Localized Defects in Classical One-Dimensional Models

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Several aspects of localized defects in the Frenkel–Kontorova, classical XY chain and analogous models with a finite range of interactions are discussed from a general point of view. Precise definitions are given for defect phase shifts (charges) and for creation, pinning, and interaction energies. Corresponding definitions are also provided for interfaces (localized regions separating two phases). For the nearest-neighbor Frenkel–Kontorova model, the various defect energies are related to areas enclosed by contours joining heteroclinic points of the area-preserving map generated by the conditions of mechanical equilibrium.

1. INTRODUCTION

This paper is a study of some properties of localized defect configurations in classical one-dimensional models of the sort used to describe incommensurate and modulated phases.[1,2] Examples include the Frenkel–Kontorova[3] model with energy

$$\Phi = \sum_n \left[V(u_n) + \tfrac{1}{2}(u_{n+1} - u_n)^2 \right] \tag{1.1}$$

where u_n is a real variable giving the position of the nth atom in a linear chain and $V(u)$ is a periodic potential; and the chiral classical XY model in a magnetic field,[4]

$$\Phi = \sum_n \left[-H \cos \phi_n - \cos(\phi_{n+1} - \phi_n - \Delta) \right] \tag{1.2}$$

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where ϕ_n is an angle associated with the nth "spin." The ground states of these and other analogous models can exhibit a periodicity or quasiperiodicity which varies in a complicated way as a function of the parameters (such as H and Δ) which enter the energy, showing some resemblance (or at least analogy) with a variety of physical systems, including some alloys,[5] ferroelectrics,[6] rare-earth magnets,[7] and the like, in which there is a one-dimensional modulation superimposed on a regular crystal structure. If the modulation period is a rational multiple of the distance between crystalline planes, one calls it "commensurate"; otherwise, it is "incommensurate." It seems likely that both of these can occur in real physical systems, and it is known that both can be exhibited (under suitable conditions) by ground states of (1.1) and (1.2).[2,4] Among the elementary excitations of these systems there are localized static defects[1,2,4,8–15] (called various names, such as kinks, solitons, discommensurations, domain walls), which play an important role in the phase transitions which occur when the periodicity of the modulation changes and in various transport and other (e.g., electronic) properties of the system. In addition, it is helpful to think of certain incommensurate (and also commensurate) configurations as consisting of an array of defects with some average separation between the center of one defect and the next defect. The occurrence of such configurations as ground states is then related to the energy required to create defects and also their interaction energy.

It might appear at first sight that the ground-state properties and defect structures of simple one-dimensional models such as (1.1) and (1.2) can have little or no relevance to three-dimensional physical systems at a finite temperature. This turns out not to be the case.[5,10] One reason, to be sure, is that modulated structures are sufficiently complicated, in comparison with ordinary crystals, that *any* source of insight is welcome! But in addition, many modulated structures in three dimensions possess planes perpendicular to the modulation direction in which the thermal average of some parameter, such as position or magnetization, is essentially constant and the modulation is exhibited in the variation of this average from plane to plane. In such cases one can plausibly treat the thermal average in each plane as a classical quantity and assume the existence of a phenomenological free energy per unit area which depends on the value of this quantity in different planes, and which is a minimum in thermal equilibrium. Within this framework, a discussion of one-dimensional models and their static defects can be carried over to corresponding properties of a three-dimensional system by simply inserting "free" before every occurrence of "energy."

In this paper we consider localized defects, in classical (nonquantum) models with short-range interactions, which relax back to some underlying

reference configuration with increasing distance from the center of the defect. While the emphasis is on static defects, the basic definitions also apply to (localized) dynamical defects. Our aim is to provide precise definitions of concepts such as the "phase shift" or "charge" associated with a defect and the various energies (creation, pinning, interaction) associated with a single defect or a small number of defects. These concepts are illustrated with a number of examples, and in the case of the Frenkel–Kontorova model they are given a geometrical interpretation using an area-preserving map of the phase plane.[8,16]

The presentation occurs in the following order. Basic definitions of configurations, energies, equilibrium, FK models, etc., are assembled in Section 2, along with the definition of a localized defect and its "phase shift" and "charge." We also define an "interface" (a localized structure at the junction of two distinct "phases"), and consider multiple defects and interfaces which are composed of more elementary defects or interfaces.

Section 3 contains definitions and some analyses of various types of defect energy: the creation energy of a single defect, its pinning energy (work required to move the defect to a new location), the interaction energy of two or more defects, and the counterparts of these quantities for interfaces.

The static defects of a Frenkel–Kontorova model with nearest-neighbor interaction are discussed in Section 4 using the area-preserving map of the phase plane which is associated with the condition of mechanical equilibrium. Using the plausible assumption that a localized defect is associated with a set of heteroclinic points at the intersections of expanding and contracting manifolds,[8] the various energies defined in Section 3 are interpreted in terms of areas inside suitable contours made up from segments of the relevant manifolds.

Previous work on one-dimensional models and uniaxial modulated systems which is closely related to the theme of this paper includes the following items.

Aubry and his collaborators have carried out a very extensive analysis of Frenkel–Kontorova and related models, with particular emphasis on minimum-energy configurations, including ground states and "elementary" defect configurations.[17] Although our analysis is deliberately not limited to minimum-energy configurations, it owes much in terms of a general point of view as well as specific ideas to Aubry's work. The use of an area-preserving map to study properties of equilibrium configurations was also initiated by Aubry.

A thermodynamic instability against the creation of localized defects is a well-known mechanism for phase transitions in uniaxial modulated systems. In this respect there have been many attempts at numerical and

approximate analytical calculations of defect creation and interaction energies for specific models.[9,18-21] Recently Fisher and Szpilka have proposed a general procedure for constructing the phase diagram of a uniaxial modulated system in the "small-fluctuation" regime.[10] The discussion is based on the assumption that the relevant long-period (or incommensurate) equilibrium or metastable states can be characterized in terms of a distribution of well-defined domain walls in a simple periodic structure. The thermodynamic stability of these states can then be discussed in terms of the creation and two-body, three-body, etc., interaction energies of the domain walls. One of the advantages of their treatment is that it provides a unified description of the equilibrium phases over a range of parameter values in the phase diagram, and a classification of the major and also the higher-order commensurate phases. (Our work is related to that just mentioned in that the procedures we present can be used for qualitative discussions and actual calculations when an appropriate phenomenological or "mean-field" description of the relevant model is available. These procedures also provide the ground work for an alternative approach to discussing the transitions between commensurate states, as in ref. 4; additional details are in ref. 20.)

The geometrical interpretation of the energy difference (sometimes known as the action) between stationary configurations for the Frenkel-Kontorova model (see Section 4) has been noted previously by Mackay et al.,[16] who were mainly interested in transport properties of points on the phase plane under successive iterations of the two-dimensional area-preserving twist map.[8,21] We find this picture very helpful in understanding various properties of the Frenkel-Kontorova model, such as the tendency to "lock" into commensurate phases, pinning of the localized defects, and the formation and completeness of the devil's staircase.[17] As the two-dimensional geometry of the phase plane plays an important role in obtaining many of these results, one might expect some qualitative changes in behavior (e.g., disappearance of the devil's staircase) for models corresponding to higher-dimensional canonical maps associated with interactions extending beyond nearest neighbors.

2. DEFINITIONS

2.1. Configurations and Energies

We shall be interested in one-dimensional systems in which the position or state of the nth particle (atom, spin, or whatever) is denoted by u_n. For example, u_n may be the displacement (possibly a vector) of the nth atom from its equilibrium position, or it could be a real variable giving the

(scalar) position of this atom relative to some (n-independent) origin. In a spin model u_n is the nth spin variable: in the (classical) XY model it is an angle measured relative to some fixed axis, in the (classical) Heisenberg model a point on the unit sphere. One can also consider cases in which u_n takes on only a discrete set of values (Ising model, Potts model).

The collection $\{u_n\}$ of these positions or angles or whatever is a doubly infinite sequence, $-\infty < n < \infty$, or *configuration*, denoted by u. Different configurations are distinguished, when necessary, by superscripts. Two configurations u and $\hat{u}$ are regarded as physically equivalent if one is obtained from the other by renumbering the particles, i.e., there is some q such that

$$\hat{u}_{n+q} = u_n \tag{2.1}$$

for all n. A configuration u is *periodic* with period Q provided Q is the smallest positive integer such that

$$u_{n+Q} = u_n \tag{2.2}$$

holds for all n. A superscript on Q will often be used to indicate which configuration has this period: Q' is the period of u', etc.

The *energy* of a configuration u is defined formally as the sum

$$\Phi(u) = \sum_{n=-\infty}^{\infty} K(u_n, u_{n-1}, ..., u_{n-r}) \tag{2.3}$$

where the *interaction K* is a real-valued, appropriately smooth function of its $r+1$ arguments. Here r is the *range* of the interaction: 1 for nearest-neighbor, 2 for next-nearest-neighbor, etc. Whereas (2.3) is not (in general) a convergent sum, it can still be used to define energy *differences* when only a finite number of the u_j are changed, or in the limit when the changes are small as $|j| \to \infty$.

An *equilibrium* or *stationary* configuration u is one for which

$$\partial \Phi / \partial u_j = 0 \tag{2.4}$$

for every j. An equilibrium configuration is *locally stable* provided it is a local minimum of Φ: all "nearby" configurations have a slightly higher, or at least not a lower energy. There are various "degrees" of local stability which can be discussed in terms of the spectrum of the infinite matrix

$$\partial^2 \Phi / \partial u_j \, \partial u_k \tag{2.5}$$

Given a sufficient degree of local stability, one can make a plausible case for the existence of localized equilibrium defects (Section 2.2 below).

However, the corresponding technical discussion goes beyond the scope of the present paper, in which we shall consider the properties of such defects assuming they exist, rather than the conditions which ensure their existence.

We have written (2.4) assuming the u_j are real numbers, but there is an obvious generalization to the case (as in the classical Heisenberg model) where the u_j are on smooth manifolds. The terms "equilibrium" and "locally stable" do not apply if the u_j are discrete variables.

The *average energy* per particle is defined as

$$\varepsilon = \lim_{M \to \infty} \lim_{N \to \infty} (N + M + 1)^{-1} \sum_{n=-M}^{N} K(u_n,..., u_{n-r}) \tag{2.6}$$

provided the limit exists and is independent of how M and N tend to infinity.

It is convenient to modify some of the preceding definitions in the case where the u_n are real numbers and the energy is unchanged if u_n is replaced by $u_n + a$ for all n, where a is some positive constant. For lack of a better name, we call this an *FK model* (for Frenkel–Kontorova). If the u_n are measured in units of a, or, equivalently, $a = 1$, as will be assumed henceforth, we require that

$$K(1 + u_n, 1 + u_{n-1},..., 1 + u_{n-r}) = K(u_n, u_{n-1},..., u_{n-r}) \tag{2.7}$$

Note that the Frenkel–Kontorova model (1.1) has this property with

$$K(u_1, u_0) = \tfrac{1}{2}(u_1 - u_0)^2 + V(u_0) \tag{2.8}$$

provided V is periodic with period 1; for example,

$$V(u) = -K(2\pi)^{-2} \cos(2\pi u) \tag{2.9}$$

For an FK model, two configurations u and $\hat{u}$ are regarded as "physically equivalent" if one is obtained from the other by renumbering the particles (2.1), or by a *shift* operation in which the same integer is added to each u_n, or by any combination of these, that is, provided there are integers q and s such that

$$\hat{u}_{n+q} = u_n + s \tag{2.10}$$

for all n. A configuration u is *periodic* with period Q provided there are integers Q and S such that

$$u_{n+Q} = u_n + S \tag{2.11}$$

and Q is the smallest positive integer for which this equation holds. Superscripts on Q and S will indicate to which configuration the "period" (Q, S) refers: thus, Q', S' refers to a configuration u'. The *winding number* or *average separation* of neighboring atoms in an FK configuration is defined by

$$\omega = \lim_{M \to \infty} \lim_{N \to \infty} (N + M + 1)^{-1} (u_N - u_{-M}) \qquad (2.12)$$

provided the limit exists and is independent of how M and N tend to infinity. For a periodic configuration (2.11),

$$\omega = S/Q \qquad (2.13)$$

The *enthalpy* of an FK configuration is obtained by replacing K in (2.3) with the modified interaction

$$K(u_n, u_{n-1}, ..., u_{n-r}) - \sigma(u_n - u_{n-1}) \qquad (2.14)$$

where σ is a "stress" or "tension."[19] (It is denoted by γ in ref. 19 and μ in many of Aubry's papers.) The equilibrium and local stability conditions for a given configuration are independent of σ, while the enthalpy per particle $\varepsilon(\sigma)$, defined by replacing K in (2.6) with (2.14), is given by

$$\varepsilon(\sigma) = \varepsilon(0) - \sigma\omega \qquad (2.15)$$

assuming ω is well defined, where $\varepsilon(0)$ is of course the energy per particle ε.

2.2. Defects and Their Phase Shifts

We shall call u' a *defect configuration* relative to a *reference configuration* u provided that, after (if necessary) a suitable renumbering of particles [see (2.1)],

$$\begin{aligned} u'_n &\to u_n & \text{as} \quad n &\to -\infty \\ u'_n &\to u_{n-q} & \text{as} \quad n &\to +\infty \end{aligned} \qquad (2.16)$$

where the left arrow means "tends to" in an appropriate sense. Typically there is some appropriate metric $d(\ ,\ )$, and $d(u'_n, u_n)$ goes to zero as $n \to -\infty$. We shall always assume that a defect is *localized* in the sense that u'_n tends to u_n, or u_{n-q}, as the case may be, sufficiently rapidly to ensure convergence of the sums in energy expressions (Section 3), and possibly other desirable properties.

The integer q in (2.16) is the *phase shift* of u' relative to u, and can be thought of as the number of extra particles which must be added to the

reference configuration to produce the defect; see Fig. 1 for an example when $q = 1$. This figure also illustrates the fact that if the reference configuration has a period Q, the phase shift can equally well be set equal to $q + vQ$, where v is any integer.

For FK models, (2.16) should be replaced with

$$
\begin{aligned}
u'_n &\to u_n + m & \text{as} \quad n &\to -\infty \\
u'_n &\to u_{n-q} + m + s & \text{as} \quad n &\to +\infty
\end{aligned}
\tag{2.17}
$$

where m and s are integers (in general, multiplying a, but we are assuming that $a = 1$), and the *phase shift* is defined as the pair (q, s). (Figure 2 illustrates the case $m = 0$, $q = 3$, $s = 1$, where the reference state is periodic with $Q = 5$, $S = 2$.) When the reference state is periodic, an equivalent phase shift is

$$
(q + vQ, s + vS)
\tag{2.18}
$$

where v is any integer. On the other hand, the quantities

$$
\tilde{q} = qS - sQ
\tag{2.19}
$$

$$
\hat{q} = q - s/\omega = \tilde{q}/S = q - sQ/S
\tag{2.20}
$$

are independent of the choice of v. Note that $\hat{q}$, which we shall call the *charge* of the defect, is also defined by the first equality in (2.20) for a nonperiodic reference configuration with a well-defined nonzero winding number.

The term "charge" is suggested by what happens if the defect u' is displaced a distance S to the right to form a defect u^*, with

$$
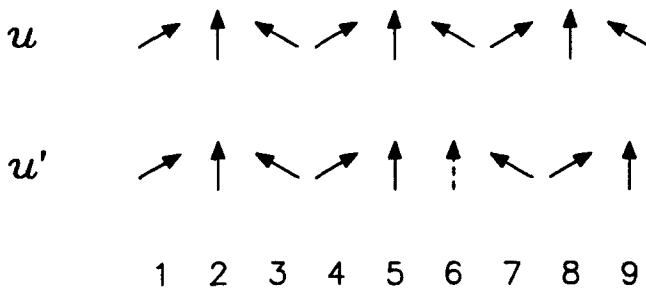u^*_{n+Q} = u'_n + S
\tag{2.21}
$$

Fig. 1. An example of a defect in a period-three configuration u of the chiral XY model. The defect configuration u' can be obtained by inserting one extra spin (indicated by the dashed arrow) in u, corresponding to a phase shift $q = 1$, or by inserting the four spins 4, 5, 6, and 7 corresponding to a phase shift $q = 4$.
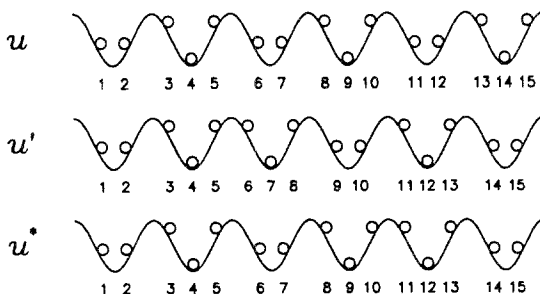
Fig. 2. Defects in a $Q = 5$, $S = 2$ configuration u of the Frenkel–Kontorova model. The configuration u' represents a defect with a phase shift $q = 3$, $s = 1$. The configuration u^* shows the defect translated to the right by two periods of the potential, with a total atomic displacement of $qS - sQ = 1$. Thus, the defect has a charge of $1/2$.

(See Fig. 2 for the case $S = 2$.) One can show that the *total atomic displacement*

$$\tilde{q} = \sum_n (u_n^* - u_n') \tag{2.22}$$

is given by (2.19). Thus, if each atom carries a unit charge, the current produced by a steady motion of the defect is the same as if the defect had a charge of $\tilde{q}/S$, whence (2.20). (This argument is taken from ref. 15.)

Note that if (2.16) or (2.17) is adopted as definition, one can just as well speak of u as a defect state relative to the reference state u', with a phase shift $-q$ or $(-q, -s)$. Similarly, u^* in (2.21) may be considered a defect state relative to u' as a reference, with phase shift $(0, 0)$, since

$$u_n^* \to u_n' \qquad \text{as} \quad |n| \to \infty \tag{2.23}$$

a consequence of (2.17), (2.21), and (2.11). While this expanded notion of a "defect" may seem strange at first, it has some technical advantages, which will emerge in Sections 3 and 4.

2.3. Multiple Defects

It is often convenient to think of a defect (or interface) as a composite object formed of two simpler defects (or interfaces). Thus, in Fig. 3 the configuration $\bar{u}$ contains both of the defects represented by u' and u'' relative to the reference configuration u.

This example suggests the following approach to thinking about how a complex defect $\bar{u}$ can be decomposed into two simpler objects. We suppose
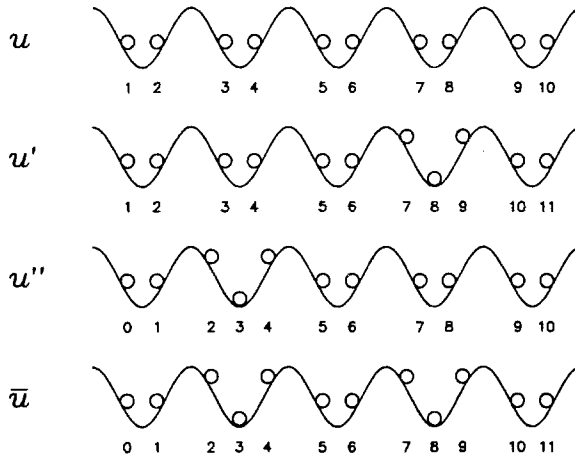
Fig. 3. An example of a two-defect configuration $\bar{u}$ relative to a period-2 reference configuration u. The corresponding single-defect configurations are u' and u''.

that $\bar{u}$, u'', u', and u are numbered in such a way that there is an integer m such that

$$u_n' \simeq u_n \quad \text{and} \quad u_n'' \simeq \bar{u}_n \quad \text{for } n \leqslant m$$

$$u_n' \simeq \bar{u}_n \quad \text{and} \quad u_n'' \simeq u_n \quad \text{for } n \geqslant m+1 \tag{2.24}$$

This is represented schematically in Fig. 4, where n is represented by horizontal distance.

Here $\simeq$ is used in a fairly loose sense; thus, for the example in Fig. 3 we would say that (2.24) holds for $m = 5$, but also (with less accuracy) for $m = 4$ or 6, or even with $m = 3$ or 7. However, we require that $\simeq$ become a strict equality in the limit as $|n|$ becomes infinite, or, in other words, that

$$u_n' \to u_n; \quad u_n'' \to \bar{u}_n \quad \text{as} \quad n \to -\infty$$

$$u_n' \to \bar{u}_n; \quad u_n'' \to u_n \quad \text{as} \quad n \to +\infty \tag{2.25}$$
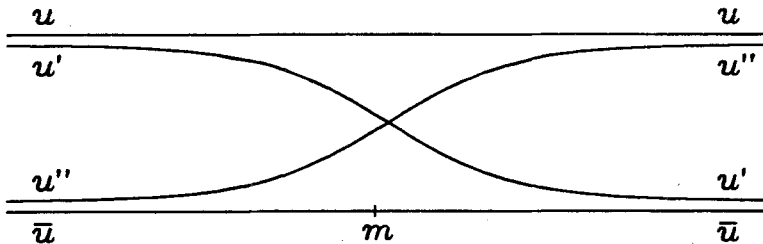

Fig. 4. The reconnection formula (2.24) or (2.25) is indicated schematically with particle position on the vertical axis plotted against particle number on the horizontal axis.

We shall call (2.25) a "reconnection" formula, because in most cases of interest to us u' and u'' can be obtained by a process suggested by (2.24): as a first approximation, let u'_n be u_n for $n \leqslant m$ and $\bar{u}$ for $n > m$; similarly let u''_n be $\bar{u}_n$ for $n \leqslant m$ and u_n for $n > m$, and then let both configurations relax to their final values. When (2.25) holds, we shall say that $\bar{u}$ "contains" the defects u' and u'', and further that the defect u' is to the right of u'', or u'' is to the left of u'. This terminology is motivated by (2.24).

Note that given $\bar{u}$ and u, the choice of u'' and u' need not be unique, especially with sufficient latitude in the use of $\simeq$ in (2.24). This ambiguity seems unavoidable, and is not serious for our subsequent discussion.

Using (2.25), one can show that the phase shift $\bar{q}$ of $\bar{u}$ (relative to u) is given by the sum of the phase shifts of u' and u'',

$$\bar{q} = q' + q'' \tag{2.26}$$

In the FK case, where the phase shift is the pair $(\bar{q}, \bar{s})$, one also has

$$\bar{s} = s' + s'' \tag{2.27}$$

Consequently, the charge $\hat{q}$, (2.20), is additive, provided ω is defined and is the same for u and $\bar{u}$. Such additivity is a plausible property for a reasonable definition of a multiple defect.

Properties of multiple defects $\bar{u}$ which contain more than two elementary defects can be discussed by iterating the reconnection procedure (2.24) or (2.25): first $\bar{u}$ is decomposed into two defects u' and u'', and one or both of these are then decomposed into two more defects, etc. Once again, the procedure does not lead unambiguously to a unique set of "elementary" defects, although in the case in which the latter are separated by distances larger than some characteristic length in which defects "relax" to the reference configuration, a suitably tight use of $\simeq$ in (2.24) can remove the ambiguity.

2.4. Interfaces

We shall call a configuration $u^{\alpha\beta}$ an *interface* between two "phases" α and β, represented by configuration u^α and u^β, provided that (after a suitable renumbering and shift, if needed)

$$\begin{aligned}
u_n^{\alpha\beta} &\to u_n^\alpha && \text{as} \quad n \to -\infty \\
u_n^{\alpha\beta} &\to u_n^\beta && \text{as} \quad n \to +\infty
\end{aligned} \tag{2.28}$$

Figure 5 shows two examples in which u^α and u^β are periodic phases whose character can be inferred from the "tails" of $u^{\alpha\beta}$. A defect as defined by
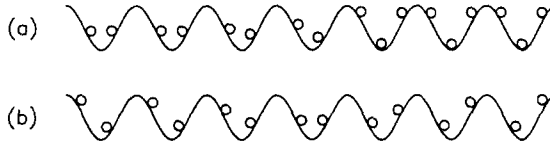
Fig. 5. Interfaces between (a) a period-2 phase (left) and a period-3 phase (right); (b) two distinct period-2 phases.

(2.16) or (2.17) can be thought of as a special case of an "interface" in which u^α and u^β are related to each other by a renumbering and/or a shift, so that they are physically equivalent, and thus identical "phases."

In the special case of an interface in an FK model between two periodic phases with equal nonzero winding number,

$$\omega = S^\alpha/Q^\alpha = S^\beta/Q^\beta \tag{2.29}$$

in an obvious notation, one can identify a *charge* $\hat{q}$ in the same manner as for a defect (Section 2.2 above). Thus, let Q be the least common multiple of Q^α and Q^β, and let S be ωQ. If the interface is shifted to the right by a distance S as in (2.21), one can show that the sum of the corresponding atomic displacements is

$$\tilde{q} = \sum_{j=1}^{Q} (u_j^\alpha - u_j^\beta) \tag{2.30}$$

and, as in (2.20), the charge is

$$\hat{q} = \tilde{q}/S \tag{2.31}$$

The equality of ω in both phases, i.e., equal density, (2.29), is essential: otherwise the interface cannot be moved along using a finite total displacement of all the atoms (and without adding or deleting atoms).

In general, a phase shift cannot be assigned to a single interface, but it can be defined for a pair of "complementary" interfaces $u^{\alpha\beta}$ and $u^{\beta\alpha}$ (see Fig. 6), which (after suitable renumbering and shifting) satisfy a "generalized reconnection" formula [compare (2.25)]:

$$\begin{aligned} u_n^{\alpha\beta} \to u_n^\alpha \quad \text{as } n \to -\infty; & \quad u_n^{\alpha\beta} \to u_n^\beta \quad \text{as } n \to +\infty \\ u_n^{\beta\alpha} \to u_n^\beta \quad \text{as } n \to -\infty; & \quad u_n^{\beta\alpha} \to u_{n-q}^\alpha + s \quad \text{as } n \to +\infty \end{aligned} \tag{2.32}$$

Then, in an FK model, (q, s) is the phase shift of the pair $u^{\alpha\beta}$, $u^{\beta\alpha}$ relative to the pair u^α, u^β; otherwise, the phase shift is q, and s should be omitted or

$$u^\alpha = \overset{\circ}{u}$$

$$u^\beta$$

$$u^{\alpha\beta}$$
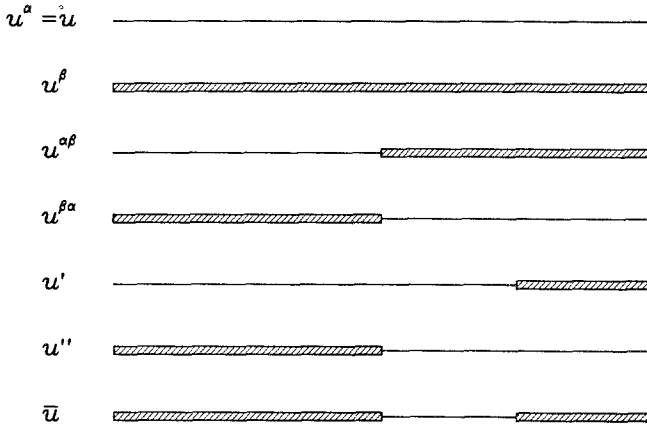
$$u^{\beta\alpha}$$

$$u'$$

$$u''$$

$$\bar{u}$$

Fig. 6.   Schematic illustration of interfaces $\alpha\beta$ and $\beta\alpha$ between phases α and β. Note that both interfaces are present in $\bar{u}$.

set equal to zero in (2.32) and the equations which follow. If u^α or u^β or both are periodic, an equivalent phase shift [compare (2.18)] is

$$(q + v^\alpha Q^\alpha + v^\beta Q^\beta, \, s + v^\alpha S^\alpha + v^\beta S^\beta) \tag{2.33}$$

where v^α and v^β are any integers, but are set equal to zero if the corresponding phase is *not* periodic.

That such a phase shift makes sense is supported by the following construction (see Fig. 6) in the case in which u^α is periodic. Let $u = u^\alpha$, and let u' and u'' be displacements of $u^{\alpha\beta}$ and $u^{\beta\alpha}$ given by the formulas

$$u'_n = v S^\alpha + u^{\alpha\beta}_{n - vQ^\alpha}, \qquad u''_n = -s + u^{\beta\alpha}_{n+q} \tag{2.34}$$

where v is some integer. Next construct a configuration $\bar{u}$ so as to satisfy (2.24): for v sufficiently positive it will be of the form suggested in Fig. 6, a segment of phase α inserted inside phase β. With the choices in (2.34) one can show, using the periodicity of $u = u^\alpha$, that the reconnection formula (2.25) is satisfied, and an additional calculation shows that the phase shift of $\bar{u}$ regarded as a defect relative to the reference state u^β is

$$(q + vQ^\alpha, \, s + vS^\alpha) \tag{2.35}$$

That is to say, the phase shift of the two interfaces combined as a defect in $\bar{u}$ is consistent with the value (or one of the values) assigned to the same pair by (2.33).
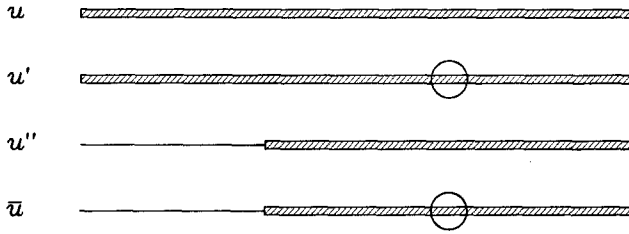
Fig. 7.   Schematic illustration of the reconnection of a defect configuration u' (the defect is indicated by a large circle) and an interface configuration u'' to yield a reference configuration u plus a configuration $\bar{u}$ containing both an interface and a defect.

A reconnection procedure of the sort just discussed can be used in other cases in which there are several interfaces present, or some mixture of interfaces and defects. As an example, see Fig. 7, where the large circle represents a defect.

3. DEFECT ENERGIES

3.1. Energy of a Single Defect

Let u' be a defect configuration relative to a reference configuration u [see (2.16) or (2.17)]. The (excess) *defect energy* can be thought of as

$$e' = e(u') = e(u'; u) = \Phi(u') - \Phi(u) \tag{3.1}$$

where we shall have to provide a more precise interpretation of the right-hand side, as the sum (2.3) diverges. We shall use the short form e' and $e(u')$ when the reference configuration is obvious from the context.
Define

$$K'_n = K(u'_n, u'_{n-1}, ..., u'_{n-r}) \tag{3.2}$$

and similarly K_n, $\bar{K}_n$, etc.: any superscript (or lack thereof) on u is transferred to K_n. The conditions (2.16) or (2.17) [note (2.7) in connection with the latter] lead to

$$\begin{aligned} K'_n &\to K_n & \text{as} \quad n &\to -\infty \\ K'_n &\to K_{n-q} & \text{as} \quad n &\to +\infty \end{aligned} \tag{3.3}$$

provided K is suitably continuous.

The simplest situation is that of zero phase shift, $q = 0$, in which case a plausible explication of (3.1) is

$$e' = \sum_{n = -\infty}^{\infty} (K_n' - K_n) \tag{3.4}$$

assuming that the convergence in (3.3) is sufficiently rapid that the sum is absolutely convergent. (We shall hereafter assume that the technical conditions required for the convergence of this and similar sums below are satisfied, as they will not be discussed in this paper and have to be checked in particular cases.)

For $q \neq 0$, we define

$$e' = -q\varepsilon + \lim_{N \to \infty} \left(\sum_{n = -N}^{N} K_n' - \sum_{n = -N}^{N-q} K_n \right) \tag{3.5}$$

The limits on the two sums are chosen such that the $N \to \infty$ limit will exist [see (3.3)]. As a consequence, the first sum has q extra terms (q may be negative), reflecting the fact that the defect has q extra particles. If each of these additional particles initially had a reference energy ε, then the right side of (3.5) would represent the work required to add them to the reference configuration. When the reference configuration u has a well-defined energy per particle, (2.6), we choose ε equal to this energy: one can then imagine that the extra particles required to form u' are particles of u "pulled in from infinity." That a compensating term $-q\varepsilon$ is needed in (3.5) can also be seen by considering a periodic configuration, where q can be altered by adding to it any integer multiple of the period Q. Such a change has no effect upon e' in (3.5) because of the fact that

$$\sum_{j = 1}^{Q} (K_j - \varepsilon) = 0 \tag{3.6}$$

Putting the matter in still another way, a "defect" in which an entire extra period of $q = Q$ particles is inserted in a reference configuration of period Q is indistinguishable from the reference configuration, and with ε the average energy per particle, (3.5) yields $e' = 0$, as it should.

One can rewrite (3.5) in the equivalent form

$$e' = \sum_{n = -\infty}^{m} (K_n' - K_n) + \sum_{n = m+1}^{\infty} (K_n' - K_{n-q}) + \Delta_m \tag{3.7}$$

where m is any integer, and Δ_m is given by

$$q = 0: \qquad \Delta_m = 0$$

$$q > 0: \qquad \Delta_m = \sum_{n=m+1-q}^{m} (K_n - \varepsilon) \tag{3.8}$$

$$q < 0: \qquad \Delta_m = \sum_{n=m+1}^{m-q} (\varepsilon - K_n)$$

[A convenient mnemonic for remembering or deriving formulas of this type is to note that the infinite sums are arranged to give absolute convergence consistent with (3.3), and Δ_m compensates for any terms which have been omitted from or duplicated in the (formal) sums for $\Phi(u') - \Phi(u)$, with a reference energy ε subtracted from each extra K_n.] Since ε is the average energy per particle, the average of Δ_m vanishes in the sense that

$$\lim_{M \to \infty} \lim_{N \to \infty} (M + N + 1)^{-1} \sum_{m=-M}^{N} \Delta_m = 0 \tag{3.9}$$

If u is a periodic configuration, then

$$\sum_{m=n}^{n+Q-1} \Delta_m = 0 \tag{3.10}$$

The *defect enthalpy* as a function of σ, $e'(\sigma)$, for an FK model, assuming that u has a well-defined winding number ω, (2.12), is obtained by replacing K'_n in the expressions above by

$$K'_n - \sigma(u'_n - u'_{n-1}) \tag{3.11}$$

[see (2.14)], along with the analogous substitution for K_n, and replacing ε by $\varepsilon(\sigma)$, (2.15). The dependence of $e'(\sigma)$ on σ is easily calculated from (3.5), noting that the first sum becomes

$$\sum_{n=-N}^{N} K'_n - \sigma(u'_N - u'_{-N-1}) \tag{3.12}$$

an analogous change takes place in the second sum, and that (2.17) applies. The final result is

$$e'(\sigma) = e' - \sigma(s - q\omega) = e' + \sigma\tilde{q}/Q$$

$$= e' + \sigma\omega\hat{q} \tag{3.13}$$

where e' is the defect energy, that is, the enthalpy for $\sigma = 0$; $\tilde{q} = S\hat{q}$ is defined in (2.19); $\hat{q}$ is the charge, (2.20); and the last equality in (3.13) assumes $\omega \neq 0$.

3.2. Pinning Energy

Let u be a locally stable, periodic reference configuration of period Q, u^0 a locally stable defect relative to u, and u^1 a translation of this defect Q particles to the right, which is to say

$$u_n^1 = u_{n-Q}^0 + S \tag{3.14}$$

for an FK model [see (2.11)]; otherwise, $S = 0$. As u_n^0 (in place of u_n') satisfies (2.17) or (2.16) as the case may be, the periodicity of u implies that

$$u_n^1 \to u_n^0 \qquad \text{as} \quad |n| \to \infty \tag{3.15}$$

Thus, one can imagine a continuous displacement of atoms carrying one defect into the other: a family of configurations u^t, $0 \leqslant t \leqslant 1$, interpolating between u^0 and u^1 with the property that u_n^t is a continuous function of t for each n, and is almost constant as $|n| \to \infty$. The corresponding defect energy $e(u^t)$ will (plausibly) possess a maximum as a function of t. Let e_m be the minimum of these maxima over all possible interpolating families u^t. The *pinning energy* e_p is defined as

$$e_p = e_m - e(u^0) \tag{3.16}$$

and can be thought of as the amount of external work which must be done to bring the defect u^0 over the lowest saddle point of the energy surface which separates it from u^1.

Under the plausible hypothesis that e_m is actually achieved in a specific saddle point configuration u^m, the pinning energy can be written as

$$e_p = \sum_{n=-\infty}^{\infty} (K_n^m - K_n^0) = e(u^m; u^0) \tag{3.17}$$

that is, it is the defect energy of u^m relative to the reference state u^0, or, equivalently, u^1. Note that the phase shift of u^m relative to u^0 or u^1 is zero.

3.3. Defect Interaction Energies

Corresponding to the reconnection formula (2.25), we define a *reconnection energy* by means of the formal expression

$$e_r(u', u''; u, \bar{u}) = \Phi(u') + \Phi(u'') - \Phi(u) - \Phi(\bar{u}) \tag{3.18}$$

interpreted as the sum

$$e_r(u', u''; u, \bar{u}) = \sum_{n = -\infty}^{\infty} (K'_n + K''_n - K_n - \bar{K}_n) \qquad (3.19)$$

which will converge absolutely [given appropriate technical conditions—see remarks following (3.4)]. The absence of phase shifts in (2.25) makes (3.19) a simpler formula than (3.5), and the former makes sense even in the absence of an average energy per particle.

The decomposition of a multiple defect into simpler defects was discussed in Section 2.3. The results of such a decomposition may not be unique. However, as long as the simpler defects are defined in some way, their energies of interaction can be obtained by a process of subtraction. Some examples will illustrate how this is done, and demonstrate the utility of (3.19) as an explicit expression for an interaction energy.

Let $u^{AB} = \bar{u}$ be a defect configuration which can be decomposed into two defects $u^A = u''$ and $u^B = u'$, all relative to the same reference configuration u, in accordance with (2.25); see also Fig. 3. One can then write

$$e(u^{AB}) = e(u^A) + e(u^B) + e_{AB} \qquad (3.20)$$

where this equation *defines* the interaction energy e_{AB}. An explicit expression in terms of (3.18) and (3.19) is

$$e_{AB} = \Phi(u^{AB}) + \Phi(u) - \Phi(u^A) - \Phi(u^B)$$

$$= e_r(u^{AB}, u; u^A, u^B) = \sum_n (K_n^{AB} + K_n - K_n^A - K_n^B) \qquad (3.21)$$

Next consider a configuration u^{ABC} containing three defects u^A, u^B, u^C, all relative to a reference u, with defect A to the left and defect C to the right of B. [For "left" and "right" in this connection, see the paragraph following (2.25).] To be more precise, assume that $u^{ABC} = \bar{u}$ can be decomposed into configurations $u^A = u''$ and $u^{BC} = u'$ satisfying (2.25), or equally well into configurations $u^{AB} = u''$ and $u^C = u'$ again satisfying (2.25); and that in turn u^{AB} can be decomposed into u^A and u^B, with u^A to the left of u^B (as in the previous paragraph), and u^{BC} can be decomposed into u^B and u^C, with u^B to the left of u^C and identical to the u^B obtained by decomposing u^{AB}. One can then define a three-defect interaction energy e_{ABC} by means of the formula

$$e(u^{ABC}) = e(u^A) + e(u^B) + e(u^C) + e_{AB} + e_{BC} + e_{ABC} \qquad (3.22)$$

where e_{AB} and e_{BC} are defined by (3.20) and its analog for u^{BC}. Note the absence of a term e_{AC} in (3.22); because of the linear ordering in these one-

dimensional systems it is most convenient to assume that such a term has been incorporated into e_{ABC}.

An explicit expression is

$$e_{ABC} = e_r(u^{ABC}, u^B; u^{AB}, u^{BC})$$

$$= \sum_n (K_n^{ABC} + K_n^B - K_n^{AB} - K_n^{BC}) \qquad (3.23)$$

where one can think of u^B as the reference configuration to which one can add an A or a C defect, or both. (Note that the value of e_{ABC} depends on the two-defect configurations u^{AB} and u^{BC}, the choice of which need not be uniquely determined by u^{ABC}.)

3.4. Energies of Interfaces

We know of no unique way an *interface energy* $e_i^{\alpha\beta}$ can be assigned to a *single* interface connecting phase α to phase β, such as those sketched in Fig. 5. However, there is a well-defined energy $e_i^{\alpha\beta} + e_i^{\beta\alpha}$ associated with *two* complementary interfaces $u^{\alpha\beta}$ and $u^{\beta\alpha}$, namely the reconnection energy

$$e_R(u^{\alpha\beta}, u^{\beta\alpha}; u^\alpha, u^\beta) = \Phi(u^{\alpha\beta}) + \Phi(u^{\beta\alpha}) - \Phi(u^\alpha) - \Phi(u^\beta) \qquad (3.24)$$

associated with the generalized reconnection formula (2.32). [We use e_R rather than e_r, (3.19), because (2.32) permits a phase shift and (2.25) does not.] In circumstances in which $u^{\alpha\beta}$ and $u^{\beta\alpha}$ are related by symmetry, it is plausible to assume that $e_i^{\alpha\beta}$ and $e_i^{\beta\alpha}$ are equal, and to assign half the total energy, (3.24), to each.

In order to make the formal expression (3.24) explicit, we need to assume that u^α and u^β have *the same average energy per particle* ε. The result is

$$e_R(u^{\alpha\beta}, u^{\beta\alpha}; u^\alpha, u^\beta) = \sum_{n=-\infty}^{m} (K_n^{\alpha\beta} + K_n^{\beta\alpha} - K_n^\alpha - K_n^\beta)$$

$$+ \sum_{n=m+1}^{\infty} (K_n^{\alpha\beta} + K_n^{\beta\alpha} - K_{n-q}^\alpha - K_n^\beta) + \Delta_m \qquad (3.25)$$

where

$$q = 0: \qquad \Delta_m = 0$$

$$q > 0: \qquad \Delta_m = \sum_{n=m+1-q}^{m} (K_n^\alpha - \varepsilon) \qquad (3.26)$$

$$q < 0: \qquad \Delta_m = \sum_{n=m+1}^{m-q} (\varepsilon - K_n^\alpha)$$

One way of deriving this is to introduce an auxiliary configuration $\bar{u}^\alpha$ with the property that $\bar{u}_n^\alpha$ tends to u_n^α and to $u_{n-q}^\alpha + s$ as n tends to $-\infty$ and $+\infty$, respectively. Then

$$e_R(u^{\alpha\beta}, u^{\beta\alpha}; u^\alpha, u^\beta) = e_r(u^{\alpha\beta}, u^{\beta\alpha}; \bar{u}^\alpha, u^\beta) + e(\bar{u}^\alpha; u^\alpha) \qquad (3.27)$$

where the right side is evaluated using (3.19) and (3.7).

The discussion of Section 3.2 above also applies to the *pinning energy* e_p of a locally stable interface $u^{\alpha\beta}$ separating two locally stable periodic phases u^α and u^β with the same average energy per particle, and the same winding number ω, (2.29), in the case of an FK model. Let Q be the least common multiple of Q^α and Q^β, and let S be ωQ for an FK model and 0 otherwise. If $u^0 = u^{AB}$ and u^1 is defined by (3.14), the discussion of Section 3.2 applies except that all defect energies are to be evaluated relative to u^0 as a reference state. Thus $e(u^1)$ should be replaced by $e(u^1; u^0)$, and $e_p = e_m$ in place of (3.16); formula (3.17) is unchanged. Note that since the pinning energy is related to *changes* in the interface energy as the interface moves, the fact that $e_i^{\alpha\beta}$ is undefined causes no problems.

Similarly, the ambiguity in the definition of single interface energies does not interfere with defining the interaction energy of two interfaces, or an interface with a defect, provided these can be obtained by a suitable application of the reconnection formula (2.25) or its generalization (2.32). For example, consider the configuration $\bar{u}$ in Fig. 6, which represents a $\beta\alpha$ interface separated from an $\alpha\beta$ interface by a region containing phase α. The interaction energy of these interfaces, which is analogous to the interaction energy of two defects, the e_{AB} of Section 3.3, is given by the reconnection energy (3.19), with u, u', u'', and $\bar{u}$ described in the paragraph containing (2.34). See Fig. 7 for another example: the interaction energy between the defect and the interface will again be given by (3.19), assuming (2.25) is satisfied.

4. DEFECTS AND AREA-PRESERVING MAPS

4.1. Maps of the Phase Plane and Phase Cylinder

In this section we restrict ourselves to FK models with nearest-neighbor interactions, $r = 1$ in (2.7), for which K satisfies the "convexity" condition

$$\partial^2 K(u_2, u_1)/\partial u_2\, \partial u_1 \leqslant c < 0 \qquad (4.1)$$

for some negative constant c.[17] Given any configuration u, define

$$p_n = \partial K(u_n, u_{n-1})/\partial u_n \qquad (4.2)$$

$$\hat{p}_n = -\partial K(u_{n+1}, u_n)/\partial u_n \qquad (4.3)$$

as "momenta" conjugate to u_n; note that in a stationary configuration, (2.4), $\dot{p}_n = p_n$.

Given that K is suitably smooth and satisfies (4.1), there is, as is well known, an area-preserving, invertible map T of the *phase plane* $\mathbb{R}^2$ onto itself with the property that for any stationary configuration $\{u_n\}$,

$$T\xi_n = \xi_{n+1} \tag{4.4}$$

where

$$\xi_n = (u_n, p_n) \tag{4.5}$$

That is to say, $\{\xi_n\}$ is an *orbit* of the map T. For the specific example of (2.8) with V given by (2.9), T is given by

$$\begin{aligned}
u_{n+1} &= u_n + p_{n+1} \\
p_{n+1} &= p_n + (K/2\pi) \sin 2\pi u_n
\end{aligned} \tag{4.6}$$

As usual, iterates of T will be denoted by T^ν, where ν is a positive or negative integer, and T^0 is the identity map. Thus, $T^{-2}\xi_n$ is ξ_{n-2}.

A general point in the phase plane will be denoted by (u, p), where u in this connection is a real number and does not denote a configuration $\{u_n\}$. By identifying values of u which differ by an integer, the phase plane is mapped onto the *phase cylinder* $S^1 \times \mathbb{R}$, and corresponding to the map T there is a map $\tilde{T}$ of the points $(\tilde{u}, p)$ of this cylinder onto itself, which is again invertible and area preserving. Thus, in the example (4.6), replace u by $\tilde{u}$, and understand the first (not the second) equation as an equality mod 1. An orbit $\{\xi_n\}$ of T in the phase plane is mapped into an orbit $\{\tilde{\xi}_n\}$ of $\tilde{T}$ on the phase cylinder. However, in the reverse operation in which the cylinder is "unrolled" onto the phase plane so that each point on the cylinder produces a collection of points with the same p value and all values of u differing from $\tilde{u}$ by integers, an orbit $\{\tilde{\xi}_n\}$ of $\tilde{T}$ will in general lead to a collection of orbits of T related to each other through the *shift operator* (or map)

$$\tau(u, p) = (1 + u, p) \tag{4.7}$$

4.2. Contracting and Expanding Manifolds, Heteroclinic Points

Consider a stationary configuration of period Q, (2.11). There is a corresponding orbit of $\tilde{T}$ on the phase cylinder made up of Q distinct points $\tilde{\xi}_j$, $1 \leqslant j \leqslant Q$, each of which is a fixed point of $\tilde{T}^Q$. As the map is area preserving, the product of the two eigenvalues of $\tilde{T}^Q$ linearized around one of these fixed points (the eigenvalues are the same for each $\tilde{\xi}_j$) is equal to 1. As Aubry and others have pointed out, a configuration which is

locally stable will, in general, correspond to the "hyperbolic" case of two real eigenvalues, one with magnitude less than and the other with magnitude greater than 1. In what follows we restrict ourselves to this situation.

Then, passing through each (hyperbolic) fixed point $\tilde{\xi}_j$ one expects to find two smooth curves which are invariant under $\tilde{T}^Q$: a *contracting* or *stable* manifold $\tilde{C}_j$ and an *expanding* or *dilating* or *unstable* manifold $\tilde{D}_j$. Any point on $\tilde{C}_j$ approaches $\tilde{\xi}_j$ under successive iterations of $\tilde{T}^Q$, while any point on $\tilde{D}_j$ approaches $\tilde{\xi}_j$ under iterations of $\tilde{T}^{-Q}$. Consequently, two contracting manifolds corresponding to different fixed points cannot intersect each other, nor can two expanding manifolds intersect each other. However, an expanding and a contracting manifold can intersect each other at *heteroclinic points* (known as "homoclinic" points if the manifolds are associated with the same fixed point), which are thus associated in a unique way with the two manifolds in question. [In exceptional cases the expanding manifold associated with one fixed point may coincide with the contracting manifold of another (or the same) fixed point.]

The map $\tilde{T}$ then maps the different (assuming $Q > 1$) contracting manifolds into each other, the different expanding manifolds into each other, and heteroclinic points onto heteroclinic points. The same holds for any iterate of $\tilde{T}$ or $\tilde{T}^{-1}$.

If the phase cylinder is "unrolled" onto the phase plane, the fixed points and manifolds just discussed are imaged in points and curves which are mapped into each other by the maps T and τ, (4.7). The fixed points of $\tilde{T}^Q$ are imaged in collections of points forming orbits, (4.4); in some cases there is just one orbit, but in general there will be more than one. Through a point ξ_n on the orbit $\{\xi_n\}$ there pass contracting and expanding manifolds C_n and D_n corresponding to their counterparts on the cylinder.

Figure 8 shows the situation schematically for $Q = 3$, $S = 2$: the points labeled 1, 2, 3 belong to one orbit and $\bar{1}$, $\bar{2}$, $\bar{3}$ to the other orbit. Heavy lines indicate expanding and light lines the contracting manifolds. The complete manifolds are extremely complex curves, and the figure only shows the portions which are "close," in terms of distance measured along the manifold, to the orbit points.

In general, C_n is not invariant under T^Q or under any iterate of T. It can, however, be identified as a contracting manifold in the sense that if α and β are any two points in C_n, then

$$T^m \alpha \to T^m \beta \qquad \text{as} \quad m \to +\infty \qquad (4.8)$$

in the sense that the Euclidean distance in the plane between $T^m\alpha$ and $T^m\beta$ tends to zero as m becomes infinite. In an analogous sense D_n is expanding: (4.8) with T^m replaced with T^{-m} holds, with α and β any two points in D_n.
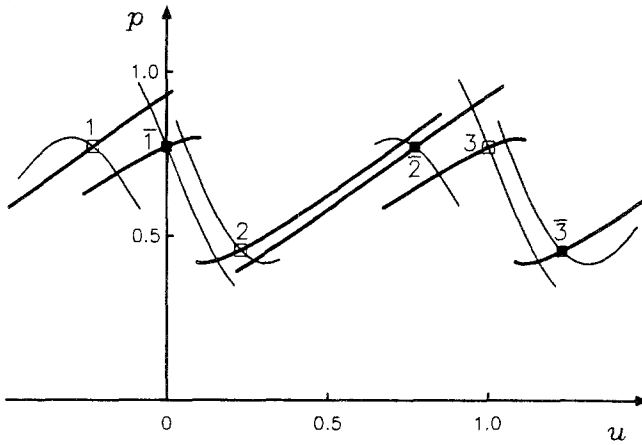
Fig. 8. Orbits with $Q = 3$, $S = 2$ and the corresponding contracting and dilating manifolds of the map T defined by Eq. (4.6) at $K = 2$. The open squares labeled 1, 2, and 3 are successive points on one orbit, and the solid squares labeled $\bar{1}$, $\bar{2}$, and $\bar{3}$ are successive points on another orbit. The heavy and light lines are the associated dilating and contracting manifolds, respectively.

As the different $\tilde{C}_j$ do not intersect each other, and if we assume (as seems plausible) that a given $\tilde{C}_j$ does not intersect itself, the corresponding contracting manifolds in the phase plane cannot intersect each other, and the same is true of the expanding manifolds. We shall again use the term "heteroclinic" point to refer to an intersection of an expanding and a contracting manifold. Note that the orbit points ξ_n obtained as images of the periodic orbit when the phase cylinder is "unrolled" are heteroclinic points under this definition.

If ξ_a and ξ_b are heteroclinic points associated with (lying on the intersection of) the *same* pair of expanding and contracting manifolds D and C and if in addition one can be obtained from the other by successive applications of the map T and/or the shift τ, i.e.,

$$\xi_b = \tau^\nu T^{\nu'} \xi_a \tag{4.9}$$

for some integers ν and ν', we shall call them *equivalent* heteroclinic points.

The preceding discussion identifies the manifolds which are useful for discussing equilibrium defects in a periodic reference configuration. The situation for nonperiodic configurations, for example, those with an irrational winding number ω, is not so clear. Nonetheless, it is plausible to assume that given a locally stable reference configuration, and perhaps in other cases as well, there is a similar network of expanding and contracting

manifolds passing through the points of the orbit and mapped into each other by T. This is the crucial feature assumed in all of the discussion below.

4.3. Equilibrium Defects and Heteroclinic Points

The physical significance of the contracting and expanding manifolds in the phase plane can be understood in terms of the example in Fig. 9. Here an external force f applied to atom 5 in the locally stable equilibrium configuration $\{u_n\}$ shown in Fig. 9a results in a configuration $\{u_n^*\}$ shown in Fig. 9b, where all atoms except 5 are in equilibrium. The corresponding points ξ_n and ξ_n^* in the phase plane are shown in Fig. 9c; note that correspondence of the horizontal positions in Fig. 9c with those in Figs. 9a and 9b. For $n = 5$ one has

$$p_5^* = \hat{p}_5^* + f \tag{4.10}$$

using (4.2) and (4.3) with asterisks added to the symbols, and hence two distinct points in the phase plane, ξ_5^* and $\hat{\xi}_5^*$, the former above the latter, since f is positive. The counterpart of (4.4),

$$\xi_{n+1}^* = T\xi_n^* \tag{4.11}$$
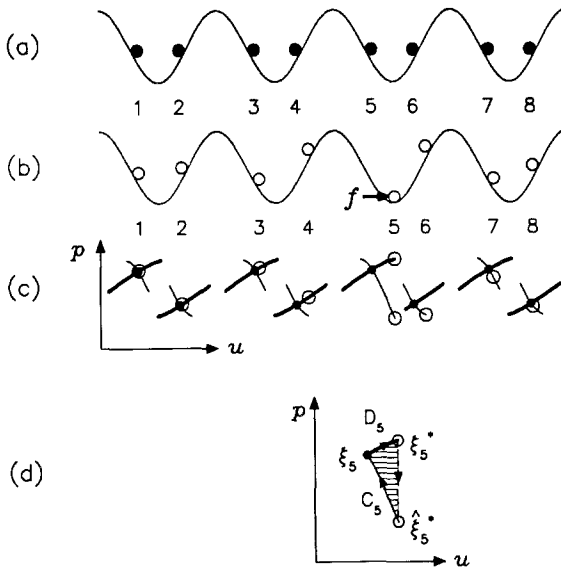
Fig. 9. A force applied to particle 5 in (a) the equilibrium configuration results in (b) displacements and (c) the phase plane. (d) Enlargement of a portion of (c). The area corresponds to the work required to change (a) to (b) (see text).

holds for all n except $n = 5$, for which one has

$$\xi_6^* = T\hat{\xi}_5^* \tag{4.12}$$

Given that $\{u_n\}$ is locally stable, it is plausible that u_n^* approaches u_n and thus ξ_n^* approaches ξ_n as $n \to -\infty$. Thus, when n is sufficiently negative, ξ_n^* should lie on the expanding manifold D_n through ξ_n. But if this is so, (4.4), (4.11), and the fact that T maps D_n onto D_{n+1} imply that ξ_n^* is on D_n for all $n \leqslant 5$. By the same reasoning, ξ_n^* falls on C_n, the contracting manifold through ξ_n, for all $n > 5$, and $\hat{\xi}_5^*$ falls on C_5.

Next, consider an equilibrium defect configuration u' satisfying (2.17) with $m = 0$, relative to a locally stable configuration u. The corresponding orbit $\{\xi_n'\}$ has the property

$$
\begin{aligned}
\xi_n' &\to \xi_n & \text{as} \quad n &\to -\infty \\
\xi_n' &\to \tau^s \xi_{n-q} & \text{as} \quad n &\to +\infty
\end{aligned}
\tag{4.13}
$$

Following the preceding discussion, we infer that ξ_n' lies on D_n and on $\tau^s C_{n-q}$ [the manifold obtained by shifting, (4.7), the contracting manifold through ξ_{n-q}]. Thus, *each point ξ_n' of the defect orbit is a heteroclinic point*, at the intersection of D_n and $\tau^s C_{n-q}$. The situation is illustrated schematically in Fig. 10a for the reference state, Fig. 10b for the defect with $q = -1$, $s = 0$, and Fig. 10c for the corresponding points and manifolds in the phase plane.
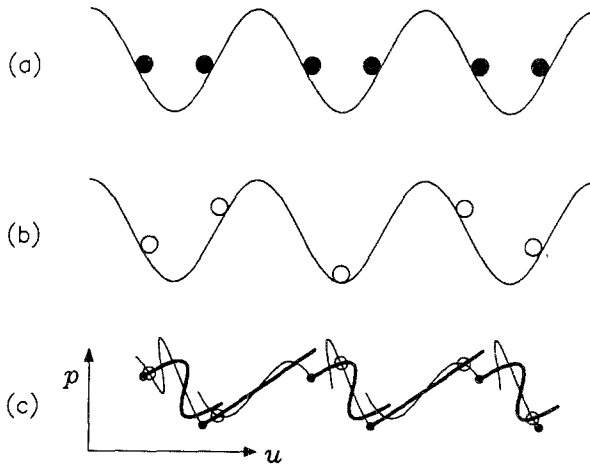

Fig. 10. (a) A reference configuration and (b) a $q = -1$, $s = 0$ defect shown in (c) the phase plane, along with segments of the dilating (heavy) and contracting (light) manifolds.

4.4. Energy Changes as Areas

By equating the energy change of a semi-infinite chain of atoms to the work done on the end atom during a quasistatic displacement, it is possible to interpret defect energies as areas in the phase plane. To begin with, consider a finite chain of atoms $M \leqslant j \leqslant N$. Let $\{u_j^t\}$ be a family of configurations depending smoothly on t for $0 \leqslant t \leqslant 1$ and satisfying the equilibrium condition (2.4) for all interior atoms $M < j < N$ and all t. With

$$\Phi_{MN}(u^t) = \sum_{j=M+1}^{N} K(u_j^t, u_{j-1}^t) \tag{4.14}$$

the energy of the finite chain, one finds by using (4.2) and (4.3), and noting that $\hat{p}_j^t = p_j^t$ in the interior of the chain,

$$\Phi_{MN}(u^1) - \Phi_{MN}(u^0) = \int_0^1 dt\, \partial \Phi_{MN}(u^t)/\partial t$$

$$= \int_{\Gamma^L} p_N^t\, du_N^t - \int_{\Gamma^R} \hat{p}_M^t\, du_M^t = W_{MN} \tag{4.15}$$

where Γ^L and Γ^R are appropriate smooth curves in the phase plane. As p_N^t and $-\hat{p}_M^t$ are the external forces which must be applied to atoms N and M to maintain mechanical equilibrium during the quasistatic transformation carrying u^0 to u^1, (4.15) has the interpretation that the energy change is equal to the work W_{MN} done by these forces.

Next consider a semi-infinite chain $-\infty < j \leqslant N$, and suppose that for all t,

$$u_n^t \rightarrow u_n^0 = u_n \qquad \text{as} \quad n \rightarrow -\infty \tag{4.16}$$

We then expect (Section 4.4 above) that for all $j \leqslant N$, $\xi_j^t = (u_j^t, p_j^t)$ lies on the expanding manifold D_j passing through ξ_j. Thus, in the limit, as M goes to $-\infty$, (4.15) yields the result

$$W_N^L = \int_{\Gamma_N^L} p\, du \tag{4.17}$$

for the work done during a displacement of atom N, where the superscript L indicates a semi-infinite configuration to the left of N, and Γ_N^L is an appropriate segment of D_N. Similarly, for a semi-infinite chain $M \leqslant j < \infty$ to the right of M (superscript R), assuming

$$u_n^t \rightarrow u_n^0 = u_n \qquad \text{as} \quad n \rightarrow +\infty \tag{4.18}$$

one obtains the expression

$$W_M = -\int_{\Gamma_M^R} p \, du \qquad (4.19)$$

where the integral is over a suitable segment Γ_M^R of the contracting manifold C_M.

As a first application of these formulas, consider the work required to move particle 5 from its position in Fig. 9a to that in Fig. 9b. This is the sum of (4.17) and (4.19) with $N = M = 5$, and is equal to

$$W_5 = \int_{\Gamma_5} p \, du \qquad (4.20)$$

where Γ_5, shown in Fig. 9d, which is enlargement of the region of the phase plane near ξ_5, consists of a segment of C_5 from ξ_5^* to ξ_5, and a segment of D_5 from ξ_5 to ξ_5^*. The direction of integration is indicated by the arrows; note that the one on C_5 properly accounts for the minus sign in (4.19). One can extend the integration path to a closed contour by adding the vertical segment, which contributes nothing to $\int p \, du$. Then W_5 is just the cross-hatched area inside the contour, and is positive, since the enclosing contour has a clockwise sense.

As a second application, we calculate the energy required to put together parts of two locally stable configurations u and $\bar{u}$ to form an equilibrium configuration u' satisfying (2.25). The process is illustrated schematically in Fig. 11. Choose some m ($m = 0$ in Fig. 11) and from the configuration u discard all atoms with $n > m$; from $\bar{u}$ discard all atoms with $n < m$. Move the end atom (numbered m) in each of the remaining semi-infinite configurations to the position u'_m and fuse them together.
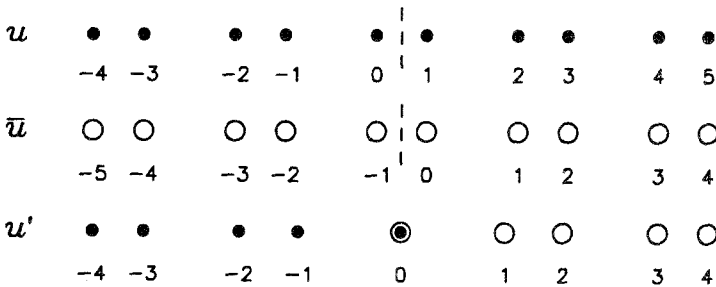

Fig. 11.   The semi-infinite configurations to the right and left of the dashed line for u and $\bar{u}$, respectively, are discarded and the atoms numbered 0 are shifted and fused together to form the configuration u'; see text.

The total work W'_m for the process just discussed is the sum of (4.17) and (4.19) with $N = M = m$, and can be written as

$$W'_m = \int_{\Gamma'_m} p \, du = \sum_{n=-\infty}^{m} (K'_n - K_n) + \sum_{n=m+1}^{\infty} (K'_n - \bar{K}_n) \qquad (4.21)$$

where Γ'_m is a path in the phase plane from ξ_m to ξ'_m via D_m, and from ξ'_m to ξ_m via $\bar{C}_m$; note that this takes proper account of the sign in (4.19). See Fig. 12, where Γ'_m consists of the two curved segments with arrows indicating the direction of integration. By adding straight line segments as shown, each of which makes zero contribution to $\int p \, du$, one can extend the integral to a closed contour and interpret W'_m as the enclosed area, or minus the area for a counterclockwise contour.

Next suppose there is another equilibrium configuration u'' satisfying (2.25). The work required to form it by the reconnection process just discussed, with the roles of u and $\bar{u}$ interchanged, is

$$W''_m = \int_{\Gamma''_m} p \, du = \sum_{n=-\infty}^{m} (K''_n - \bar{K}_n) + \sum_{n=m+1}^{\infty} (K''_n - K_n) \qquad (4.22)$$

where Γ''_m is a path in the phase plane connecting ξ_m to ξ''_m via $\bar{D}_m$, and ξ''_m to ξ_m via C_m. By adding W'_m to W''_m, we obtain the reconnection energy (3.19):

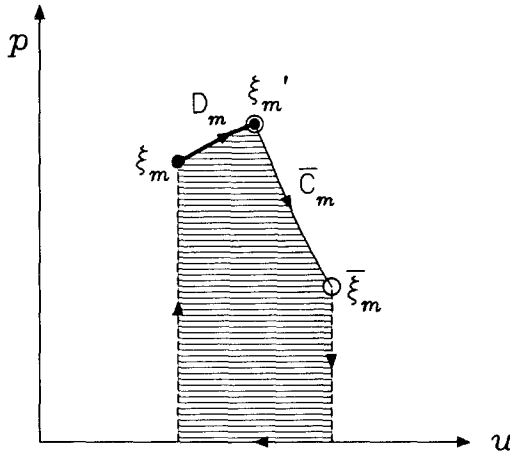$$e_r(u', u''; u, \bar{u}) = W_m = W'_m + W''_m = \int_{\Gamma_m} p \, du \qquad (4.23)$$

Fig. 12.   The work done during the shifting process of Fig. 11 is shown as a contour integral (note arrows) in the phase plane.

where Γ_m, the union of Γ'_m and Γ''_m, is the contour indicated in Fig. 13, and W_m is the area it encloses (W_m is negative for a counterclockwise contour).

The reconnection *energy* (3.18) does not depend on the order of its first two (or second two) arguments: interchanging u' and u'' leaves e_r unchanged. But the reconnection *formula* (2.25) which determines the contour Γ_m does not have this symmetry! Thus, it is useful to note the following rule for Γ_m does not have this symmetry! Thus, it is useful to note the following rule for Γ_m in (4.23). If a configuration u^l to the left of the semicolon in e_r approaches a configuration u^r to the right of the semicolon as $n \to +\infty$, connect ξ_m^l and ξ_m^r in the phase plane with a C manifold with an arrow *from* ξ_m^l *to* ξ_m^r. If, on the contrary, u^l and u^r approach each other as $n \to -\infty$, use a D manifold with arrow *to* ξ_m^l *from* ξ_m^r.

A third application is to an equilibrium defect u' in a periodic (Q, S) locally stable reference state u, and the translation u^* of this defect defined by (2.21). From (2.23) we see that for every n, ξ'_n and ξ_n^* are heteroclinic points for the same pair of contracting and expanding manifolds, as indicated schematically in Fig. 14, and thus they are equivalent heteroclinic points in the notation of Section 4.2. As u' and u^* have the same defect energy, the net work required to move an atom quasistatically from u'_n to u_n^*, transforming u' into u^*, is zero; that is,

$$\int_\Gamma p \, du = 0 \tag{4.24}$$

where Γ consists of a segment of the expanding manifold from ξ_n^* to ξ'_n. If these two segments intersect at only one point between the ends, as in
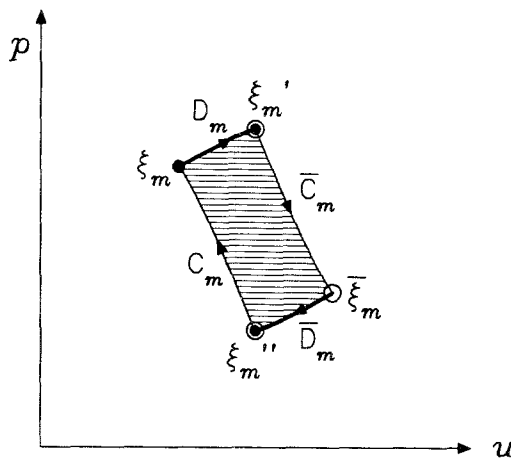

Fig. 13.   The reconnection energy (4.23) as a contour integral in the phase plane.
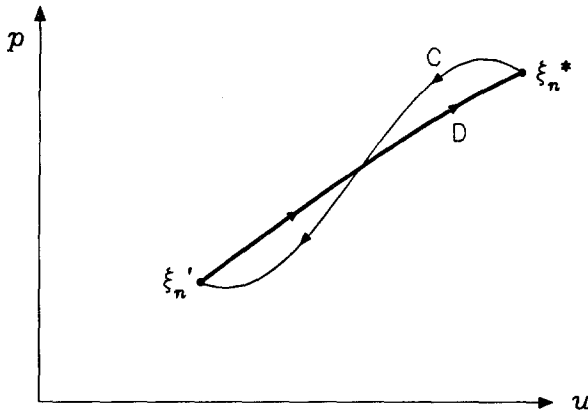
Fig. 14. The segments of contracting and expanding manifolds connecting two heteroclinic
points associated with a defect and its translation.

Fig. 14, the areas of the two loops thereby created must be equal. (In order
to visualize moving the atom from u'_n to u^*_n it may be convenient to
imagine it split in two parts, one connected to particles to the left of it and
the other to particles to its right. The two half-particles can be moved
independently and then reunited at the end.)

4.5. Single-Defect Energies

In all the examples considered below, we assume that the reference
and defect configurations are equilibrium configurations related through a
network of expanding and contracting manifolds as discussed in Sec-
tion 4.3. This is plausible provided the reference configuration is locally
stable, but this last is not a necessary condition.

The simplest situation is that in which the defect u' has zero phase
shift: $(q, s) = (0, 0)$ in the notation of Section 2.2. We can then let $\bar{u}$ be the
same as the reference configuration u in the discussion leading up to (4.21);
from this equation and (3.4) we infer that the defect energy is

$$e' = e(u') = W'_m = \int_{\Gamma'_m} p \, du \qquad (4.25)$$

where Γ'_m consists of D_m from ξ_m to ξ'_m and C_m from ξ'_m back to ξ_m. (See
the example in Fig. 15, where e' is the area of the cross-hatched region.)
Although this closed contour depends on m, the area it encloses does not,
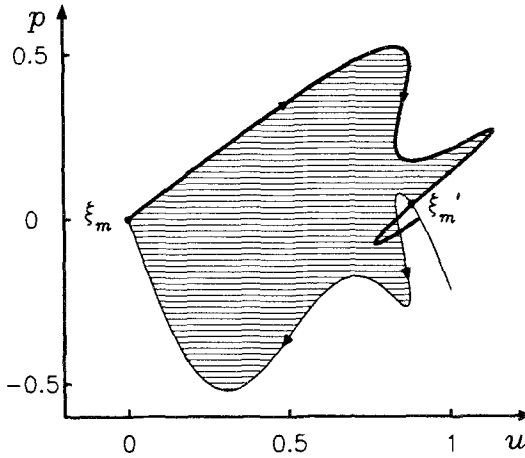due to the fact that T is area preserving.

Fig. 15. The area of the cross-hatched region enclosed by the expanding and contracting manifolds is the energy of a $q = s = 0$ defect in the $Q = 1$, $S = 0$ ground state of the Frenkel–Kontorova model with $K = 2$ in (2.9).

When u' has a nonzero phase shift (q, s), we define $\bar{u}$ by

$$\bar{u}_n = u_{n-q} + s \tag{4.26}$$

so that u' satisfies (2.25). Once again, (4.21) applies, with

$$\bar{K}_n = K_{n-q} \tag{4.27}$$

and

$$\bar{C}_m = \tau^s C_{m-q} \tag{4.28}$$

$$\bar{\xi}_m = \tau^s \xi_{m-q} \tag{4.29}$$

Combining (4.21) with (3.7) yields

$$e' - \Delta_m = W'_m = \int_{\Gamma'_m} p \, du \tag{4.30}$$

with Δ_m defined by (3.8). Unlike the case of zero phase shift, W'_m and Δ_m can depend on m. However, the *average* of Δ_m is zero, (3.9); thus

$$e' = \langle W \rangle = \lim_{N \to \infty} (2N + 1)^{-1} \sum_{m=-N}^{N} W_m \tag{4.31}$$

or, if u is periodic of period Q,

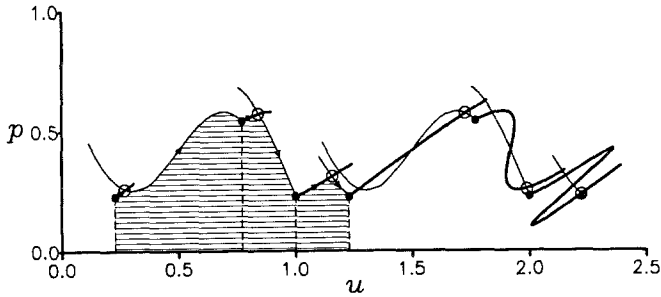$$e' = Q^{-1} \sum_{m=j}^{j+Q-1} W_m \tag{4.32}$$

Fig. 16. Energy of a $q = -1$, $s = 0$ defect (open circles) in a $Q = 3$, $S = 1$ configuration (solid-circles). The area of the cross-hatched region, whose width is $\Delta u = 1$, is three times the energy of the defect.

This is illustrated for a $q = -1$, $s = 0$ defect (open circles) in a $Q = 3$, $S = 1$ reference configuration (solid circles) in Fig. 16. The cross-hatched area is $3e'$. Note that while the actual positions of the defect heteroclinic points will vary if m is increased by Q, nevertheless

$$W_m = W_{m+Q} \tag{4.33}$$

because the map T is area preserving, and thus the right side of (4.32) is, as expected, independent of j.

Figure 17 shows a second example: a $q = 2$, $s = 1$ defect in a $Q = 5$, $S = 2$ reference configuration. The right side of (4.32) is $1/5$ the total cross-hatched area in Fig. 17a, or in Fig. 17b, where two of the "windows" in Fig. 17a have been translated backward using τ^{-1} (which of course leaves their areas unchanged). The choice of the defect heteroclinic point at which the expanding and contracting manifolds of a given "window" intersect is arbitrary: one can replace it with an equivalent point (as defined in Section 4.2 above) without changing the area.

4.6. Pinning Energy

The pinning energy e_p of a defect u^0 [see (3.17)] is equal to the defect energy of a saddle point configuration u^* [denoted u^m in (3.17)] relative to u^0. As u^* has zero phase shift relative to u^0, we can employ the equivalent of (4.25) and write

$$e_p = W_m^* = \int_{\Gamma_m^*} p \, du \tag{4.34}$$

where Γ_m^* is a contour from ξ_m^0 to ξ_m^* along an expanding manifold D, and from ξ_m^* back to ξ_m^0 along a contracting manifold C.
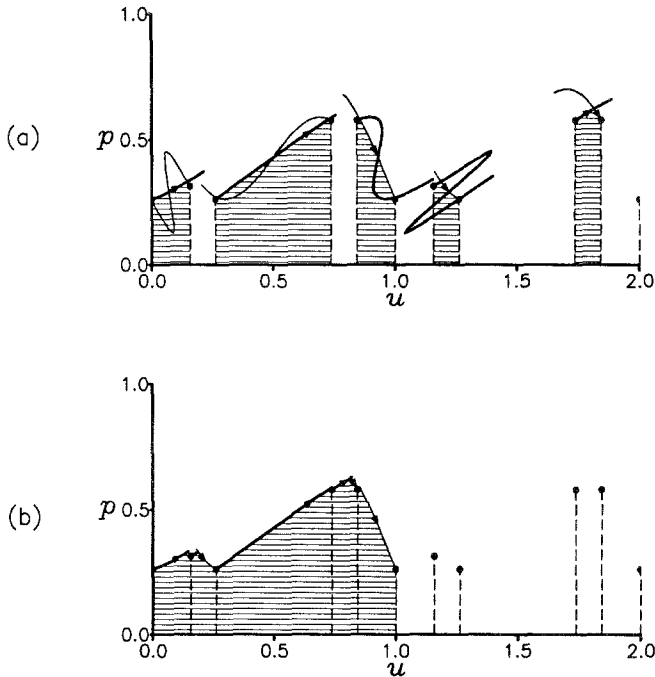
Fig. 17. Energy of a $q = 2$, $s = -1$ defect in a $Q = 5$, $S = 2$ reference configuration. (a) Defect orbit and contracting and dilating manifolds for one period of the reference configuration. The energy of the defect is one-fifth the sum of the areas of the five cross-hatched columns. (b) Same as in (a), except that the two columns in the interval $1 \leqslant u < 2$ are shifted back to the interval $0 \leqslant u < 1$ to make a connected domain.

As an example, in Fig. 18 the solid circles represent a $Q = 1$, $S = 1$ reference configuration u, the open circles a $q = -1$, $s = 0$ defect u^0, and the open squares the corresponding translated defect, (3.14). In the right half of the figure the open circle and square are heteroclinic points of the contracting and expanding manifolds C and D, and on the segments of these manifolds connecting these two points there is a third heteroclinic point, a solid square. Making the plausible assumption that this third point corresponds to an atom in the appropriate saddle point configuration, (4.34) tells us that e_p is the area of the cross-hatched loop, or equivalently that of the dotted loop—the two are equal; see the discussion following (4.24). The same construction applied to the loops joining the open circle and square in the left of the figure must yield the same answer for e_p, since T preserves areas.

It is not obvious that the heteroclinic point for the saddle point configuration must be at an intersection of the segments of the two manifolds
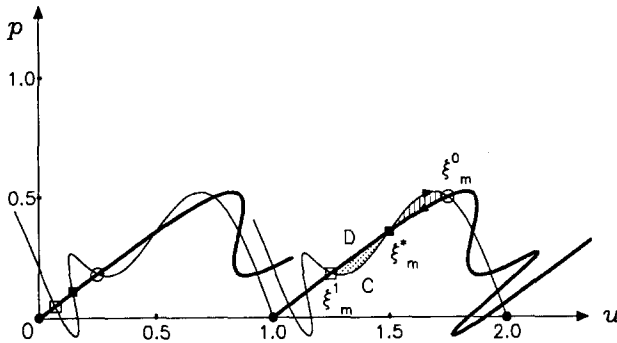
Fig. 18.   A $q = -1$, $s = 0$ defect in the $Q = S = 1$ ground state of the Frenkel–Kontorova model (2.9) with $K = 2$. Here ξ^0 and ξ^1 are two defected orbits related by a translation, and ξ^* is a "saddle point" defect orbit. The pinning energy is the area of the cross-hatched or of the dotted region.

connecting ξ_m^0 and ξ_m^1. And even if it is, there could be several intersections, in contrast to Fig. 18. Formula (4.34) remains valid, but applying it requires that ξ_m^* be correctly identified!

   The pinning energy of an interface (Section 3.4) between phases α and β can be discussed in a similar manner provided (2.29) is satisfied. The points $\xi_m^{\alpha\beta}$ in the phase plane associated with the interface configuration $u^{\alpha\beta}$, which satisfies (2.28), fall on the intersection of the manifolds D_m^α and C_m^β associated with u^α and u^β, respectively. The same is true of the translated interface (Section 2.4) and the intermediate saddle point configuration u^*. The pinning energy is again given by (4.34) with contour Γ_m^* equal to D_m^α from $\xi_m^{\alpha\beta}$ to ξ_m^* and C_m^β from ξ_m^* back to $\xi_m^{\alpha\beta}$, and is thus the area inside a closed contour in the phase plane. Once again, it may not be easy to identify the heteroclinic point ξ_m^* associated with the correct saddle point configuration.

4.7. Interaction Energy of Two Defects

   By combining (3.21) with (4.23), the interaction energy of two defects u^A and u^B in a configuration u^{AB}, relative to a reference configuration u, can be expressed as a contour integral

$$e_{AB} = e_r(u^{AB}, u; u^A, u^B) = \int_{\Gamma_m} p \, du \qquad (4.35)$$

as in Fig. 13, which is reproduced in Fig. 19 with the vertices and manifolds appropriately labeled. Note that Γ_m has been constructed by the rule which follows (4.23) assuming that the defect u^A is to the *left* of u^B in
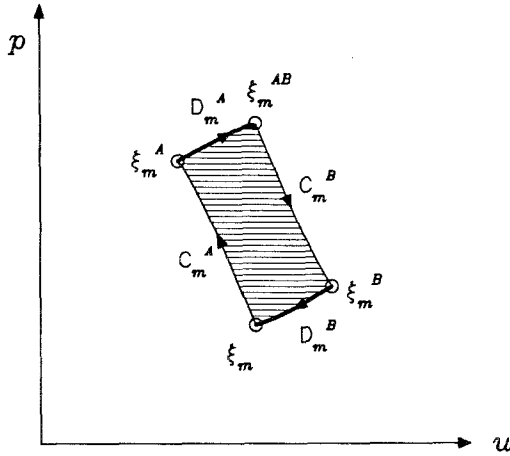
Fig. 19.   Contour (schematic) whose area is the interaction energy e_{AB} of (4.35).

the terminology of Section 2.3, which is to say that u_n^{AB} tends to u_n^A as $n \to -\infty$, and to u_n^B as $n \to +\infty$.

An example is shown in Fig. 20. The reference configuration u has to satisfy (2.25); in particular,

$$u_n^A \to u_n^{AB} \to -1; \qquad u_n^B \to 0 \qquad\qquad \text{as} \quad n \to -\infty$$
$$u_n^A \to 0; \qquad\qquad u_n^B \to u_n^{AB} \to +1 \qquad \text{as} \quad n \to +\infty$$
$$(4.36)$$

Portions of the corresponding manifolds in the phase plane are sketched in Fig. 20b with symbols for the heteroclinic points corresponding to those in Fig. 20a, and Fig. 20c is a simplified version of Fig. 20b with the heteroclinic points labeled with Greek letters.

The various defect energies, in the notation of (3.20), can then be identified, as in Sections 4.4 and 4.5, with areas inside contours in Fig. 20c as follows: $e(u^A)$ corresponds to $\alpha \to \zeta \to \beta \to \alpha$; $e(u^B)$ corresponds to $\beta \to \theta \to \gamma \to \beta$; $e(u^{AB})$ corresponds to $\alpha \to \zeta \to \eta \to \theta \to \gamma \to \beta \to \alpha$. Thus, we see that the interaction energy e_{AB} defined by (3.20) corresponds to the cross-hatched area within $\zeta \to \eta \to \theta \to \beta \to \zeta$, which is just the reconnection energy (4.35) (see Fig. 19). (Note that in the present example the manifolds C_m^A, C_m^B, D_m^A, and D_m^B are all independent of m.)

As an application of (4.35), consider the case in which the defects A and B are relatively far apart, with A to the left of B, and m labels some particle approximately midway between them. It is then plausible that ξ_m, ξ_m^A, ξ_m^B, and ξ_m^{AB} are quite close together in the phase plane, and that the segments of C_m^A and C_m^B which connect them (Fig. 19), and which cannot
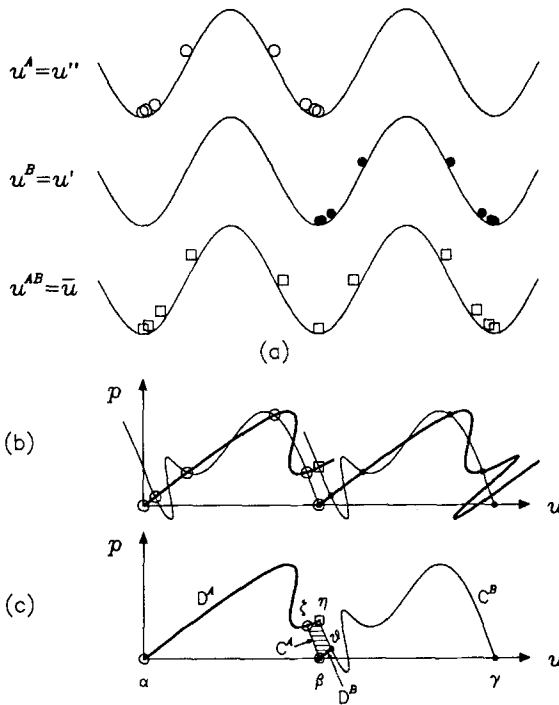
Fig. 20. (a) Single-defect configurations u^A, u^B and a two-defect configuration u^{AB} relative to a $Q = 1$, $S = 0$ reference state (not shown). (b) The corresponding dilating and contracting manifolds in the phase plane. (c) A simplified version of (b) with the cross-hatched area equal to the defect interaction energy e_{AB}.

intersect each other, are approximately parallel straight lines, and likewise the segments of D_m^A and D_m^B. This means that Γ_m is, to a good approximation, a parallelogram, with area

$$e_{AB} \simeq \delta p_m^A \, \delta u_m^B - \delta p_m^B \, \delta u_m^A \qquad (4.37)$$

where δ indicates the deviation of the corresponding quantity from the reference value: δu_m^B is $u_m^B - u_m$, etc. Formula (4.37) is valuable in that it expresses the interaction energy of two well-separated defects in terms of properties of the individual defects.[4,20]

4.9. Step Width in σ for Ground States

The dependence of winding number ω on stress σ for the ground states of a Frenkel–Kontorova model satisfying the "convexity condition" (4.1) has been discussed in refs. 17. Typically, one expects a "devil's staircase" in

which for every rational $\omega = S/Q$ (Q and S have no common divisors), the minimum-enthalpy configuration u is independent of the stress σ in the range

$$\sigma'_\omega \leqslant \sigma \leqslant \sigma''_\omega \qquad (4.38)$$

In simple cases σ'_ω and σ''_ω are determined by the values of σ at which the defect enthalpies $e'_\omega(\sigma)$ and $e''_\omega(\sigma)$ of the *retarded* and *advanced discommensurations* (Aubry's terminology), u' and u'', become zero. In the notation of (3.13) this means that

$$e'_\omega + \sigma'_\omega \tilde{q}'/Q = 0 = e''_\omega + \sigma''_\omega \tilde{q}''/Q \qquad (4.39)$$

where we have added a subscript ω, and superscripts to distinguish the two values of $\tilde{q}$ associated with u' and u''. In fact, u' and u'' are minimum-energy[13] configurations with phase shifts chosen so that

$$\tilde{q}' = q'S - s'Q = 1$$
$$\tilde{q}'' = q''S - s''Q = -1 \qquad (4.40)$$

This corresponds [(2.20)] to charges $1/S$ and $-1/S$, respectively. Combining (4.39) with (4.40) yields the expression

$$\sigma''_\omega - \sigma'_\omega = Q(e'_\omega + e''_\omega) \qquad (4.41)$$

which gives the width of the step (4.38) in terms of the sum of the defect energies of u' and u''.

   Both e'_ω and e''_ω can be expressed as integrals over appropriate paths as in Section 4.5. However, one gains additional insight by using the fact that if $\bar{u}$ is defined by

$$\bar{u}_n = u_{n-q'} + s' \qquad (4.42)$$

and is hence physically equivalent to u, then u' and u'' with appropriate numbering satisfy the reconnection formula (2.25). Therefore, $e'_\omega + e''_\omega$ is the reconnection energy (3.18) given by (4.23):

$$e'_\omega + e''_\omega = e_r(u', u''; u, \bar{u}) = \int_{\Gamma_m} p \, du \qquad (4.43)$$

where Fig. 13 shows the contour Γ_m.

   As a first example, consider the case $Q = 1$, $S = 1$ sketched in Fig. 21a, where u, $\bar{u}$, u', u'' are shown using open and solid squares (square containing a dot where the two coincide) and open solid circles, respectively, and

(a)

$\square\, u$ $\blacksquare\, \bar{u}$

$\bigcirc\, u'$ $\bullet\, u''$
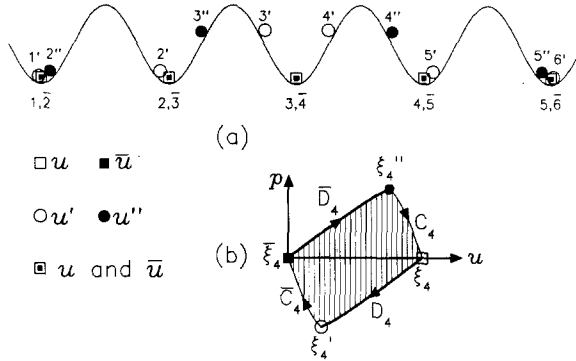
$\boxdot\ u$ and $\bar{u}$

(b)

Fig. 21. The width of the $Q = S = 1$ step in the phase diagram is the cross-hatched area in (b) corresponding to the points, shown in (a), of the retarded (u') and advanced (u'') elementary defects relative to the $Q = S = 1$ ground state u and its translation $\bar{u}$.

the particle numbers, carrying superscripts to avoid confusion, are consistent with (2.25). Figure 21b shows a portion of the phase plane; comparison with Fig. 19 shows that $e'_\omega + e''_\omega$ in (4.43) is the area of the cross-hatched region inside the contour. The contour would look rather different if $m = 2$ were used instead of $m = 4$, but the enclosed area would be the same. More generally, ξ'_4 can be replaced with any other equivalent heteroclinic point (Section 4.2), and the same holds for ξ''_4.

A second example is the $Q = 5$, $S = 2$, $\omega = 2/5$ case sketched in Fig. 22, with atoms numbered consistently with (2.25). Using the same symbols, a portion of this diagram is shown on an expanded scale in Fig. 23a, while
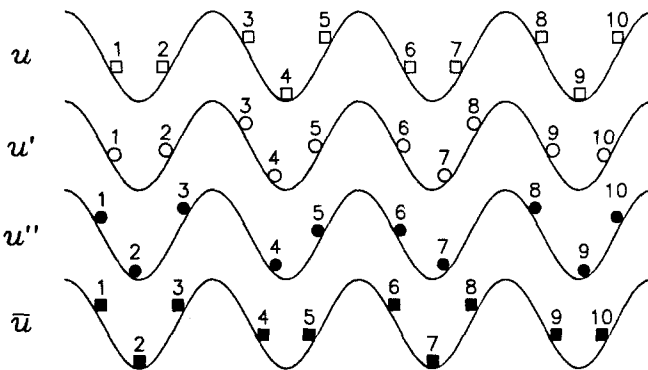

Fig. 22. Advanced (u'') and retarded (u') defects relative to a $Q = 5$, $S = 2$ ground state u and its translate $\bar{u}$.
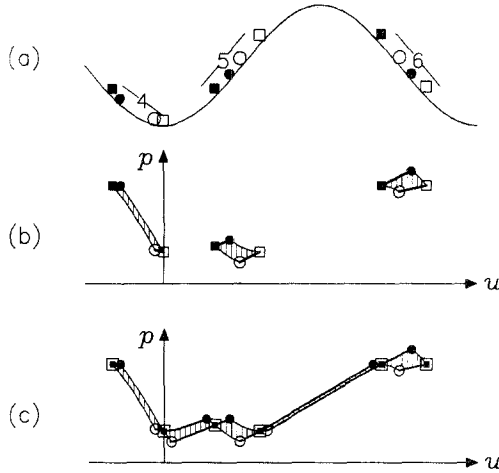
Fig. 23. (a) Part of Fig. 22 shown on an expanded scale, with atoms for the different configurations placed in the same potential troughs. (b) Connecting the corresponding positions in the phase plane with suitable manifolds yields "bubbles," each of which has an area equal to the width of the $\omega = 2/5$ step in the devil's staircase. (c) The same is true of additional "bubbles," again formed from contracting and diluting manifolds.

Fig. 23b indicates corresponding points in the phase plane connected by contours Γ_m (compare Fig. 13), each of which encloses an area equal to $e'_\omega + e''_\omega$. Just as in the earlier discussion of single-defect energies (Fig. 17), it is possible to use translation to produce a string of five "bubbles" covering a unit interval in u, Fig. 23c, whose total area is the step width (4.41). Again, the choice of "bubbles" is not unique, since the ξ'_m (or ξ''_m) can be replaced with other equivalent heteroclinic points.

ACKNOWLEDGMENTS

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