described in ref. 11. The spin Hamiltonian (16) belongs to the class of Ising models studied by Bak and Bruinsma.[12] Aubry[11] showed that such Ising modes can be mapped onto models of type I (in general, with long-range interatomic inter-

actions). Applying his prescription to the specific case (16), one obtains model I with (6). On the other hand, the latter can be mapped back onto the former under the condition (3). Thus, the equivalence of models I and II with (6) is established. [The spin model (16) has been studied by Ishimura[13] and the phase diagram for ground states has been obtained in some detail, which is consistent with the results computed from Aubry's analytic expressions mentioned in the preceding paragraph.]

APPENDIX. DERIVATION OF (12)

It must be shown that any ground state of model I, with γ in the range (3), satisfies the set of inequalities (12). We begin with the first inequality,

$$u_j \leqslant u_{j+1} \tag{A.1}$$

and note that it will be satisfied when $\gamma = 0$ because the ground state will be of the form

$$\bar{u}_j = \bar{x} \tag{A.2}$$

for all j, where $\bar{x}$ is some (absolute) minimum of V^*: this state clearly minimizes both the V and W contributions to H.

Suppose next that $\gamma > 0$. Then there is a $\sigma < 0$ such that

$$\bar{W}_0(y) = W_0(y) - \sigma y \tag{A.3}$$

has a (unique) minimum at $y = 0$. Let $\bar{H}$ be the energy function obtained by replacing W_0 with $\bar{W}_0$. For any configuration u of $N+1$ atoms numbered $j = 0, 1, \ldots, N$ it is the case that

$$\bar{H}(u) = H(u) - \sigma(u_N - u_0) \tag{A.4}$$

Now $\bar{u}$, (A.2), is clearly a ground state of $\bar{H}$, and if u is a ground state of H, we have the inequalities

$$\bar{H}(u) + \sigma(u_N - u_0) = H(u) \leqslant H(\bar{u}) = \bar{H}(\bar{u}) \leqslant \bar{H}(u) \tag{A.5}$$

upon noting that $\bar{u}_n = \bar{u}_0$. Since σ is negative, we conclude that

$$u_N \geqslant u_0 \tag{A.6}$$

The first inequality in (12) is then a consequence of the following result.

Lemma. Let $\{u_j\}$, $0 \leqslant j \leqslant N$, be any set of real numbers satisfying $u_0 \leqslant u_N$, and let $\{x_j\}$ be the same set of numbers rearranged in increasing order,

$$x_0 \leqslant x_1 \leqslant \cdots \leqslant x_N \tag{A.7}$$

Let $W(y)$ be a convex function with the property $W(y) > W(0)$ whenever y is negative. Then

$$\sum_{j=1}^{N} W(x_j - x_{j-1}) \leqslant \sum_{j=1}^{N} W(u_j - u_{j-1}) \tag{A.8}$$

and if for some j it is the case that $u_j < u_{j-1}$, the inequality (A.8) is strict.

The lemma, whose proof is given below, implies (A.1), for the following reason. If u is a ground state of H, then it satisfies (A.6), and since W_0 is strictly convex with a positive minimum, $W = W_0$ obviously satisfies the conditions of the lemma. Were (A.1) not valid, (A.8) would hold as a strict inequality, making the $\{x_j\}$ a state of lower energy than the $\{u_j\}$, contradicting the assumption that u is a ground state; note that the contribution to H from $V = V^*$ is the same for the $\{x_j\}$ and the $\{u_j\}$.

The second inequality in (12) can be handled in exactly the same manner by defining

$$\hat{u}_j = j - u_j \tag{A.9}$$

$$\hat{W}_0(y) = W_0(1 - y) \tag{A.10}$$

$$\hat{V}^*(x) = V^*(-x) \tag{A.11}$$

and noting that, because of the periodicity of V^*,

$$\hat{H}(\hat{u}) = H(u) \tag{A.12}$$

where $\hat{H}$ is obtained by using $\hat{W}_0$ and $\hat{V}^*$ in place of W_0 and V^*. The minimum $\hat{\gamma}$ of $\hat{W}_0$ is equal to $1 - \gamma$, and thus the previous argument applied to $\hat{H}$ yields (A.1), with $\hat{u}$ in place of u, as long as $\gamma \leqslant 1$. This then translates, using (A.9), into the second inequality in (12).

The lemma is proved as follows. Define the quantities

$$\alpha_j = x_j - x_{j-1}; \qquad \beta_j = u_j - u_{j-1} \tag{A.13}$$

The α's are nonnegative numbers, and the β's can be expressed as linear combinations of the α's through the formula

$$\beta_j = \sum_k B_{jk} \alpha_k \tag{A.14}$$

Here we assume that $B_{jk} = 0$ if either $\beta j = 0$ or $\alpha_k = 0$. If $\beta_j > 0$, then the nonzero B_{jk} are all $+1$; if $\beta_j < 0$, the nonzero B_{jk} are all -1. For a given k, let J_k^+ and J_k^- be the sets of j values for which $B_{jk} = +1$ and -1, respectively.

Condition (A.6) implies that for every k for which $\alpha_k > 0$, J_k^+ is not empty, and contains either the same number of elements as J_k^- or one more. (One way to see this is to draw a graph of u_j as a function of j, connecting successive points with straight lines.) The desired inequality

$$\sum_{j=1}^{N} W(\alpha_j) \leqslant \sum_{j=1}^{N} W(\beta_j) \tag{A.15}$$

can be obtained by showing that the partial derivative of the left side with respect to any nonzero α_k does not exceed to corresponding partial derivative of the right side, that is,

$$W'(\alpha_k) \leqslant \sum_j B_{jk} W'(\beta_j) \tag{A.16}$$

This can be rearranged in the form

$$W'(\alpha_k) + \sum_{j \in J_k^-} W'(-|\beta_j|) \leqslant \sum_{j \in J_k^+} W'(\beta_j) \tag{A.17}$$

If J_k^+ contains one more element than J_k^-, (A.17) follows from the observation that $W'(y)$ is monotone increasing in y, and the arguments of W' on the left side are obviously not greater than those on the right side. If J_k^- has as many elements as J_k^+ (which means—see above—that J_k^- is not empty), one simply discards one of the terms on the left side whose argument is negative, noting that in such a case W' is necessarily negative.

If W is not differentiable, one employs a similar argument with finite differences replacing derivatives. This is in any case a more "elegant" approach, though harder to explain. The strict inequality in (A.15) when some β_j is negative comes by noting that this condition leads to a corresponding strict inequality in (A.17) for some k.

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