

GROUND STATE PROPERTIES OF FRENKEL-KONTOROVA MODELS WITH
SCALLOPED POTENTIALS

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ABSTRACT

GROUND STATE PROPERTIES OF FRENKEL-KONTOROVA MODELS WITH SCALLOPED POTENTIALS

In this thesis, the ground state configuration of the Frenkel-Kontorova model with a scalloped external potential is investigated. The method of effective potentials of Griffiths and Chou is extended by a novel approach involving the Burgers' equation of fluid dynamics. This approach is then employed to predict the effective potential at the end of a semi-infinite harmonic chain of particles in a periodic scalloped external potential. We explicitly construct the ground state configuration of particles, where the period of the particle spacing is close to that of the external potential. Our results are in agreement with previous exact results for this problem, thereby validating our method of approach.

ÖZET

PARÇALI PARABOLİK POTANSİYELLİ FRENKEL-KONTOROVA MODELLERİNDE TEMEL HAL ÖZELLİKLERİ

Bu tezde dış potansiyeli oluklu (parçalı parabolik) olan bir Frenkel-Kontorova modelinin temel hal parçacık konfigürasyonu araştırılmaktadır. Griffiths ve Chou'nun efektif potansiyeller metodu, akışkanlar dinamiğinden bilinen Burgers denklemini içeren bir yöntemle geliştirilmiştir. Bu yaklaşım daha sonra periyodik oluklu bir dış potansiyel içinde duran yarı-sonsuz bir harmonik parçacık zincirinin ucundaki efektif potansiyelin bulunmasında kullanılmıştır. Parçacık diziliminin periyodunun dış potansiyelinkine yakın olduğu durumlar için temel hal konfigürasyonunu net biçimde oluşturduk. Bulduğumuz sonuçların geçerliliği, bu problem için daha önce ortaya konmuş tam çözümle tutarlılık göstermektedir.

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LIST OF SYMBOLS/ABBREVIATIONS

a	Half-period of the external potential
$\mathcal{H}$	Hamiltonian, total energy
k	Elastic constant
l	Mean spacing of atoms
s_i	Propagation speed of shock i
t	Time, reciprocal of elastic constant
T	Mapping of adjacent particle positions
u_i	Absolute coordinates of particle i
$\mathcal{U}^{(n)}$	Velocity field associated with an effective potential
$V^{(n)}$	Effective potential at the end of a chain of $n + 1$ particles
V_o	External potential
W	Inter-atomic interaction
x_i	Burgers coordinates of particle i
$\hat{x}_i$	Well coordinates of particle i
Δ_i	Intensity of shock i
λ	Overall slope of a shock train
λ^*	Steady state value of λ
λ_o	Strength of the external potential
μ	Equilibrium length of the spring
ν_i	Location of a node i
τ	Duration of an evolution
ξ_i	Location of a shock front i
FK	Frenkel-Kontorova

1. INTRODUCTION

Complex models with many degrees of freedom arise in the analysis of solids. While complicated models account for many effects which need not be negligible, they are difficult to solve and most importantly it is usually not possible to draw qualitative conclusions about the phenomena involved. Among the phenomena investigated via the *Frenkel-Kontorova* (FK) model are, the dynamics of a dislocation core in a solid, crystal growth, approximate description of DNA dynamics and friction on a microscopic level [1, 2, 3, 4].

The FK model is a simple, low dimensional nonlinear model widely used for the description of various phenomena in the physics of the condensed state. The model consists of an infinite chain of particles with nearest-neighbor interaction, immersed in an external periodic potential field, as shown in Fig. 1.1. The total energy of such a system can be written as,

$$\mathcal{H} = K + V_{int} + V_{ext} \quad , \quad (1.1)$$

where V_{int} is the inter-atomic potential, V_{ext} is the external periodic potential with period $2a$, and K is the total kinetic energy.

If the lowest energy configuration, which will be referred to as the *ground state* of such a system, is investigated, the kinetic energy term may be disregarded. The

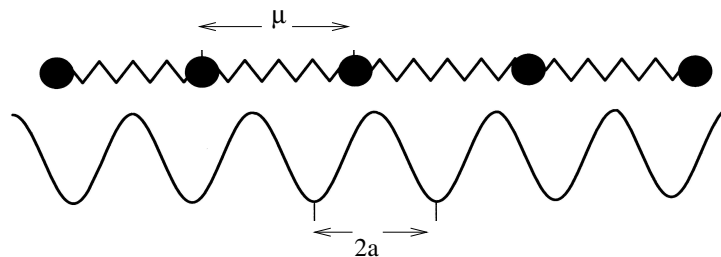


Figure 1.1. An illustration of the Frenkel-Kontorova model with sinusoidal potential and harmonic interaction.

external potential is usually the first term in the Fourier expansion of a complicated potential function. The inter-atomic interaction is often assumed to be elastic, which is the first order approximation of a more complicated force field around the equilibrium point. The elastic inter-atomic potential may be written as,

$$V_{int} = \frac{1}{2}k(u_i - u_{i-1} - \mu)^2 \quad , \quad (1.2)$$

where k and μ correspond to the elastic constant and the equilibrium spacing, respectively. The elastic interaction between particles can be interpreted as neighboring particles being connected by a spring of constant k and unstretched length μ .

The main factor that makes this system nontrivial is that there are two competing length scales: the period of the external potential and the equilibrium spacing of the elastic interaction. This can result in two possible types of ground states, commensurate and incommensurate. Commensurate ground states exhibit periodic ground states with the average inter-particle spacing l having the property that $l/2a$ is rational, whereas for incommensurate ground states we have $l/2a$ irrational. Note that l is not necessarily equal to μ . In fact the requirement of a minimum energy stable configuration can induce a highly complex l - μ dependence, as will be shown later.

The case with $\mu = 2a$ is relatively simple. The lowest energy configuration is obtained when every period of the external potential is occupied by a single particle situated at the potential minimum in that period, thereby inducing no strains in the springs. This is the simplest example of a commensurate ground state, where $l = \mu$ and $l/2a = 1$.

In a more complicated commensurate ground state, where $\frac{l}{2a} = \frac{r}{s}$ with r and s co-prime, the configuration is periodic with period $2ar = ls$. The location of particles are related such that [5],

$$u_{i+s} = u_i + sl \quad . \quad (1.3)$$

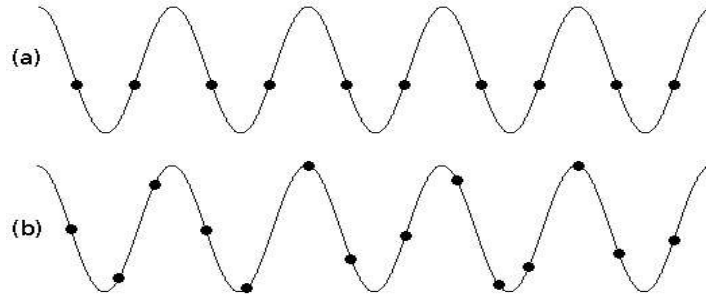


Figure 1.2. Examples to the two types of ground states shown: (a) Commensurate
(b) Incommensurate.

Commensurate and incommensurate ground states also display another interesting difference. The particle locations in a commensurate ground state are such that the configuration is *locked*, *i.e.* the particles are allowed to sit at definite, finitely spaced locations on the external potential. Another ground state configuration cannot be achieved by changing the u_i 's continuously, so that there is a certain energy barrier between ground state configurations. On the other hand, incommensurate ground states allow *sliding solutions* where all locations relative to the external potential are possible, and so there is an infinite set of nearby ground state configurations that allows the particle chain to slide, *i.e.* there is no potential barrier. Fig. 1.2 illustrates the two types of ground state configurations.

The relative strength of the external potential to the elastic constant together with the equilibrium spacing μ , or equivalently the average spacing l , determines whether a system will exhibit a commensurate or an incommensurate ground state. For irrational $l/2a$, if the external potential is weak and the elastic interaction is stiff, the effect of the springs on the average spacing dominates and the configuration is incommensurate. When the strength of the potential increases beyond some critical point, a phenomenon called *transition by breaking of analyticity* [6] occurs and the ground state becomes commensurate. The name originates from the fact that the *hull function* that determines the allowable locations that particles can take, is analytic in the case of an incommensurate ground state and ceases to be analytic at the incommensurate-commensurate transition. Moreover, Aubry and De Laeron [7] proved that $l/2a$ uniquely determines commensurate ground states when the external potential is convex.

The ground state configuration of a FK chain with a sinusoidal potential has been extensively studied [6, 8, 9, 10]. The equations for stationary configurations for this case reduce to what is called the *standard map*. With a general external potential V and harmonic interaction of nearest neighbors, the total energy of the chain becomes,

$$\mathcal{H} = \sum_i \frac{1}{2} k (u_i - u_{i-1} - \mu)^2 + V(u_i) \quad . \quad (1.4)$$

Minimization of the total energy of the chain requires that the difference equation,

$$k(u_{i+1} + u_{i-1} - 2u_i) = V'(u_i) \quad (1.5)$$

yields the static force equilibrium condition.

Aubry [6] showed that this second order difference equation may be transformed into a two dimensional map. This map allows the representation of a stationary configuration by a trajectory of a nonlinear dynamical system. With p_i defined as,

$$p_i \equiv u_i - u_{i-1} \quad (1.6)$$

Eq. 1.5 becomes,

$$p_{i+1} = p_i + \frac{1}{k} V'(u_i) \quad (1.7)$$

$$u_{i+1} = u_i + p_{i+1} \quad . \quad (1.8)$$

Eqs. 1.7 and 1.8 define the map from (u_i, p_i) to (u_{i+1}, p_{i+1}) . Trajectories generated by this map, corresponding to different relative strengths of the external potential and the elastic constant in the case of a sinusoidal external potential are depicted in Fig. 1.3.

Aubry also showed that the requirement of minimum energy configurations selects a subset of the possible trajectories. Continuous looking sets of points (invariant tori) in the map correspond to incommensurate phases where the configuration is not pinned

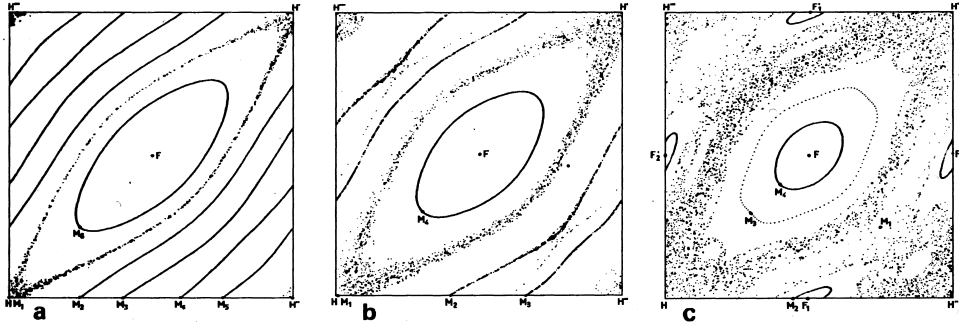


Figure 1.3. Maps corresponding to different relative strengths as: (a) $k/\lambda = 13.333$, (b) $k/\lambda = 10$, and (c) $k/\lambda = 8$ with a sinusoidal external potential [9].

(locked). Commensurate phases with rational $l/2a$ correspond to discrete trajectories. Observe that models where the elastic constant is smaller relative to the external potential amplitude, discrete orbits of commensurate phases dominate.

In this thesis, we will theoretically investigate the FK model with a piecewise parabolic external potential, henceforth to be referred as a *scalloped* potential, given as,

$$V_{ext}(u) = \frac{1}{2}\lambda \left[u - 2a \text{Int} \left(\frac{u+a}{2a} \right) \right]^2, \quad (1.9)$$

using a novel solution technique. Since the potential is convex, the model turns out to exhibit only commensurate ground states with $\frac{l}{2a}$ rational [7]. The problem was exactly solved by Aubry [11] and the phase diagram was calculated as well. We will therefore use the known exact solution of Aubry to validate our approach.

The novel technique we introduce in this thesis is an extension of the method of effective potentials, first proposed by Griffiths and Chou [8], who applied their method to the problem of determining the ground state configuration of the chain. We will show that a deeper structure underlies the method of Griffiths and Chou and this will be used to provide an exact analytical solution of the effective potentials as well as the ground state particle solutions for the FK model with a scalloped potential. We would like to note, that the analytical description of the effective potential is original, and a direct consequence of our method, while the work of Griffiths and Chou was mostly

numerical in nature, being primarily concerned with mapping out the phase diagram of the complex dependence of l on μ and λ .

In the first chapter, we set up the background of our work. We start with briefly discussing Aubry's exact solution and its consequences in the first section. The following two sections will be concerned with the method of effective potentials and our novel approach that we use to extend this method.

In the second chapter, the application of our method to the FK model with a scalloped potential is rigorously carried out. The ground state configuration and the boundary of the associated phase is found to be in accordance with the exact results of Aubry, thereby validating our method of approach.

2. THEORY AND BACKGROUND

2.1. Aubry's Exact Solution for a Scalloped Potential

The configuration of particles in the chain will be represented by the set of coordinates $\{u_i\}$. The energy of a particle at location u_i due to the external potential is defined as,

$$V_o(u_i) = \frac{1}{2}\lambda_o (u_i - 2m_i a)^2 \quad , \quad (2.1)$$

where

$$m_i = \text{Int}\left(\frac{u_i + a}{2a}\right) \quad . \quad (2.2)$$

Then the energy of the infinite chain, with a spring constant k_o can be written as,

$$\mathcal{H}(\{u_i\}) = \sum_i \left[\frac{1}{2}\lambda_o (u_i - 2m_i a)^2 + \frac{1}{2}k_o (u_{i+1} - u_i - \mu)^2 \right] \quad . \quad (2.3)$$

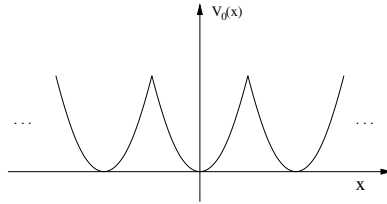


Figure 2.1. The scalloped potential $V_o(x)$.

Ground state configurations require that $\partial\mathcal{H}/\partial u_i = 0$, *i.e.* no net force on the chain. Imposing this condition on Eq. 2.3 we obtain,

$$\left(\frac{\lambda_o}{k_o} + 2\right) u_i - u_{i+1} - u_{i-1} = 2m_i a \frac{\lambda_o}{k_o} \quad . \quad (2.4)$$

This equation determines u_{i+1} in terms of u_i and u_{i-1} recursively. Because of Eq. 2.2, Eq. 2.4 is a non-linear difference equation. If $\{m_i\}$ were known a priori, the set of equations 2.4 would be linear, and could be solved to yield $\{u_i\}$. One possibility would be to choose the set $\{m_i\}$ at random, which would yield a trajectory $\{u_i\}$, but then we would still have to check that Eq. 2.2 is satisfied. Note that Eqs. 2.2 and 2.4 only yield an equilibrium configuration that is not necessarily stable, nor of lowest energy. A powerful theorem due to Aubry [6] provides the necessary and sufficient condition for the lowest energy configuration:

Theorem: For any ground state of model 2.3 with atomic mean distance l , there exists a number α called the phase such that u_i and $(il + \alpha)$ belong to the same closed interval $[p_i a, (p_i + 1)a]$ with $p_i = \text{Int } u_i/a$.

The theorem asserts that the location $(il + \alpha)$ of an atom in the unperturbed chain ($\lambda_o = 0$), is in the same potential well¹ as the location u_i of the atom in the perturbed chain ($\lambda_o > 0$). Thus,

$$m_i = \text{Int} \left(\frac{il + \alpha + a}{2a} \right) \quad . \quad (2.5)$$

and we can solve Eq. 2.4 for the set $\{u_i\}$.

The difference equation Eq. 2.4 can be solved using discrete Fourier transforms (see Appendix A) to yield

$$u_i = A \sum_{n=-\infty}^{+\infty} \eta^{|n|} m_{n+i} \quad , \quad (2.6)$$

where the constants A and η are found as,

$$\eta = 1 + \frac{1}{2} \frac{\lambda_o}{k_o} - \frac{1}{2} \frac{\lambda_o}{k_o} \sqrt{1 + 4 \frac{k_o}{\lambda_o}} \quad (2.7)$$

¹The assertion of the theorem is even stronger. The two positions are claimed to be within the same *half*-well, but for our purposes it does not make any difference.

and

$$A = 2a \frac{1 - \eta}{1 + \eta} \quad . \quad (2.8)$$

Eqs. 2.5 and 2.6 determine the so called *hull function* $u_i = f(x)$ relating the location of the i^{th} particle u_i in the perturbed chain to its location $x = il + \alpha$ in the unperturbed chain as,

$$f(x) = A \sum_{n=-\infty}^{+\infty} \eta^{|n|} \text{Int} \left(\frac{x + a + nl}{2a} \right) \quad . \quad (2.9)$$

The hull function determines the locations that atoms are allowed to sit inside the wells, so to speak. Eq. 2.9 readily shows that $f(x) - x$ is periodic, *i.e.* $\{u_i\}$ is a *periodically modulated* structure, with period $2a$. The hull function and the corresponding configuration for a case with $\lambda_o = 0.8$ and $\frac{l}{2a} = \frac{1}{3}$ are shown in Fig. 2.2. Also, commensurate ground state configurations with various mean spacings are depicted in Fig. 2.3.

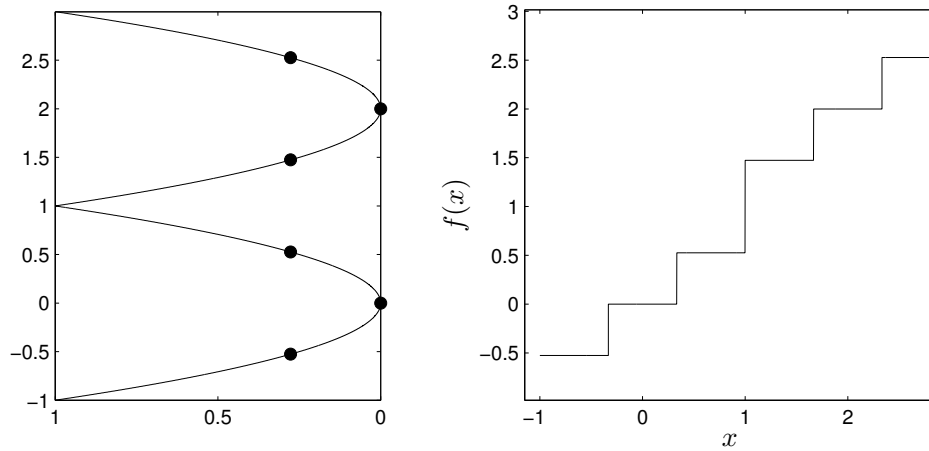


Figure 2.2. The hull function for a model with $\lambda_o = 0.8$ and $\frac{l}{2a} = \frac{1}{3}$, and the corresponding configuration of particles.

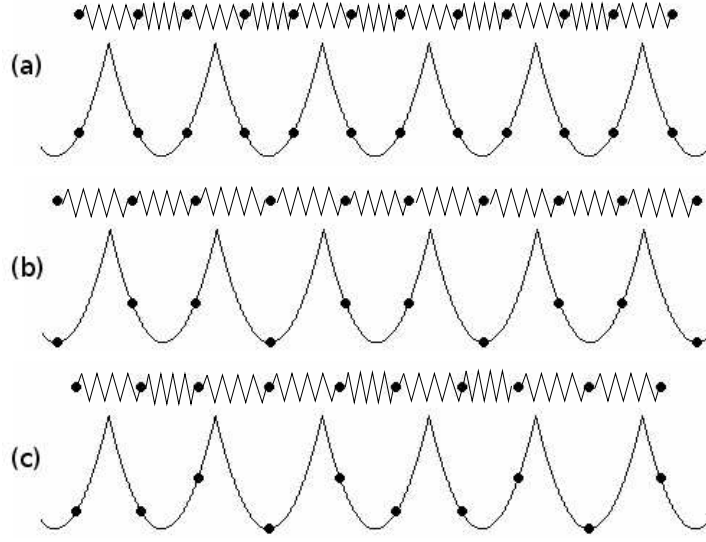


Figure 2.3. Ground state configuration of particles for (a) $\frac{l}{2a} = \frac{1}{2}$ (b) $\frac{l}{2a} = \frac{2}{3}$ (c) $\frac{l}{2a} = \frac{3}{5}$. Note that each structure is periodic with the denominator of its respective $\frac{l}{2a}$.

In terms of the variables m_i , the total energy of the chain becomes

$$\tilde{\mathcal{H}}(\{m_i\}) = \frac{1}{2} \sum_{ij} K(i-j)(m_i - m_j)^2 - 2\mu a(m_N - m_0) \quad , \quad (2.10)$$

where 0 and N are the indices of the two ends of the chain, and

$$K(i-j) = 2a^2 \frac{\lambda_o}{k_o} \frac{1-\eta}{1+\eta} \eta^{|i-j|} \quad . \quad (2.11)$$

The energy per atom as the number of particles N on the chain grows infinite becomes,

$$\varphi(l) \equiv \lim_{N \rightarrow \infty} \frac{\tilde{\mathcal{H}}(\{m_i\})}{N} = \psi(l) - \mu l \quad , \quad (2.12)$$

where

$$\psi(l) = \sum_{n=1}^{\infty} K(n) \psi_n(l) \quad , \quad (2.13)$$

and

$$\psi_n(l) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N (m_{i+n} - m_i)^2 \equiv \langle (m_{i+n} - m_i)^2 \rangle \quad . \quad (2.14)$$

Note that, the quantity $(m_{i+n} - m_i)$ can take only two values:

$$m_{i+n} - m_i = \text{Int} \frac{nl}{2a} = s_n$$

or

$$m_{i+n} - m_i = s_n + 1 \quad .$$

If the probability that $(m_{i+n} - m_i) = s_n$ is p_n , then the average value of $(m_{i+n} - m_i)$ is found as,

$$\langle m_{i+n} - m_i \rangle = p_n s_n + (1 - p_n)(s_n + 1) \quad . \quad (2.15)$$

Alternatively, by linearity of arithmetic means, we have

$$\langle m_{i+n} - m_i \rangle = \left\langle m_{i+n} - \frac{(i+n)l}{2a} \right\rangle - \left\langle m_i - \frac{il}{2a} \right\rangle + \frac{nl}{2a} = \frac{nl}{2a} \quad . \quad (2.16)$$

Eqs. 2.15 and 2.16 combine to yield:

$$p_n = 1 + s_n - \frac{nl}{2a} \quad . \quad (2.17)$$

Hence, rewriting Eq. 2.14 we obtain,

$$\begin{aligned} \psi_n(l) &= p_n s_n^2 + (1 - p_n)(s_n + 1)^2 \\ &= \frac{nl}{2a} [2 \text{Int}(nl/2a) + 1] - [\text{Int}(nl/2a)]^2 - \text{Int}(nl/2a) \quad . \end{aligned} \quad (2.18)$$

It can be easily checked that $\psi_n(l)$ is a convex function with discontinuous first derivative for $\frac{nl}{2a}$ an integer. Since $K(n)$ defined by Eq. 2.11 is positive, $\psi(l)$ (Eq. 2.13) is also a convex function, and so is $\varphi(l)$ due to Eq. 2.12.

For a ground state configuration, the energy per particle should be a minimum. Since $\varphi(l)$ is a convex function, setting $\varphi'(l) = 0$ will yield the minimum condition. The derivative of $\psi(l)$ is readily found from Eq. 2.13 as,

$$\psi'^{\pm} = \frac{1}{2a} \sum_{n=1}^{\infty} nK(n) \left[2 \text{Int}^{\pm} \left(\frac{nl}{2a} \right) + 1 \right] \quad , \quad (2.19)$$

where $\pm$'s are used as a shorthand notation for the values of a function immediately to the right or left of a point. From Eq. 2.12, the minimization of the average particle energy requires that,

$$\mu = \psi'^{\pm}(l) \quad . \quad (2.20)$$

Therefore, μ is a series of step functions as a function of l , discontinuously increasing whenever $\frac{nl}{2a}$ is an integer, that is at points where $\frac{l}{2a}$ is rational. The function $l(\mu)$ is therefore, what is called a *Devil's staircase* (see Fig. 2.4).

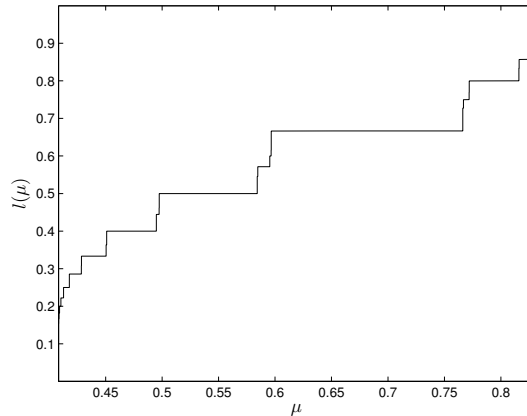


Figure 2.4. The mean spacing of atoms versus the equilibrium spring length for $a = 1$ and $\lambda_o = 0.8$. Note the intervals over which the value of l is constant.

For each rational value $\frac{l_r}{2a} = \frac{r}{s}$ with r and s two irreducible integers, the step width of the discontinuous increase in μ is found as,

$$\delta\mu(l_r) \equiv \psi'^+(l_r) - \psi'^-(l_r) = \frac{1}{a} \sum_{p=1}^{\infty} K(ps)ps \quad . \quad (2.21)$$

After calculating the sum on the right hand side and substituting K from Eq. 2.11, the expression for step widths is obtained:

$$\delta\mu\left(2a\frac{r}{s}\right) = 2a \frac{(1-\eta)^3}{(1+\eta)\eta} \frac{s\eta^s}{(1-\eta^s)^2} \quad . \quad (2.22)$$

The important result of this discussion is that for rational $\frac{l}{2a}$, there are intervals of μ such that $\psi'^-(l_r) < \mu < \psi'^+(l_r)$, where the average inter-atomic distance l is the same (locked) over the whole interval. These intervals define the *commensurate* phases with the order parameter l . An example phase diagram is shown in Fig. 2.5.

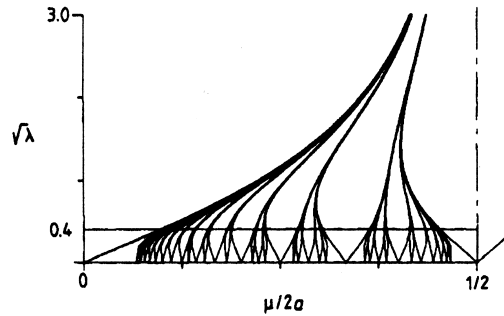


Figure 2.5. The diagram of commensurate phases. Each rational value of $\frac{l}{2a}$ has a corresponding region of stability. Regions up to commensurability $s = 10$ are depicted only [11].

2.2. The Method of Effective Potentials

A powerful numerical method to find the ground state configuration of the FK chain was proposed by Griffiths and Chou [8], the method of *effective potentials*.

It is useful to first consider a system with only two particles connected by a spring, with positions u and u' , subjected to different periodic potentials $V_o(u)$ and

$U_o(u')$, respectively. The inter particle interaction will be denoted by $W(u, u')$ with,

$$W(u, u') = \frac{1}{2}k(u - u' - \mu)^2 \quad (2.23)$$

in the elastic interaction case. This definition of the elastic interaction requires that u is on the right of u' . The total energy of the system is,

$$\mathcal{H}(u, u') = U_o(u') + W(u, u') + V_o(u) \quad . \quad (2.24)$$

We are looking for the lowest energy configuration $\{u, u'\}$. For a fixed position u of the second atom, the lowest energy is given by,

$$\min_{u'} \mathcal{H}(u, u') = V_o(u) + \min_{u'} \{W(u, u') + U_o(u')\} \quad . \quad (2.25)$$

This lowest energy of the two particle chain, with the fixed position of the particle on the right, is the definition of the effective potential $V(u)$:

$$V(u) = V_o(u) + \min_{u'} \{W(u, u') + U_o(u')\} \quad . \quad (2.26)$$

The interpretation of the term *effective potential* is now immediate. It is the combined effect that the right-hand particle is subjected to, lumping together the external potential V_o and the effects due to what is on the left as mediated by the spring. Hence, the derivative of the effective potential is proportional to the force that should be applied in order to hold the fixed atom at that position.

The minimization on the right hand side of Eq. 2.26 also yields the mapping between the particle positions u and u' . The mapping $u' = T(u)$ is defined for each fixed position u of the atom on the right and yields the position u' of the atom on the left which minimizes the total energy.

Particularly, the potentials that both particles are subjected to, could be the same, as is the case for a FK chain. Then the transformation Eq. 2.26 could be

iterated a large number of times to yield the effective potential that the rightmost atom experiences, in a free-end semi-infinite chain. The case for a three particle chain will be shown, then the result is to be generalized to a chain of n particles.

The total energy of a system with three particles, all submersed in an external potential V_o is given as,

$$\mathcal{H}(u_2, u_1, u_0) = V_o(u_0) + W(u_0, u_1) + V_o(u_1) + W(u_1, u_2) + V_o(u_2) \quad (2.27)$$

The ground state configuration, with respect to a fixed position u_2 of the last atom, is obtained through the minimization of the total energy with respect to u_0 and u_1 as,

$$V^{(2)}(u_2) = V_o(u_2) + \min_{u_0, u_1} \{V_o(u_1) + W(u_1, u_2) + V_o(u_0) + W(u_0, u_1)\} \quad . \quad (2.28)$$

Note that the effective potential V is labeled with a superscript to indicate how many particles there are to the left.

One should observe in Eq. 2.28 that the minimization with respect to u_0 , together with $V_o(u_1)$ will yield $V^{(1)}(u_1)$,

$$V^{(1)}(u_1) = V_o(u_1) + \min_{u_0} \{V_o(u_0) + W(u_0, u_1)\} \quad . \quad (2.29)$$

This means that what is to the left of particle 1 can be disregarded and be accounted for using the effective potential that particle 1 sees. Hence, Eq. 2.28 can be rewritten as,

$$V^{(2)}(u_2) = V_o(u_2) + \min_{u_1} \{V^{(1)}(u_1) + W(u_1, u_2)\} \quad . \quad (2.30)$$

This result can be generalized as,

$$V^{(n)}(u_n) = V_o(u_n) + \min_{u_{n-1}} \{V^{(n-1)}(u_{n-1}) + W(u_{n-1}, u_n)\} \quad . \quad (2.31)$$

Eq. 2.31 determines the effective potential acting on the rightmost particle in a chain of $n + 1$ particles (n springs) all immersed in the same periodic external potential $V_o(u)$. We recall that all atoms in the chain, except the rightmost one whose position is fixed, are relaxed such that the total energy obtains its lowest value. Furthermore, since the energy of such a chain would remain invariant under a rigid translation of all particles by one period of the periodic external potential, the effective potential is also a periodic function with the same period.

Note that one can consider another effective potential, *i.e.* the potential seen from the end of the last spring but *before* the addition of the last particle. This effective potential will be denoted by a *minus* sign in the superscript, and defined as,

$$V^{(n)-}(u_n) = \min_{u_{n-1}} \{V^{(n-1)}(u_{n-1}) + W(u_{n-1}, u_n)\} \quad . \quad (2.32)$$

A nonlinear functional transformation $\mathcal{K}$ can be defined as,

$$\mathcal{K}V^{(n)}(u) = V^{(n+1)}(u) \quad . \quad (2.33)$$

Griffiths and Chou argue that, when n is large, $\mathcal{K}^n V$ reaches a steady state [8]. On assumptions about the steady state behaviour of this transformation $\mathcal{K}V^*(u)$, they propose a solution to the nonlinear eigenvalue of the transformation,

$$\mathcal{K}V^*(u) = V^*(u) + \epsilon \quad , \quad (2.34)$$

where ϵ is the average energy per particle, which in turn yields the steady state mapping T^* relating the locations of adjacent particles. The ground state configuration in its entirety can then be constructed by application of this map iteratively as,

$$u_{n-i} = T^{*i}(u_n) \quad . \quad (2.35)$$

We suggest another transformation in the following section, where the assumption of

steady state will have to be modified.

As an aside, so far only a semi-infinite chain which is bounded at its right-hand edge has been considered. The case with a chain that is bounded on its left-hand edge can be treated similarly. If we were to call the corresponding effective potentials $V_R(u)$ and $V_L(u)$, respectively, then the combined effective potential $\hat{V}(u)$ for a particle in a doubly infinite chain will be given by,

$$\hat{V}(u) = V_R(u) + V_L(u) - V_o(u) \quad , \quad (2.36)$$

where V_o is subtracted since it is accounted for both in V_R and V_L . When the periodic external potential V_o is half-wave symmetrical, the left and right effective potentials are related as [8],

$$V_L(u) = V_R(-u) \quad . \quad (2.37)$$

However, it can be shown that the effective potential of a semi-infinite chain is equally useful in finding the ground state configuration as the effective potential of a doubly-infinite chain. The effect of the initial point u_n on the locations of the particles u_{n-i} will diminish as $i \rightarrow \infty$ in the mapping of Eq. 2.35. Therefore $\{u_{n-i}\}$ will give the ground state configuration of a doubly infinite chain for large i . We will thus be only concerned with the effective potential at the free end of a semi-infinite chain.

2.3. Effective Potentials and Burgers' Equation

2.3.1. The Minimization Equation

By virtue of the effective potential concept, the total energy of a chain of particles can be written in terms of the positions of the two rightmost particles only, lumping the energy due to the rest of the chain into the effective potential the left-hand particle

sees. The total energy becomes,

$$\mathcal{H}(u, u') = V_{\circ}(u) + W(u, u') + V(u') \quad , \quad (2.38)$$

where $V(u')$ is the effective potential acting on the atom to the immediate left of the atom at the free end at position u . The mapping $u' = T(u)$ corresponds to the point u' that minimizes the total energy as,

$$\frac{\partial W(u, u')}{\partial u'} + \frac{\partial V}{\partial u'} = 0 \quad . \quad (2.39)$$

For a harmonic interaction between particles, we can write

$$W(u, u') = \frac{1}{2}k_{\circ}(u - u' - \mu)^2 \quad , \quad (2.40)$$

in which case the extremization Eq. 2.39 becomes,

$$u = u' + \mu + \frac{1}{k_{\circ}}V'(u') \quad , \quad (2.41)$$

and it is required that,

$$V''(u') > -k_{\circ} \quad (2.42)$$

or equivalently,

$$\frac{\partial u}{\partial u'} > 0 \quad (2.43)$$

for the point u' to be a minimum.

Let us discuss the mapping between adjacent particles in the case of a simple effective potential. Consider an effective potential $V(u')$ given as,

$$V(u') = 1 - \cos\left(\frac{\pi}{a}u'\right) \quad , \quad (2.44)$$

which is periodic with period $2a$. With this effective potential, Eq. 2.39 becomes,

$$u = u' + \mu + \frac{1}{k_o} \frac{\pi}{a} \sin\left(\frac{\pi}{a}u'\right) \quad . \quad (2.45)$$

Observe that, the map $u' = T(u)$ is multi-valued if k_o is small enough. The situation is depicted in Fig. 2.6. At points where the map is triple valued, one of the values do not

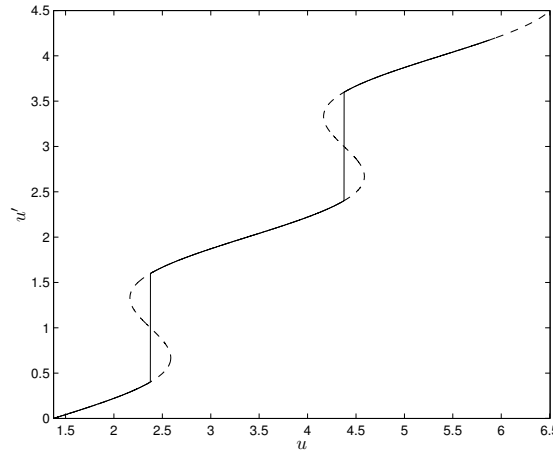


Figure 2.6. The mapping $u' = T(u)$ in the case of a sinusoidal effective potential.

Dashed lines represent the multivalued map while solid lines represent the lowest energy map found by an equal area rule.

qualify as a minimum energy configuration since the map has negative derivative, therefore not satisfying the stability condition Eq. 2.43. The two other points correspond to local minima with different energies. Since the ground state is the configuration of the *lowest* energy, only one of the points correspond to the ground state, thereby yielding a single valued map. Where the map is discontinuous is to be determined by an equal area rule. The equal area rule ensures the continuity of the effective potential due to the derivative of the effective potential appearing in Eq. 2.41, because a discontinuity in the effective potential means an infinite force.

2.3.2. The Evolution of Effective Potentials

In this section, we will rigorously investigate how the effective potential evolves upon the augmentation of the chain by one particle. Let us write down the partition function of the semi-infinite chain, with particle n at the free end:

$$\mathcal{Z}^{(n)}(u_n) = \int_{-\infty}^{+\infty} du_0 \dots du_n e^{-\beta \{V_o(u_n) + \sum_{i=0}^{n-1} [V_o(u_i) + \frac{1}{2}k_o(u_i - u_{i-1} - \mu)^2]\}} \quad , \quad (2.46)$$

with β being the inverse temperature. The expression Eq. 2.46 for the partition function can be rewritten in the form of a recursion relation as follows:

$$\begin{aligned} \mathcal{Z}^{(n)}(u_n) &= e^{-\beta V_o(u_n)} \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \frac{1}{2}k_o(u_n - u_{n-1} - \mu)^2} e^{-\beta V_o(u_{n-1})} \int_{-\infty}^{+\infty} du_{n-2} \dots \\ &= e^{-\beta V_o(u_n)} \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \frac{1}{2}k_o(u_n - u_{n-1} - \mu)^2} \mathcal{Z}^{(n-1)}(u_{n-1}) \quad . \end{aligned} \quad (2.47)$$

Now define,

$$\mathcal{Z}^{(n)-} = \mathcal{Z}^{(n)} e^{\beta V_o(u_n)} \quad . \quad (2.48)$$

With this definition, Eq. 2.47 becomes,

$$\mathcal{Z}^{(n)-}(u_n) = \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \frac{k_o}{2}(u_n - u_{n-1} - \mu)^2} \mathcal{Z}^{(n-1)}(u_{n-1}) \quad . \quad (2.49)$$

If we now define a free energy F as

$$\mathcal{Z}^{(n)} = e^{-\beta F^{(n)}(u_n)} \quad , \quad (2.50)$$

then Eq. 2.49 reads,

$$e^{-\beta F^{(n)}(u_n) + \beta V_o(u_n)} = \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \frac{k_o}{2}(u_n - u_{n-1} - \mu)^2} e^{-\beta F^{(n-1)}(u_{n-1})} \quad , \quad (2.51)$$

where we also made use of the definition Eq. 2.48.

In the zero temperature limit ($\beta \rightarrow \infty$), a saddle point approximation approach might be taken for the integral in Eq. 2.51. The exponent is to be expanded around its minimum point, u_{n-1}^* , which yields

$$e^{-\beta F^{(n)}(u_n) + \beta V_o(u_n)} = \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \left[\frac{k_o}{2} (u_n - u_{n-1}^* - \mu)^2 + F^{(n-1)}(u_{n-1}^*) + \alpha (u_{n-1} - u_{n-1}^*)^2 \right]} \quad , \quad (2.52)$$

where $\alpha (u_{n-1} - u_{n-1}^*)^2$ in the exponent is due to the second order term in the expansion. Eq. 2.52 yields, after integration,

$$e^{-\beta F^{(n)}(u_n) + \beta V_o(u_n)} = e^{-\beta \left[F^{(n-1)}(u_{n-1}^*) + \frac{k_o}{2} (u_n - u_{n-1}^* - \mu)^2 \right]} \sqrt{\frac{\pi}{\alpha \beta}} \quad . \quad (2.53)$$

The exponential dominates the square root as $\beta \rightarrow \infty$, so taking the logarithm of both sides we obtain,

$$F^{(n)}(u_n) = V_o(u_n) + \frac{1}{2} k_o (u_n - u_{n-1}^* - \mu)^2 + F^{(n-1)}(u_{n-1}^*) \quad , \quad (2.54)$$

which is exactly the definition of the effective potential as in Eq. 2.31 since u_{n-1}^* is defined to be the point that minimizes the right hand side. So we can conclude that, the effective potential of Griffiths and Chou is the zero temperature limit of the free energy as defined in Eq. 2.50.

With the discussion of the free energy aside for a moment, we will return to Eq. 2.49. Since we can multiply the partition function by a constant without affecting the physics of the problem, we will normalize the Gaussian inside the integral as,

$$\mathcal{Z}^{(n)-}(u_n) = \sqrt{\frac{\beta k_o}{2\pi}} \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \frac{k_o}{2} (u_n - u_{n-1} - \mu)^2} \mathcal{Z}^{(n-1)}(u_{n-1}) \quad . \quad (2.55)$$

We will substitute τ for $\frac{1}{k_o}$, the reason will be clear shortly. Also note that if the harmonic interaction is to be viewed as if it is mediated by an elastic strip made of some material, the equilibrium length of the strip is directly proportional to the

reciprocal of the elastic constant. Therefore, μ can be regarded as a function of τ as,

$$\mu(\tau) = c\tau \quad , \quad (2.56)$$

where c is a positive constant. With these modifications, Eq. 2.55 becomes

$$\mathcal{Z}^{(n)-}(u_n, \tau) = \sqrt{\frac{\beta}{2\pi\tau}} \int_{-\infty}^{+\infty} du_{n-1} e^{-\beta \frac{1}{2\tau} (u_n - u_{n-1} - \mu(\tau))^2} \mathcal{Z}^{(n-1)}(u_{n-1}) \quad . \quad (2.57)$$

We can use different coordinates x in which the position of the rightmost particle is described with respect to the free end of the unstretched spring, simplifying the exponent in the integral of Eq. 2.57. With the transformations,

$$\begin{aligned} u_n &= x_n + \mu(\tau) \\ u_{n-1} &= x_{n-1} \end{aligned} \quad (2.58)$$

we can rewrite Eq. 2.57 as,

$$\mathcal{Z}^{(n)-}(x_n + \mu, \tau) = \sqrt{\frac{\beta}{2\pi\tau}} \int_{-\infty}^{+\infty} dx_{n-1} e^{-\beta \frac{1}{2\tau} (x_n - x_{n-1})^2} \mathcal{Z}^{(n-1)}(x_{n-1}) \quad . \quad (2.59)$$

The right hand side of Eq. 2.59 is the solution to the well-known linear diffusion equation. The function,

$$\tilde{\mathcal{Z}}^{(n)-}(x_n, \tau) = \mathcal{Z}^{(n)-}(x_n + \mu, \tau) \quad (2.60)$$

is the solution to the diffusion equation,

$$\frac{\partial \tilde{\mathcal{Z}}^{(n)-}}{\partial t} = \frac{1}{2\beta} \frac{\partial^2 \tilde{\mathcal{Z}}^{(n)-}}{\partial x_n^2} \quad , \quad (2.61)$$

at time $t = \tau$, with the initial condition

$$\tilde{\mathcal{Z}}^{(n)-}(x_n, 0) = \mathcal{Z}^{(n-1)}(x_{n-1}) \quad , \quad (2.62)$$

The continuous time parameter t such that $0 < t < \tau$ corresponds to a variable spring constant k such that $\infty > k > k_o$. Moreover, since the spring length μ depends on time as $\mu(t) = ct$, the flow of time corresponds to an elastic strip gradually growing until it has the right length μ . With this interpretation, the coordinates x defined by the transformation Eq. 2.58 refer to a frame that is moving with speed c , along with the open end of the unstretched strip. The transformation Eq. 2.58, that only involves the pair at the end of the chain, can be generalized as,

$$\begin{aligned} u_n &= x_n + (n-1)\mu + \mu(t) \\ u_{n-1} &= x_{n-1} + (n-1)\mu \end{aligned} \quad (2.63)$$

which applies to every part of the chain. This moving coordinate frame will be referred to as the *Burgers frame* henceforth.

With the *Cole-Hopf transformation* [12, 13],

$$v(x_n, t) = -\frac{1}{\beta} \frac{\partial}{\partial x_n} \log \tilde{\mathcal{Z}}^{(n)-}(x_n, t) = \frac{\partial}{\partial x_n} \tilde{F}^{(n)-}(x_n, t) \quad , \quad (2.64)$$

the diffusion equation is equivalent to the *Burgers' equation* of fluid dynamics, in terms of the new function $v(x_n, t)$ as (see Appendix B),

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x_n} = \frac{1}{2\beta} \frac{\partial^2 v}{\partial x_n^2} \quad . \quad (2.65)$$

This is the general form of Burgers' equation, taking the effects of viscosity into account. In the limit $T \rightarrow 0$, the right hand side vanishes and we obtain the *inviscid* Burgers' equation (also known as *Riemann's equation*):

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x_n} = 0 \quad . \quad (2.66)$$

We will refer to the inviscid Burgers' equation simply as the Burgers' equation since we only consider this case.

Recalling that in the zero temperature limit, the free energy is equal to the effective potential, $v(x_n, t)$ defined by Eq. 2.64 becomes,

$$v(x_n, t) = \frac{\partial}{\partial x_n} \tilde{V}^{(n)-}(x_n, t) \equiv \mathcal{U}^{(n)}(x_n, t) \quad , \quad (2.67)$$

where $\tilde{V}$ represents V transformed into the coordinates of the moving frame. Hence, the derivative of the effective potential is a profile that evolves with Burgers' equation upon the addition of one *spring* (no particle).

2.3.3. The Inviscid Burgers' Equation

The inviscid Burgers' equation is a member of a family of scalar non-linear conservation laws with the differential form:

$$v_t + \varphi(v)_x = 0 \quad , \quad (2.68)$$

where subscripts denote partial differentiation with respect to the corresponding variable and $\varphi(v)$ is the flux function associated with the conserved quantity v . Note that Eq. 2.68 may be rewritten as

$$v_t + c(v)v_x = 0 \quad , \quad (2.69)$$

where

$$c(v) = \varphi'(v) \quad . \quad (2.70)$$

One approach to solve Eq. 2.69 would be to consider the left hand side of the equation as the total derivative of $v(x, t)$ [14] along a curve in the (x, t) plane with

slope,

$$\frac{dx}{dt} = c(v) \quad (2.71)$$

since the total derivative of v is,

$$\frac{dv}{dt} = v_t + \frac{dx}{dt} v_x \quad . \quad (2.72)$$

Along the curve $x(t)$, the function $v(x, t)$ is constant according to Eq. 2.69. Hence, $c(v)$ in Eq. 2.71 is also constant meaning the curve $x(t)$ is a straight line. Thus the general solution of Eq. 2.69 depends on the construction of a family of straight lines in the (x, t) plane, each line with slope $c(v)$ corresponding to the value of v on it [14]. These straight lines are called the *characteristic lines* of the problem.

The expression for a characteristic line originating from the point $(x_0, 0)$ is found easily as

$$\begin{aligned} x(t) &= x_0 + t \frac{dx}{dt} \\ &= x_0 + tc(v_0(x_0)) \quad , \end{aligned} \quad (2.73)$$

since $\frac{dx}{dt}$ is constant, and its value is given by Eq. 2.71 where v_0 represents the initial waveform $v(x_0, 0)$. Since points on the initial waveform move with a velocity $c(v_0(x_0))$ on the characteristics, the function $c(v)$ will be called a *velocity field*. Initial and final velocity fields are related as,

$$c(v(x, t)) = c(v(x_0, 0)) \quad , \quad (2.74)$$

where x_0 is given by the *characteristic equation* Eq. 2.73. The solution to Eq. 2.69 can be implicitly found using Eqs. 2.73 and 2.74. We will now turn to the specific case of the inviscid Burgers' equation.

The inviscid Burgers' equation is a member of the family Eq. 2.68 with the flux function:

$$\varphi(v) = \frac{1}{2}v^2 \quad , \quad (2.75)$$

which yields for Eq. 2.69,

$$v_t + vv_x = 0 \quad , \quad (2.76)$$

meaning that the velocity field $c(v)$ is the function v itself, *i.e.* c is the identity function. The characteristic equation is therefore found as,

$$x(t) = x_0 + tv(x_0, 0) \quad (2.77)$$

and the solution to the inviscid Burgers' equation can be implicitly obtained from,

$$v(x, t) = v(x_0, 0) \quad , \quad (2.78)$$

with x_0 given by Eq. 2.77. Fig. 2.7 depicts a general waveform after evolution with Burgers' equation.

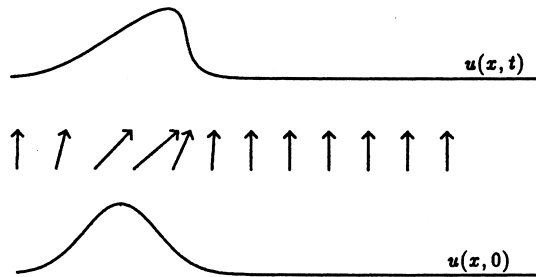


Figure 2.7. A general waveform and its new shape after evolution according to Burgers' equation. Characteristic lines are also depicted by arrows [15].

The method described above has an interesting consequence. It can be shown that if there is a point $x(0)$ at $t = 0$ where the initial waveform has $\frac{\partial v(x(0), 0)}{\partial x} < 0$, characteristic lines in the vicinity of that point will cross after a finite amount of time

t_c at the point $x(t_c)$ [15]. For times $t > t_c$, the solution will be multi-valued at the point $x(t)$. While this kind of solution can make sense in some contexts, we will only be interested in the *weak* solution corresponding to the aforementioned situation.

Burgers' equation is actually the differential form of a conservation law. The solution to a conservation has the property that its integral over the whole space is a constant in time, *i.e.* it is conserved. In this perspective, the weak solution associated with a smooth solution can be found by an equal area rule. The multi-valued smooth solution is replaced by a function which changes discontinuously at the multi-valued point. The location of this discontinuity must be chosen so as to make the area under the discontinuous function and the multi-valued function the same, due to the conservation of the integral of the function. The discontinuity introduced as such due to the intersection of characteristics, will be referred to as a *shock* henceforth. The case is depicted in Fig. 2.8.

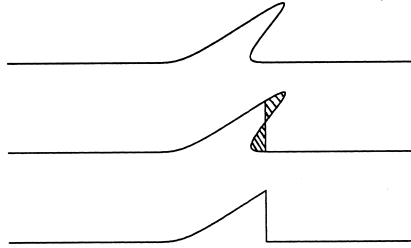


Figure 2.8. The equal area rule and shock formation in Burgers profiles illustrated [15].

The shock solution is a weak solution to Burgers' equation only if it propagates in an appropriate manner. This has to do with the weak solution having to satisfy the area conservation constraint at all times. This condition requires that the propagation speed of a shock front is given by [15],

$$s = \frac{\varphi(v^-) - \varphi(v^+)}{v^- - v^+} = \frac{v(x^-) + v(x^+)}{2} \quad , \quad (2.79)$$

with $-$ and $+$ denoting the immediate left and right of the shock, respectively.

2.3.4. The Minimization Equation as a Characteristic Equation

Since we have rigorously proven that the derivative of the effective potential is a velocity field that evolves according to Burgers' equation, we expect that the mapping between the positions of adjacent particles to have the form of a Burgers type characteristic equation. We can readily rewrite the minimization equation, Eq. 2.41 of Section 2.3.1, in the notation and coordinates introduced in Section 2.3.2 as

$$x_n = x_{n-1} + t\mathcal{U}(x_{n-1}, 0) \quad , \quad (2.80)$$

which has the form that we expected. Let us rewrite this equation in another form for a physical interpretation:

$$-\frac{x_n - x_{n-1}}{t} = -\mathcal{U}(x_{n-1}, 0) \quad . \quad (2.81)$$

The left hand side of this equation is the stress in the spring, and the right hand side is the force required to keep the particle at x_{n-1} fixed. The interpretation is easy now. A chain with free end at position x_{n-1} is to be augmented by the addition of another spring. In the Burgers evolution perspective, where the spring is an elastic strip slowly growing in time, the strain in the strip (therefore x_n) at all times should be adjusted in such a way that the particle at position x_{n-1} (therefore the rest of the chain) is stationary throughout the evolution.

3. APPLICATION OF THE BURGERS EVOLUTION METHOD TO SCALLOPED POTENTIALS

3.1. The Velocity Fields of FK Models with Scalloped Potentials

In this section, we are going to employ the *Burgers evolution* method inside the framework of effective potentials proposed by Griffiths and Chou, to the problem of Frenkel-Kontorova model with a scalloped external potential.

The potential is,

$$V_o(x) = \frac{1}{2}\lambda_o \left[x - 2a \operatorname{Int}\left(\frac{x+a}{2a}\right) \right]^2 \quad (3.1)$$

where $2a$ and $\lambda_o > 0$ are the period and the strength of the potential respectively. This kind of potential constitutes of a periodic sequence of parabolic potential wells of width $2a$, with their bottoms right on top of $x = 2ak$, where k is an integer, as shown in Fig. 3.1(a). In the context of the evolution of effective potentials, we will consider the derivative of this potential, rather than the potential itself, which is a series of ramps as shown in Fig. 3.1(b). The x -intercepts correspond to well troughs. Due to the symmetry of the *unit* well, the shock fronts² are centered on the horizontal axis, and the total area under the profile is zero, by continuity and periodicity of $V_o(x)$.

The particle chain of the model, along with the effective potential, will be grown to the right. Each step of growth consists of attaching a spring to the rightmost particle, and then a new particle onto the right-hand end of the spring. From the perspective of the effective potential, the first part corresponds to the evolution of the profile of the rightmost particle according to Burgers' equation, whereas the second part is the addition of a new profile corresponding to the external potential, on top of the old

²There is actually no need to refer to these discontinuities as *shocks* before incorporating them into the notion of Burgers evolution. Nevertheless, in order to keep the discussion simple, it is preferable to avoid referring to the same object with different names.

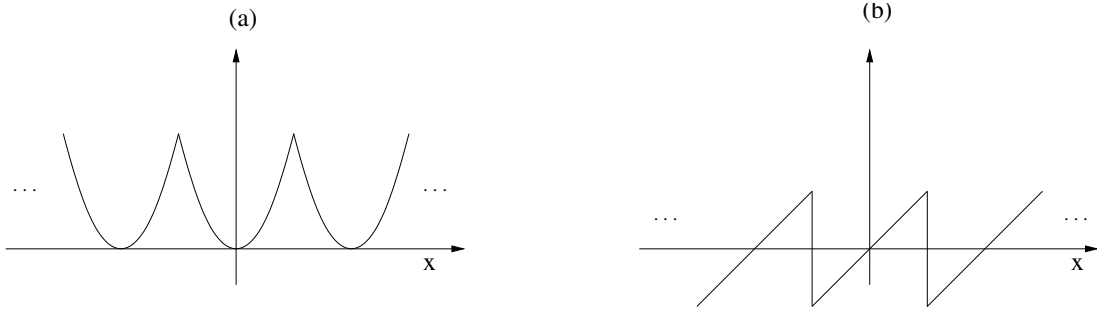


Figure 3.1. (a) The piecewise parabolic scalloped potential of our model. (b) The piecewise linear profile corresponding to the scalloped potential.

one. Since the effective potential is also periodic with period $2a$, we will carry on our discussion about these effective potentials or profiles, referring to a window of width $2a$.

Whenever a new particle is added to the chain, the profile of Fig. 3.1(b) will be added on top of whatever the current one is. Or, speaking in terms of what is seen inside a window of width $2a$, this corresponds to the addition of a pair of line segments of slope λ_o , separated by a shock front of intensity $2a\lambda_o$, as depicted in Fig. 3.2. At any step of evolution, it turns out that, the profile is a series of line segments with the same slope, separated by shocks of different magnitudes and propagation speeds. The justification of this statement is not immediate, however it will become clear after a detailed treatment of the evolution of profiles, which we turn to next.

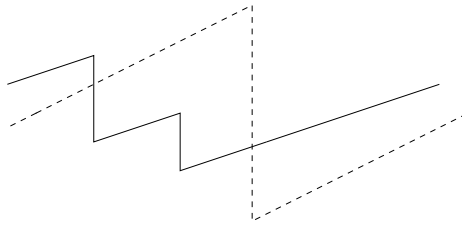


Figure 3.2. The coincidence of a new profile on top of one that has already gone through a few steps of growth.

3.2. Shock Trains and Their Evolution

A piecewise linear profile with the description above will be called a *shock train*. At any instant of its evolution, a shock train is completely determined by a set of parameters [16]. The overall slope of the segments is clearly one of the parameters. Each line segment is part of an infinite line on which it lies (see Fig. 3.3). Since the

segments are confined between shocks, the position of all the shocks determine the intervals that the segments occupy, on their respective lines. Finally, given the slope, the lines are determined by their x -intercepts. Hence, if there are n shocks in one period, then $2n + 1$ parameters are required to determine the shock train completely.

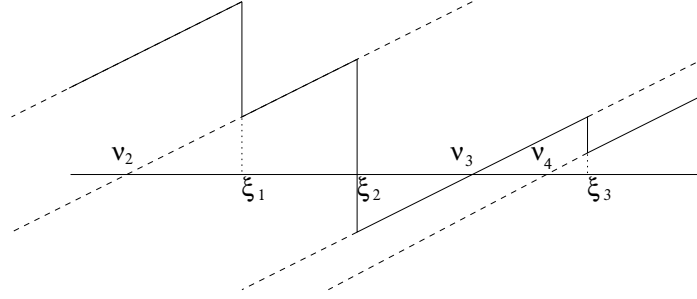


Figure 3.3. An example shock train.

We will use the symbol λ for the slope, since it is related to the potential strength that we named λ_0 . Shock positions are to be represented by the set of symbols $\{\xi_i\}$, likewise the x -intercepts by $\{\nu_i\}$. The latter will be referred to as *nodes* throughout the thesis. We label the shocks such that $\xi_j > \xi_i$ whenever $j > i$.

We will begin the treatment on time evolution by examining what happens to a line with x -intercept ν as time goes on. The general expression for such a line is,

$$v_{line}(x, t) = \lambda(t)(x - \nu) \quad .$$

Since the segments of the profile lie on such lines, the results will apply for each of the segments. If the evolution of this line is to obey Burgers' equation, taking the necessary derivatives, we find that

$$\frac{\partial \lambda}{\partial t} = -\lambda^2 \quad ,$$

which means

$$\lambda(t) = \frac{\lambda(0)}{1 + t\lambda(0)} \quad . \tag{3.2}$$

That is, $\lambda(t)$ is the harmonic mean of $\lambda(0)$ and $\frac{1}{t}$. This result is not surprising, if we

note that t corresponds to the reciprocal of the spring constant. After all, $\lambda(t)$ is the combined strength of the spring force and the force due to the external potential, both of which are harmonic.

We thus find that the line segments of the shock train flatten with time, according to

$$v_{line}(x, t) = \frac{\lambda(0)}{1 + t\lambda(0)}(x - \nu) \quad .$$

What becomes of the shock fronts that confine them is determined by the shock speeds. We discussed earlier that, discontinuities in the velocity field travel with instantaneous speeds given by,

$$s(x_i, t) = \frac{u(\xi_i^-, t) + u(\xi_i^+, t)}{2} \quad . \quad (3.3)$$

Given the geometrical description of a shock train in terms of line segments, the instantaneous speed of any shock is easily found as, (see Fig. 3.3)

$$s_i(t) = \lambda(t) \left(\xi_i(t) - \frac{\nu_i + \nu_{i+1}}{2} \right) \quad . \quad (3.4)$$

The shock speeds are actually constant in time, as can be demonstrated easily as follows: Taking the derivative of the shock speed, we have,

$$\begin{aligned} \frac{ds_i(t)}{dt} &= \frac{d\lambda(t)}{dt} \left(\xi_i(t) - \frac{\nu_i + \nu_{i+1}}{2} \right) + \lambda(t) \frac{d\xi_i(t)}{dt} \\ &= -\lambda^2(t) \left(\xi_i(t) - \frac{\nu_i + \nu_{i+1}}{2} \right) + \lambda(t) s_i(t) \\ &= -\lambda(t) s_i(t) + \lambda(t) s_i(t) = 0 \quad . \end{aligned}$$

The *intensity* of a shock front i is defined as,

$$\Delta_i \equiv u(\xi_i^-) - u(\xi_i^+) \quad , \quad (3.5)$$

that is, the height of the shock front. In terms of the profile parameters, at an arbitrary time t , the intensity of shock i directly follows from the profile parametrization, Fig. 3.3,

$$\Delta_i(t) = \lambda(t) (\nu_{i+1} - \nu_i) \quad . \quad (3.6)$$

When two shocks collide, they coalesce into a single shock [15]. During a time interval such that a collision involving the i^{th} shock does not occur, it drifts with a uniform speed s_i , and the corresponding trajectory is,

$$\xi_i(t) = \xi_i(t_0) + s_i(t - t_0) \quad , \quad (3.7)$$

where $\xi_i(t_0)$ is the location of the shock at t_0 .

At the instant t_c when two shocks collide, there are two shocks, shocks i and $i + 1$, with speeds s_i and s_{i+1} , and intensities $\Delta_i(t_c)$ and $\Delta_{i+1}(t_c)$, right on top of each other at the position $\xi_i(t_c) = \xi_{i+1}(t_c)$ (see Fig. 3.4). The speed of the resulting shock front is the position of its midpoint along the vertical direction. Thus, the speed of the resultant shock is readily found from simple geometrical calculations as,

$$s' = s_i - \frac{\Delta_{i+1}}{2} \quad \text{or alternatively,}$$

$$s' = s_{i+1} + \frac{\Delta_i}{2} \quad . \quad (3.8)$$

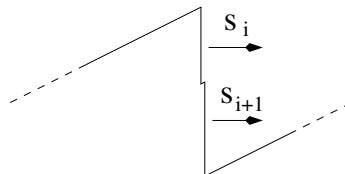


Figure 3.4. Two shocks at the instant of collision.

When two shocks collide, one of the shocks disappears and the most convenient way to describe the situation is this³ : To shock i is assigned the new speed and intensity, while shock $i + 2$ replaces shock $i + 1$, $i + 3$ replaces $i + 2$ etc. As a matter of fact, removing the ξ and ν belonging to shock $i + 1$ from the parameter set of the profile at the instant of collision, results in the required modification of the speed and intensity of the i^{th} shock.

In summary, Burgers evolution of a shock train involves the overall slanting of the line segments down to a slope of some value λ^- , with the shocks drifting around with their respective speeds, colliding on occasion according to the description given above. This concludes the discussion about shock dynamics, in the case of a piecewise parabolic scalloped potential.

3.3. Insertion of a New Particle

The evolution of the shock profile was only one step of the growth of the chain by one particle. The addition of the profile corresponding to the new particle will modify the parameters of the shock train, and requires special attention.

First of all, the introduction of a new shock into the window, clearly does not disturb the positions of the other shocks (see Fig. 3.5). The nodes, however, will shift due to the addition of the two ramps of slope λ_0 on the two sides of the new shock. The shift can be found by simple addition of the analytical equation of the newly introduced line segments, to the equation corresponding to the ones that were already there. The only point to note here is that, depending on their locations, some of the present segments are to be summed with the new segment that is to the left of the newly inserted shock, while the others with the segment on the right. The addition of the corresponding ramp to each of the resident segments, will result in a shift of the nodes of those segments. Upon summation of the equation of the i^{th} segment with the ramp on whichever side segment i is, with respect to the new shock, we obtain the

³There is also a description where a shock mass, hence a momentum, is defined and the shocks become inelastically colliding particles.

equation relating the position of node i before and after the operation:

$$\nu_i^+ = \frac{\lambda^-}{\lambda^- + \lambda_o} \nu_i^- + \frac{\lambda_o}{\lambda^- + \lambda_o} b_i \quad . \quad (3.9)$$

Here, b_i stands for the x -intercept of the newly introduced ramp relevant to the i^{th} segment, while λ^- is the value of the overall slope of the shock train after Burgers evolution, as we mentioned earlier. As a remark, Eq. 3.9 can be rewritten as,

$$\nu_i^+ - b_i = \frac{\lambda^-}{\lambda^- + \lambda_o} (\nu_i^- - b_i) \quad ,$$

indicating that nodes are *attracted* toward their respective b_i 's, since λ^- is strictly smaller than $\lambda^- + \lambda_o$.

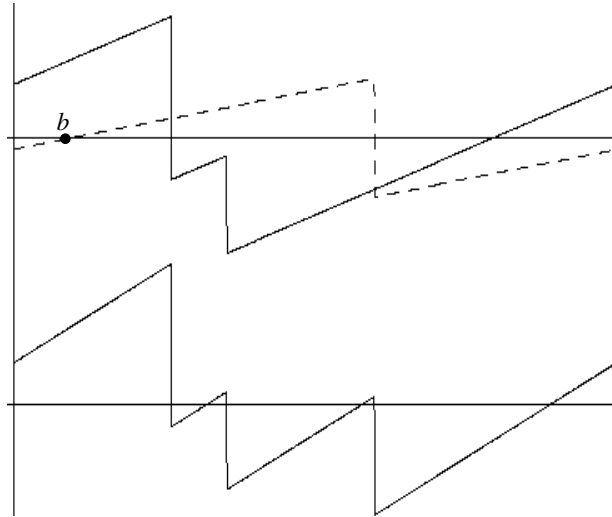


Figure 3.5. The current profile and the newly introduced one shown together in the upper half. The resulting profile after the addition of the ramps is shown in the bottom half.

Notice, however, that one segment is dissected by the new shock, into two segments (see Fig. 3.5). The formula of Eq. 3.9 applies for both of these segments, but with different b 's. The shift of each segment is governed by the ramp on the relevant side of the new shock, therefore the relevant x -intercept. Thus, *two* shifted nodes will emerge from the one belonging to the dissected segment, one for each x -intercept on the two sides of the new shock, which are $2a$ apart. Hence, since a new shock is added to the profile, a new node also appears, as expected.

3.4. Fixed Point of the Profile Slope and Aubry's η

Every time a new particle is attached onto the spring, the slope of the profile will increase by λ_o , since the particle experiences the external potential (see Fig. 3.6 for an example). Combined with the overall flattening due to Burgers evolution, the slope of the shock train corresponding to a long chain of particles will reach a limiting value. Making use of Eq. 3.2, the equation that this limiting value λ^* , of the slope is:

$$\frac{\lambda^*}{1 + \tau\lambda^*} + \lambda_o = \lambda^* \quad , \quad (3.10)$$

where τ is the duration of each Burgers evolution (which is equal to $\frac{1}{k_o}$ in the light of our previous discussion of the evolution of the effective potential). This equation is equivalent to the quadratic equation

$$\lambda^{*2} - \lambda_o\lambda^* - \frac{\lambda_o}{\tau} = 0 \quad , \quad (3.11)$$

with the solution

$$\lambda^* = \frac{1}{2}\lambda_o \left(1 + \sqrt{1 + \frac{4}{\tau\lambda_o}} \right) \quad . \quad (3.12)$$

The other solution of the quadratic equation is unphysical.⁴

Notice that λ^* , by definition (Eq. 3.10), corresponds to the slope of the profile, *just after* the addition of a new particle. The slope just before the addition of a new particle is therefore,

$$\lambda^{*-} \equiv \lambda^* - \lambda_o \quad , \quad (3.13)$$

⁴When the spring is too stiff, *i.e.* $\tau \rightarrow 0$, λ^* turns out negative. With the given circumstances, the limiting value of the slope cannot be negative. Furthermore, the condition that $\tau \rightarrow \infty$ must correspond to the limiting value being λ_o itself, which it doesn't, for the *unphysical* solution of the quadratic equation.

which yields,

$$\lambda^{*-} = \lambda^* - \lambda_o = \frac{1}{2}\lambda_o \left(1 + \sqrt{1 + \frac{4}{\tau\lambda_o}} \right) \quad (3.14)$$

through usage of Eq. 3.12. Now, the definition of λ^* also requires that,

$$\lambda^{*-} = \frac{\lambda^*}{1 + \tau\lambda^*} \quad .$$

Therefore, the factor $\frac{1}{1+\tau\lambda^*}$ generated by the Burgers evolution of a profile with initial slope λ^* becomes,

$$\begin{aligned} \frac{1}{1 + \tau\lambda^*} &= \frac{\lambda^{*-}}{\lambda^*} \\ &= \frac{1}{\lambda^*} \frac{\lambda^*}{1 + \tau\lambda^*} \\ &= \frac{\frac{\lambda_o}{2} \left(-1 + \sqrt{1 + \frac{4}{\tau\lambda_o}} \right)}{\frac{\lambda_o}{2} \left(1 + \sqrt{1 + \frac{4}{\tau\lambda_o}} \right)} \\ &= \frac{\left(-1 + \sqrt{1 + \frac{4}{\tau\lambda_o}} \right)^2}{\frac{4}{\tau\lambda_o}} \\ &= 1 + \frac{\tau\lambda_o}{2} - \frac{\tau\lambda_o}{2} \sqrt{1 + \frac{4}{\tau\lambda_o}} \equiv \eta \end{aligned} \quad (3.15)$$

which, we note, is the parameter η defined in the context of Aubry's exact solution (Eq. 2.7).

3.5. Steady State of the Velocity Field

At this point, we know that the velocity field corresponding to the effective potential seen by the rightmost particle is a shock train with slope λ^* given by Eq. 3.12. However, the overall slope of the velocity field is not the only quantity that converges to a steady state value as the particle chain grows.

With each augmentation of the particle chain, the profile parameters transform according to Eqs. 3.7, 3.8 and 3.9. Going back to these equations and keeping in mind that shock speeds and intensities change while the *nodes* of the profile remain stationary or disappear under Burgers evolution, the transformation of nodes is expected to play a crucial role in the steady state behaviour of the entire velocity field.

The transformation (Eq. 3.9) of nodes is linear, with the slope parameter η smaller than one. In fact, in the light of our previous discussion of the relation between Aubry's η and λ^* , the transformation of nodes becomes,

$$\nu_i^+ = \eta \nu_i^- + (1 - \eta) b_i \quad . \quad (3.16)$$

Since $0 < \eta < 1$, the nodes of the profile will tend to lose relevance to their initial condition and reach a steady state as the length of the chain gets larger. We expect that the velocity field, and hence the effective potential, reaches a steady state.

However, the steady state is not necessarily one where the profile parameters cease changing upon the addition of each new particle. There can be a *set* of steady state profiles with a finite number s of elements, where the elements of the set come in succession upon the addition of s new particles. Then the sequence will repeat itself. This is a kind of steady state that we will call *s-periodic*. Moreover, there can be an overall shift imposed on the successive steady state profile sets, as well.

Let us consider a case that is *s-periodic*. Then, we are looking for profiles for the n^{th} and the $(n + s)^{th}$ particles that are of the same shape, only shifted with respect to each other. Formally,

$$\mathcal{U}^{(n+s)}(x_{n+s}) = \mathcal{U}^{(n)}(x_n - \delta) \quad (3.17)$$

where δ is the shift between the $(n + s)^{th}$ and the n^{th} profiles. Recall that we have previously introduced the notation with superscripts, indicating which particle the

effective potential belongs to.

In order to find a mathematical expression for the shift between the profiles of the n^{th} and $(n + s)^{th}$ steps we have to find a point on the profiles, with the same identity, so that what we are trying to calculate is the shift in the position of that special point. An obvious candidate for this is the position of the most recently added shock in each of the profiles.

Remembering that the coordinate system with respect to which the shock trains evolve with Burgers' equation, drifts along with the loose end of the unstretched spring (see Section 2.3.2), the kinks of the external potential will coincide on different points in that frame each time a particle is inserted, although they are apart by a distance of $2a$ in the absolute coordinates. The frame will have drifted by a distance $s\mu$ in the process of going from the n^{th} particle to the $(n + s)^{th}$ particle so, any point that is fixed with respect to the external potential will seem to have shifted by an amount $-s\mu$ inside the Burgers frame, so to speak. However, we are not talking about the shift in the position of an individual point, but a sequence of similar points that are a distance $2a$ apart. Therefore, one must compensate for however many whole $2a$'s that $s\mu$ might comprise, in order to find the difference in the positions where a new shock coincides in the n^{th} and $(n + s)^{th}$ frames, with respect to the fundamental interval $[-a, a]$:

$$\delta = -s\mu + 2a \operatorname{Int}\left(\frac{s\mu}{2a}\right) \quad . \quad (3.18)$$

Notice that, by definition δ is negative and corresponds to a shift to the left. However, since the effective potential is periodic by $2a$, a shift of δ_- such that

$$-2a < \delta_- < 0$$

is indistinguishable from a positive shift of

$$\delta_+ = \delta_- + 2a \quad .$$

The shift calculated in Eq. 3.18 corresponds to δ_- . The two values of the shift are equally mentionable in this regard,

$$\delta_- = -s\mu + 2a \operatorname{Int}\left(\frac{s\mu}{2a}\right) \quad \text{and,} \quad (3.19)$$

$$\delta_+ = -s\mu + 2a \left[\operatorname{Int}\left(\frac{s\mu}{2a}\right) + 1 \right] \quad . \quad (3.20)$$

However, the one with the smaller absolute value is more useful. Since, the order of the profile parameters ξ and ν is invariant under their relevant transformations, *i.e.* their paths do not cross, the smaller shift is directly observable from the trajectories of each individual profile parameter in the process of advancing s steps. Refer to Fig. 3.9 for an illustration.

3.6. Application to the 1-periodic Case

3.6.1. Profiles of the 1-periodic Steady State

In this section, we will start to investigate the case of a 1-periodic steady state of the effective potential. The length of the spring will be written as

$$\mu = 2a - \sigma \quad , \quad (3.21)$$

where⁵

$$0 \leq \sigma < 2a \quad . \quad (3.22)$$

To begin with, imagine the situation with $\mu = 2a$, *i.e.* $\sigma = 0$. From one particle to the next one, the Burgers frame will have moved by exactly $2a$. Therefore, every time a new particle is inserted, the ramp profile it introduces will fit perfectly into the

⁵The case with negative σ is very similar and has been left out for convenience.

frame just as the 0^{th} particle. The result is that the profile of each step is a single ramp, only losing some of its strength due to Burgers evolution but not moving. The process is depicted in Fig. 3.6. This result tells us that, since $\mu = 2a$, in the ground state configuration, all particles are located at the bottom of the potential wells and the springs connecting them are unstretched.

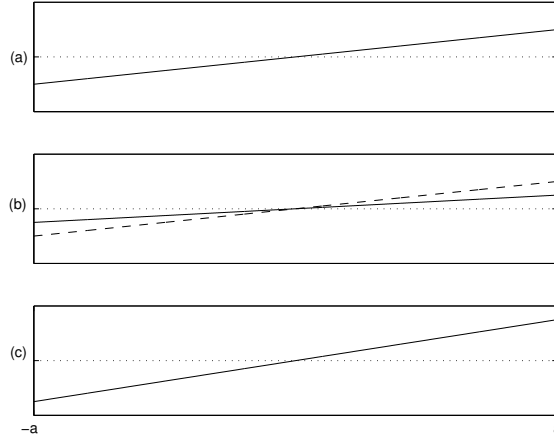


Figure 3.6. (a) The initial ramp. (b) The initial ramp after evolution and the new one (dashed). (c) After the addition of the new ramp.

With the spring length given as $\mu = 2a - \sigma$, the Burgers frame will drift by a distance a bit less than the period, between the addition of two adjacent particles. Consider the addition of two ramp profiles that are little misaligned. The resulting profile will have two closely spaced shocks with opposite directions of speed. This profile will immediately evolve back into a single ramp profile, only shifting a little during the process of the shocks coming together (see Fig. 3.7). This is why we expect a 1-periodic steady state for such a value of the spring length.

We should point out the fact that, the case with two shocks immediately colliding to yield a single ramp profile is not the only 1-periodic steady state. There is a family of such steady states with a variety of number of shocks. The common property is that, in every segment of Burgers evolution from the addition of one particle to the next, there is a specific pair of shocks that collide to destroy one of the shocks. When a new particle is added, an additional shock is created and the original number of shocks is regained, and the process repeats. Actually, the simplicity of the case with a μ close

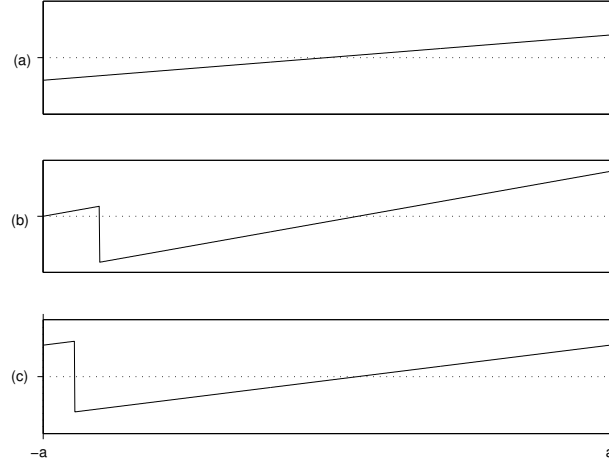


Figure 3.7. (a) The initial ramp after evolution. (b) Upon addition of a new ramp.

Note the shock on the boundary of the window. (c) The two shocks coalesce, resulting in a profile with a single ramp but shifted to the right.

to $2a$ is that, new shocks are created with a negative speed, bound to collide with one main shock front. Even in a situation with many shocks, all of them approach that main shock front, and the one closest to the main shock is absorbed in the course of evolution. We will be able to justify this statement shortly. An example profile belonging to such a situation is shown in Fig. 3.8. Also, Fig. 3.9 will be of help in picturing the situation, in which the position of shock fronts are traced as the particle chain is successively augmented by four particles.

Earlier on, we argued that the steady state profiles turn out to be displaced by a constant amount for successive steps. By focusing on the location of the most recently added shock, the corresponding shift between two successive profiles must therefore satisfy,

$$\begin{aligned}
 \delta_+ &= -(2a - \sigma) + 2a \operatorname{Int}\left(\frac{2a - \sigma}{2a}\right) + 2a \\
 &= \sigma + 2a \left[1 - \operatorname{Int}\left(\frac{\sigma}{2a}\right) - 1\right] \\
 &= \sigma
 \end{aligned} \tag{3.23}$$

since $\sigma < 2a$.

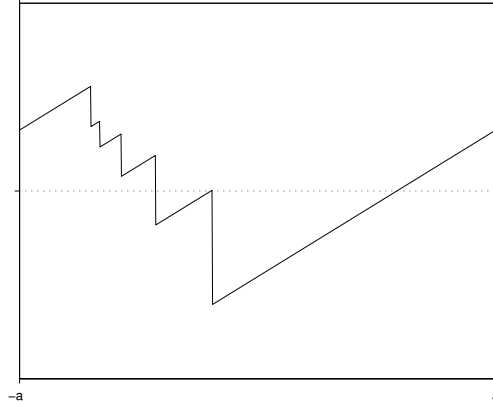


Figure 3.8. A 1-periodic steady state profile with a larger shock count. The rightmost shock is the most recently added one, whereas the pair farthest to the left will be colliding next.

We are now going to calculate the steady state profile, *i.e.* the parameters $\{\xi\}$ and $\{\nu\}$ on the previous assumption of 1-periodicity, for an arbitrary number of shocks κ (not counting the one that is constantly being created and destroyed).

3.6.2. Recursion Relation for Nodes in the Steady State

Recall that when a new particle, particle n , is added to the chain the nodes of the profile of the n^{th} evolution shift to new positions given by,

$$\nu_i^{(n)+} = \eta \nu_i^{(n)-} + (1 - \eta) b_i^{(n)} \quad (3.24)$$

where $b_i^{(n)}$ is the position of the x -intercept of the newly added ramp, associated with the node that is being transformed.

The profiles corresponding to the n^{th} and $(n + 1)^{st}$ particles are related by a mere shift. This means, whenever a new particle is inserted, the ν 's of the profile will transform in such a way that, for the evolution of the next spring, they assume the role of the ν which had been their left-neighbor. So,

$$\nu_{i-1}^{(n+1)} = \eta \nu_i^{(n)} + (1 - \eta) b_i^{(n)} \quad . \quad (3.25)$$

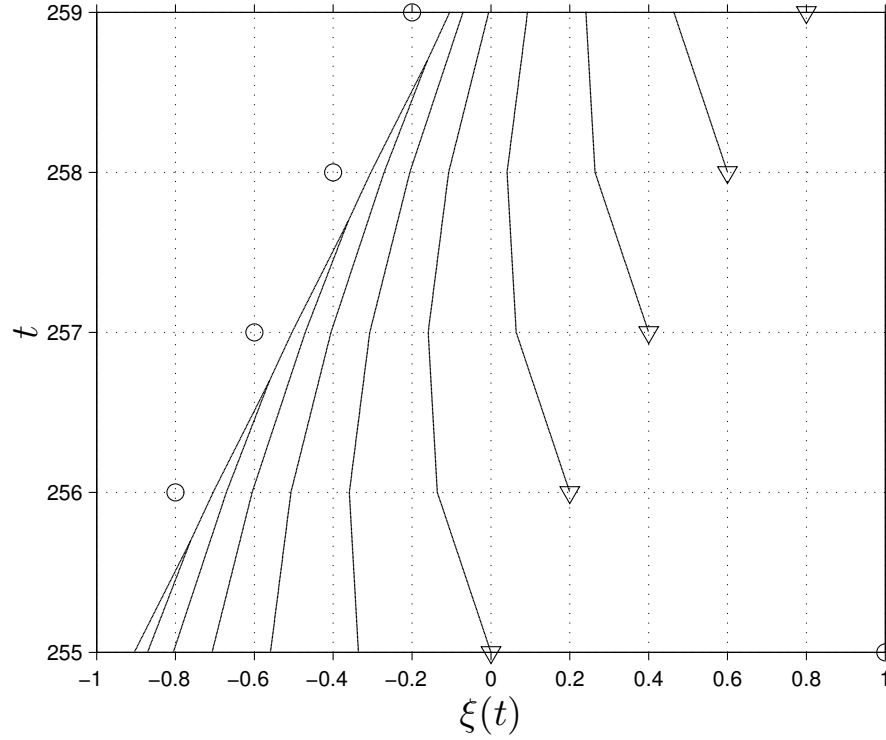


Figure 3.9. Tracing of shock fronts in the course of successive insertion of 4 particles, particles 256 to 259 with $a = 1$ and $\mu = 1.8$. The vertical axis is time with $\tau = 1$ so that integers correspond to particle number. The circle and triangle on each horizontal line represent the position of the x -intercept and shock front that are introduced by the insertion of the corresponding particle respectively. Note the shift by 0.2 after each evolution.

Incorporating also the shift,

$$\nu_{i-1}^{(n+1)} = \nu_{i-1}^{(n)} + \sigma \quad , \quad (3.26)$$

we have the recursion,

$$\nu_{i-1}^{(n)} = \eta \nu_i^{(n)} + (1 - \eta) b_i^{(n)} - \sigma \quad . \quad (3.27)$$

Now that this relation only involves quantities belonging to the n^{th} evolution, we can

drop the superscripts to ease the notation.⁶ Rewriting Eq. 3.27, we find,

$$\nu_{i-1} = \eta \nu_i + (1 - \eta)b_i - \sigma \quad . \quad (3.28)$$

Here, the recursion relation is not of much use as long as the x -intercept associated with each step of the recursion is different, *i.e.* as long as b has an index i . It turns out that this is not exactly the case, as we show next.

Recall that when a new shock is introduced, it dissects one of the segments in the profile, creating two segments out of it, with two corresponding nodes. One of these nodes is attracted to the x -intercept b that is to the right of the new shock, while the other is attracted to the left. The intercept to the left, also attracts all the other nodes corresponding to the $\kappa - 1$ shocks to the left thereby simplifying the recursion relation. If the shocks are labelled from right to left, starting from the right-bound node with an index 0 and $-1, -2, \dots, -\kappa$ for the ones to the left, as shown in Fig. 3.10, then all the κ left-bound nodes transform with the same b as,

$$\nu_{-k-1} = \eta \nu_{-k} + (1 - \eta)b - \sigma \quad , \quad k = 0, 1, \dots, \kappa - 1 \quad . \quad (3.29)$$

The transformation regarding the only right-bound node involves the ramp that is to the right of the new shock, which intercepts the x -axis at $b + 2a$. Therefore,

$$\nu_0 = \eta \nu_0 + (1 - \eta)(b + 2a) - \sigma \quad . \quad (3.30)$$

Before solving the recursion, Eq. 3.29, note that the position of ν_0 can be found in terms of b , using Eq. 3.30,

$$\nu_0 = b + 2a - \frac{\sigma}{1 - \eta} \quad . \quad (3.31)$$

⁶However, it should not be forgotten that b_i depends on the length of the chain.

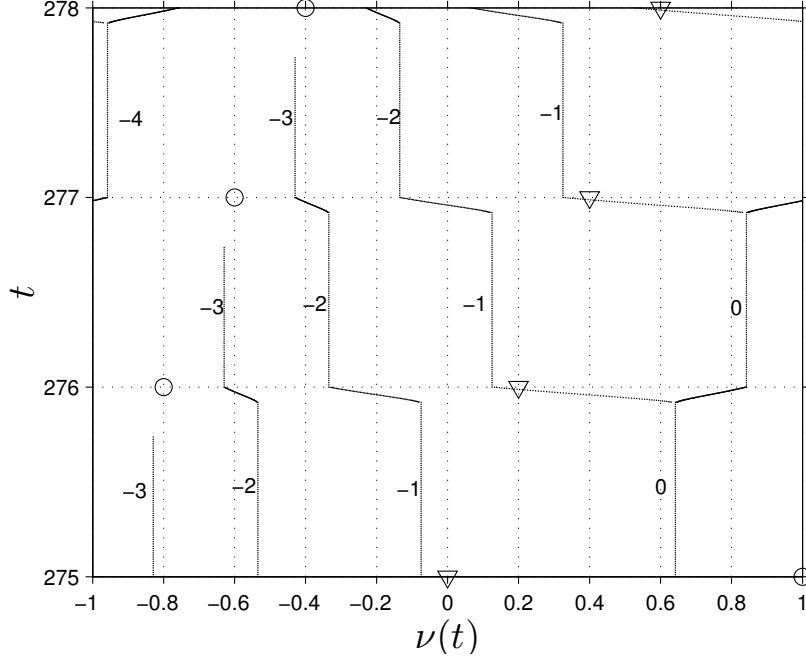


Figure 3.10. Tracing of nodes during chain augmentation, to demonstrate how the labelling is done. Nodes shift upon the insertion of a new particle. Shifts are shown by oblique line segments as if they happen continuously in a short time interval, just for illustration purposes. Node $-\kappa$ disappears in the middle of each evolution due to the collision of two shocks. Observe that one of the nodes yield two upon insertion, which is the one belonging to the segment in the profile that is dissected.

Now, using the recursion relation, we find, for the k^{th} shock to the left,

$$\begin{aligned}
 \nu_{-k} &= \eta^k \nu_0 + [(1 - \eta)b - \sigma] \sum_{j=0}^{k-1} \eta^j \\
 &= \eta^k \nu_0 + [(1 - \eta)b - \sigma] \frac{1 - \eta^k}{1 - \eta}
 \end{aligned} \tag{3.32}$$

and using Eq. 3.31,

$$\begin{aligned}
 \nu_{-k} &= \eta^k \nu_0 + (\nu_0 - 2a) (1 - \eta^k) \\
 &= \nu_0 - 2a (1 - \eta^k) .
 \end{aligned} \tag{3.33}$$

An interesting consequence of this equation is that, if the number of shocks is large,

then the 0^{th} nodes in each period become an accumulation point of nodes immediately to the right of them.

Having found the nodes of the steady state profile, our next task is to calculate the position of the shock fronts.

3.6.3. Recursion Relation for Shock Fronts in the Steady State

In finding the positions of the ν 's of the steady state profile, we based our calculations upon the fact that the steady state profile at each evolution step is invariant up to a constant shift in the 1-periodic case. A similar approach will be employed to find the corresponding shock positions $\xi_i^{(n)}$, *i.e.* the position of shock i right at the beginning of the n^{th} evolution.

At any evolution step, a new shock is inserted initially, and a pair collides during the Burgers evolution, so as to leave the overall number of shocks unchanged. In the labelling scheme we employed before, the newly-introduced shock of an evolution step gets to be labelled with -1 . The pair of shocks that collide turn out to be shocks $-\kappa$ and $(-\kappa - 1)$ owing to the simplicity of the 1-periodic case. Recall from Fig. 3.10, that node $-\kappa$ disappears during the evolution, meaning that shock $-\kappa$ is absorbed by the one on its left. The remaining shocks, *i.e.* the shocks labelled from -1 to $(-\kappa + 1)$ start out from their respective positions $\xi_{-k}^{(n)}$ and drift with their corresponding speeds s_{-k} for a duration $\tau = \frac{1}{k_o}$. Due to the imposed 1-periodicity of the steady state, each shock must end up in the position of the $(-k - 1)^{st}$ shock of the next step of evolution. That is,

$$\xi_{-k-1}^{(n+1)} = \xi_{-k}^{(n)} + s_{-k}^{(n)}\tau \quad , \quad k = 1, 2, \dots, -\kappa + 1 \quad . \quad (3.34)$$

But in our labelling scheme, shocks with the same index are of the same identity, they just belong to different steps in the growth of the chain. Since the only difference between two steps is a shift, speeds and intensities are not affected. Here, s_{-k} does not have to carry a superscript for this reason.

Due to the shift between the successive profiles we can say that,

$$\xi_{-k-1}^{(n+1)} = \xi_{-k-1}^{(n)} + \sigma \quad (3.35)$$

thus yielding for $\xi_{-k-1}^{(n)}$,

$$\xi_{-k-1}^{(n)} = \xi_{-k}^{(n)} + s_{-k}\tau - \sigma \quad . \quad (3.36)$$

We drop again the superscripts, provided we are careful not to disregard the n dependence of b .

From our previous discussion on Burgers evolution of these profiles, we know that,

$$s_{-k} = \lambda \left(\xi_{-k} - \frac{\nu_{-k} + \nu_{-k+1}}{2} \right) \quad . \quad (3.37)$$

Incorporating this relation into Eq. 3.36 with the steady state value λ^* for the potential strength, we get,

$$\begin{aligned} \xi_{-k-1} &= (1 + \tau\lambda^*)\xi_{-k} - \tau\lambda^* \frac{\nu_{-k} + \nu_{-k+1}}{2} - \sigma \\ &= \frac{\xi_{-k}}{\eta} - \frac{1-\eta}{\eta} \frac{\nu_{-k} + \nu_{-k+1}}{2} \quad . \end{aligned} \quad (3.38)$$

Referring to Eq. 3.33 for the ν_{-k} 's we can write this expression in terms of ν_0 . However, the expression for ξ_{-k-1} simplifies when ν_0 is expressed in terms of ξ_{-1} . This is easily carried out, because both are related via b . First, one should realize that b in Eq. 3.31 belongs to the n^{th} particle, whereas ξ_{-1} of the n^{th} evolution step is due to the $(n-1)^{st}$ particle. Thus,

$$\xi_{-1} = b + a - \sigma. \quad (3.39)$$

Now, Eq. 3.31 must be invoked to write ν_0 in terms of b , and then in terms of ξ_{-1}

through Eq. 3.39, which yields,

$$\nu_0 = \xi_{-1} + a - \sigma \frac{\eta}{1 - \eta} \quad (3.40)$$

where all quantities refer to the n^{th} evolution step.

Turning back to Eq. 3.38, exploiting Eqs. 3.33 and 3.40 in that order, upon simplification we have,

$$\begin{aligned} \xi_{-k-1} &= \frac{\xi_{-k}}{\eta} - \frac{1 - \eta}{\eta} [\nu_0 - 2a + a\eta^{k-1}(1 + \eta)] - \sigma \\ &= \frac{\xi_{-k}}{\eta} - \frac{1 - \eta}{\eta} [(\xi_{-1} - a) + a\eta^{k-1}(1 + \eta)] \end{aligned} \quad (3.41)$$

The absence of σ in this equation should not be surprising, since all the information about the shift in steady state is absorbed in ξ_{-1} .

Now, the relation of Eq. 3.41 can be recursed k times in order to express ξ_{-k-1} in terms of ξ_{-1} only,

$$\xi_{-k-1} = \xi_{-1} - a(1 - \eta^k) \quad , \quad k = 1, 2, \dots, \kappa - 1 \quad . \quad (3.42)$$

Eqs. 3.31 and 3.33 determined all the ν 's at a given evolution step. By virtue of Eqs. 3.39 and 3.42 we also know all the shock positions except for shock 0. However, we have one more constraint which we now use to obtain ξ_0 , given the remaining profile parameters, *i.e.* the ξ 's and ν 's.

The area under the profile at any instant has to be zero, since Burgers' equation is the conservation law regarding the velocity field, and the ramps that are constantly being added have zero area beneath them. The corresponding constraint equation in

terms of the profile parameters is (refer to Appendix C for its derivation),

$$\sum_{i=-\kappa}^0 \xi_i (\nu_{i+1} - \nu_i) = 2a (a + \nu_{-\kappa}) \quad (3.43)$$

with the summation limits adapted to the labelling scheme we employed for this case. Turning this equation around to obtain an expression for ξ_0 we get,

$$\xi_0 = \frac{2a (a + \nu_{-\kappa})}{\nu_1 - \nu_0} - \frac{1}{\nu_1 - \nu_0} \sum_{i=-\kappa}^{-1} \xi_i (\nu_{i+1} - \nu_i) \quad (3.44)$$

where

$$\nu_1 = \nu_{-\kappa} + 2a \quad .$$

Now, Eqs. 3.33 and 3.42, plus Eq. 3.40 can be invoked to express the ν 's and ξ 's in Eq. 3.44, to finally obtain,

$$\xi_0 = \xi_{-1} + \frac{1}{\eta^{\kappa-1}} \left[a \frac{(1 + \eta^{\kappa-1})(1 + \eta^{\kappa})}{1 + \eta} - \sigma \frac{1}{1 - \eta} \right] \quad . \quad (3.45)$$

We finally have the complete information to calculate the effective potential seen from one end of a very long chain. We are in a position to find out the mapping that will provide us with the positions of the particles in the ground state. But before going on to the discussion about the ground state configuration, we have a few more remarks to make.

3.6.4. Remarks on Shock Count and the Phase Boundary

Throughout all these arguments, we assumed some number κ of shocks in the steady state profile. This number is expected to depend on the potential strength λ_0 and the spring length μ , but we have not shown yet how the dependence comes about. We are going to turn to this matter now.

We pointed out earlier that, at each evolution, shocks $(-\kappa - 1)$ and $-\kappa$ collide. Each evolution lasts for a time τ , and the collision takes place during this time. When the parameters λ_0 and μ are adjusted such that the pair has barely enough time to collide, the steady state profile still has κ shocks, but this is some kind of boundary. When λ is chosen just a little smaller or μ just a little larger beyond this point, the steady state profile is not one with κ shocks anymore, but one with $\kappa + 1$. The steady state is on the boundary of a domain of κ shocks and $\kappa + 1$ shocks, so to speak. The condition that the steady state is inside a domain of κ shocks is that the required collision time is smaller than τ , and greater than zero, of course. Since the collision takes place between shocks $(-\kappa - 1)$ and $-\kappa$, the mathematical expression is,

$$0 < \frac{\xi_{-\kappa-1} - \xi_{-\kappa}}{s_{-\kappa} - s_{-\kappa-1}} < \tau \quad . \quad (3.46)$$

Substituting,

$$s_i = \lambda^* \left[\xi_i - \frac{\nu_i + \nu_{i+1}}{2} \right]$$

for the shock speeds, we arrive at the condition,

$$0 < \frac{\xi_{-\kappa-1} - \xi_{-\kappa}}{-(\xi_{-\kappa-1} - \xi_{-\kappa}) + \frac{\nu_{-\kappa-1} - \nu_{-\kappa+1}}{2}} < \tau \lambda^* \quad . \quad (3.47)$$

We have previously derived all the formulae required to substitute for the quantities appearing here. After substituting for the ξ 's and ν 's from Eqs. 3.33 and 3.42, we find

$$0 < \frac{a\eta^{2\kappa-2}(1-\eta^2)}{a(1-\eta)(1+\eta^{2\kappa-1}) - \sigma(1+\eta)} - 1 < \frac{1-\eta}{\eta} \quad , \quad (3.48)$$

which is equivalent to,

$$a \frac{1-\eta}{1+\eta} (1 - \eta^{2\kappa-2}) < \sigma < a \frac{1-\eta}{1+\eta} (1 - \eta^{2\kappa}) \quad . \quad (3.49)$$

This equation determines the interval of possible values for μ , given the number of

shocks and λ_o , since $\eta = \eta(\lambda_o)$ and $\mu = \mu(\sigma)$. It can also be turned around to give the number of shocks in the steady state, given λ_o and μ . Rearranging terms, we obtain,

$$\eta^{2(\kappa-1)} > \frac{\sigma(1+\eta)}{a(1-\eta)} - 1 > \eta^{2\kappa} \quad . \quad (3.50)$$

Now we exploit the fact that logarithm to base η is a monotonically decreasing function when $\eta < 1$ to get,

$$\kappa - 1 < \frac{1}{2} \log_{\eta} \left(\frac{\sigma(1+\eta)}{a(1-\eta)} - 1 \right) < \kappa \quad . \quad (3.51)$$

Thus, the number of shocks follows,

$$\kappa = \text{Int} \left[\frac{1}{2} \log_{\eta} \left(\frac{\sigma(1+\eta)}{a(1-\eta)} - 1 \right) \right] + 1 \quad . \quad (3.52)$$

Eqs. 3.46 to 3.49 are all equivalent, and they correspond to the condition that a collision takes place, *i.e.* a 1-periodic steady state is attainable. Focusing on Eq. 3.49 is more convenient for the following argument. Since $\eta < 1$, there always exists an interval of σ values that satisfy Eq. 3.49, no matter what the number of shocks is. Therefore a 1-periodic steady state ought to be attainable for all κ . Hence, as $\kappa \rightarrow \infty$, Eq. 3.49 defines the phase boundary for a given η . With σ_c standing for this critical value of σ ,

$$\sigma_c = a \frac{1-\eta}{1+\eta} \quad . \quad (3.53)$$

We find that the phase boundary of the 1-periodic solutions coincides with Aubry's formula for step widths, Eq. 2.22, with $s = 1$.

3.6.5. Justification of the Assumed Collision Sequence

Owing to the simplicity of the situation, we were able to convince ourselves that the pair of shocks that collide during each evolution are the shocks $-\kappa$ and $(-\kappa - 1)$.

We will now show that this is really the case.

The time required by shocks $-\kappa$ and $(-\kappa - 1)$ to collide was already found in Eq. 3.48 and the constraint that a collision must actually take place within a time interval τ was imposed in order to find the condition on μ . Similarly, we can write the collision times for the other shock pairs and see if they really do not have enough time to collide.

Representing the collision time between shocks $-k$ and $-k + 1$ by t_{-k}^{-k+1} ,

$$t_{-k}^{-k+1} = \frac{1}{\lambda^*} \frac{\xi_{-k} - \xi_{-k+1}}{-\xi_{-k} + \xi_{-k+1} + \frac{\nu_{-k} - \nu_{-k+2}}{2}}$$

following similar arguments as before for the pair that actually collides. But now k ranges from $-\kappa$ to -2 (we disregard the time required for shock -1 to collide with shock 0 , since they are actually moving away from each other). The expressions for $\xi_{-k} - \xi_{-k+1}$ and $\nu_{-k} - \nu_{-k+2}$ can be found from Eqs. 3.33 and 3.42 as,

$$\xi_{-k} - \xi_{-k+1} = a\eta^{k-2}(\eta - 1)$$

and,

$$\nu_{-k} - \nu_{-k+2} = 2a\eta^{k-2}(\eta^2 - 1) \quad .$$

Putting these into the expression for t_{-k}^{-k+1} , and substituting for λ^* in terms of η we find,

$$\begin{aligned} t_{-k}^{-k+1} &= \tau \frac{\eta}{1 - \eta} \frac{a\eta^{k-2}(\eta - 1)}{a\eta^{k-2}(1 - \eta + \eta^2 - 1)} \\ &= \frac{\tau}{1 - \eta} \quad . \end{aligned}$$

Since $\eta < 1$, the time required for the other pairs to collide is larger than the duration of each evolution τ . Thus, we are justified in not expecting them to collide. Moreover,

these times do not depend on the particular pair that is to collide.

3.6.6. The Ground State Configuration of the Chain

We argued in Section 2.3 that the velocity field associated with particle n , just before the addition of that particle, is found by Burgers evolution of the velocity field right after the addition of the $(n-1)^{st}$ particle. Associated with this evolution, there is a characteristic equation (Eq. 2.80) that relates the position of particles n and $(n-1)$. Therefore the velocity field just before the addition of the n^{th} particle determines the position of particle $(n-1)$ as a function of the position of particle n . For the case of scalloped potentials, the mapping is found as follows.

Every point x_n on the velocity field $\mathcal{U}^{(n)}(x_n, \tau)$ just before the addition of the n^{th} particle is the result of the propagation of one or many points (if x_n is on a shock) on the initial velocity field $\mathcal{U}^{(n)}(x_{n-1}, 0)$ right after the addition of the $(n-1)^{st}$ particle.⁷ That is,

$$x_n = x_{n-1} + \tau \mathcal{U}^{(n)}(x_{n-1}, 0) \quad . \quad (3.54)$$

In the case of a shock train as the velocity field, one must consider Eq. 3.54 segment by segment. Recall that, the nodes of a shock train either disappear or stay stationary under Burgers evolution. Therefore, a point x_{n-1} on one segment of the initial shock train is still on the same segment of the evolved profile if that segment does not disappear due to a collision during the evolution. Then, Eq. 3.54 can be rewritten in terms of line segments as,

$$x_n = x_{n-1} + \tau \lambda^* \left(x_{n-1} - \nu_{i+1}^{(n)} \right) \quad , \quad \xi_i^{(n)}(\tau) < x_n < \xi_{i+1}^{(n)}(\tau) \quad . \quad (3.55)$$

where the regions that this equation holds, are bounded by the shocks positions *at the end* of the n^{th} evolution. Written in terms of the parameter η , Eq. 3.55 determines the

⁷Note that, due to the coordinate transformation defined in Eq. 2.63, at $t = 0$, $x_n = x_{n-1}$.

mapping between x_n and x_{n-1} as,

$$x_{n-1} = \eta x_n + (1 - \eta) \nu_{i+1}^{(n)} \quad , \quad \xi_i^{(n)}(\tau) < x_n < \xi_{i+1}^{(n)}(\tau) \quad , \quad (3.56)$$

Note that this equation only applies for the segments that do not disappear until the end of the evolution. Indeed, the segments that disappear contain the points that are absorbed in the shocks, which are of no value for the mapping. We know that for our case, the segment to disappear is the $-\kappa^{th}$, corresponding to the interval

$$\xi_{-\kappa-2}^{(n)}(\tau) < x_n < \xi_{-\kappa-1}^{(n)}(\tau) \quad . \quad (3.57)$$

Therefore, in Eq. 3.56, i ranges from $-\kappa$ to -2 , and the mapping governed by $\nu_{-\kappa-1}^{(n)}$ should be given explicitly as,⁸

$$x_{n-1} = \eta x_n + (1 - \eta) \nu_{-\kappa-1}^{(n)} \quad , \quad \xi_{-\kappa-2}^{(n)}(\tau) < x_n < \xi_{-\kappa}^{(n)}(\tau) \quad . \quad (3.58)$$

For convenience, we will combine Eqs. 3.56 and 3.58:

$$x_{n-1} = \begin{cases} \eta x_n + (1 - \eta) \nu_{i+1}^{(n)} & , \quad \xi_i^{(n)}(\tau) < x_n < \xi_{i+1}^{(n)}(\tau) \quad , \quad i = -\kappa, \dots, -2 \\ \eta x_n + (1 - \eta) \nu_{-\kappa-1}^{(n)} & , \quad \xi_{-\kappa-2}^{(n)}(\tau) < x_n < \xi_{-\kappa}^{(n)}(\tau) \end{cases} \quad (3.59)$$

Since we can calculate the profile parameters *at the beginning* of each evolution through our recursion formulae, we must write the intervals in Eq. 3.59 in terms of the ξ 's at the beginning of the evolution. Due to the overall shift of the steady state profiles, we immediately have that,

$$\xi_i^{(n)}(\tau) = \xi_{i-1}^{(n+1)} = \xi_{i-1}^{(n)} + \sigma \quad ,$$

⁸We chose to consider $\nu_{-\kappa-1}$ instead of ν_0 , which actually correspond to the same segment of the mapping due to the periodicity of the effective potential, for the sake of clarity of the discussion that follows.

so that the intervals become,

$$\xi_{left}^{(n)} < x_n - \sigma < \xi_{right}^{(n)} \quad . \quad (3.60)$$

With the new expression for the intervals, we rewrite Eq. 3.59:

$$x_{n-1} = \begin{cases} \eta x_n + (1 - \eta)\nu_{i+1} & , \quad \xi_{i-1} < x_n - \sigma < \xi_i & , \quad i = -\kappa, \dots, -2 \\ \eta x_n + (1 - \eta)\nu_{-\kappa-1} & , \quad \xi_{-\kappa-3} < x_n - \sigma < \xi_{-\kappa-1} \end{cases} \quad (3.61)$$

where we again dropped the superscripts because all profile parameters refer to the beginning of the n^{th} evolution as they should.

Earlier, we argued that the velocity field reaches a stable steady state. Therefore we also expect that this mapping will have a stable fixed point, thereby yielding the ground state configuration of the chain when it is iterated a large number of times.

Recall that the velocity field reaches a steady state with an overall drift in the Burgers frame. This means that if we were to look for a fixed point of the mapping in this frame, we would end up with a fixed *line* instead. In order to compensate for this drift, we define a new coordinate system as,

$$\hat{x}_n \equiv x_n - n\sigma \quad . \quad (3.62)$$

Note that, if $\hat{x}_n$ is written in terms of absolute coordinates using the transformation Eq. 2.63,

$$\hat{x}_n = u_n - n(\mu + \sigma) = u_n - 2an \quad , \quad (3.63)$$

meaning that the new coordinate frame moves by one potential well for each particle. Hence, we will call these coordinates by the name *well coordinates*.

Keeping in mind that the profile parameters at the beginning of the n^{th} evolution refer to the time that the $(n-1)^{st}$ particle is added, they transform to the well coordinates as,

$$\begin{aligned}\hat{\xi}_i^{(n)} &= \xi_i^{(n)} - (n-1)\sigma \\ \hat{\nu}_i^{(n)} &= \nu_i^{(n)} - (n-1)\sigma \quad .\end{aligned}$$

Using these relations, Eq. 3.61 can be transformed into the well coordinates as,

$$\hat{x}_{n-1} = \begin{cases} \eta \hat{x}_n + (1-\eta)\hat{\nu}_{i+1} + \eta\sigma & , \quad \hat{\xi}_{i-1} < \hat{x}_n < \hat{\xi}_i \\ \eta \hat{x}_n + (1-\eta)\hat{\nu}_{-\kappa-1} + \eta\sigma & , \quad \hat{\xi}_{-\kappa-3} < \hat{x}_n < \hat{\xi}_{-\kappa-1} \end{cases} \quad , \quad i = -\kappa, \dots, -2 \quad (3.64)$$

We need to invoke the relations that yield the profile parameters in order to calculate the mapping. The recursion relations for ν 's and ξ 's, Eqs. 3.33 and 3.42, are linear transformations with unit slope, therefore they are invariant under the transformation to the new coordinates. The remaining relations, Eqs. 3.31, 3.39 and 3.45, depend only on b , so their transformation is also trivial. According to Eq. 3.63 however, we can make use of the new coordinates to choose our axes such that

$$\hat{b} = 0 \quad .$$

With this condition, the complete set of relations we need become:

$$\hat{\nu}_{-k} = -\sigma \frac{\eta}{1-\eta} + 2a\eta^k \quad , \quad k = 0, 1, 2, \dots, \kappa \quad (3.65)$$

$$\hat{\xi}_{-k} = a\eta^{k-1} \quad , \quad k = 1, 2, \dots, \kappa \quad (3.66)$$

$$\hat{\xi}_{-\kappa-1} = \hat{\xi}_0 - 2a = a \frac{1 + \eta^{2\kappa-1}}{\eta^{\kappa-1}(1+\eta)} - \sigma \frac{1}{\eta^{\kappa-1}(1-\eta)} \quad . \quad (3.67)$$

Using Eq. 3.65, the mapping Eq. 3.64 can be rewritten as,

$$\hat{x}_{n-1} = \begin{cases} \eta \hat{x}_n + 2a(1-\eta)\eta^{k-1} & , \quad \hat{\xi}_{-k-1} < \hat{x}_n < \hat{\xi}_{-k} \quad , \quad k = 2, \dots, \kappa \\ \eta \hat{x}_n & , \quad \hat{\xi}_{-\kappa-3} < \hat{x}_n < \hat{\xi}_{-\kappa-1} \quad . \end{cases} \quad (3.68)$$

It is clear that, in this coordinate system, $\hat{\xi}_{-k}$ given by Eq. 3.66 are all to the right of zero, *i.e.* $\hat{b}$. As for $\hat{\xi}_{-\kappa-1}$, the case is not that obvious. Observe that, when σ has its largest possible value, $\hat{\xi}_{-\kappa-1}$ is the farthest to the left it can be. We have already found the largest value σ can have in Eq. 3.49. Substituting this value for σ in Eq. 3.67 we find that,

$$\hat{\xi}_{-\kappa-1}^{min} = a \frac{\eta^\kappa}{1+\eta} \quad ,$$

which is clearly larger than zero. Example shock locations for a case $\kappa = 5$ are depicted in Fig.3.11.

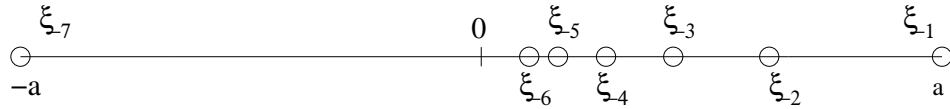


Figure 3.11. Shock locations in a coordinate system with $\hat{b} = 0$ for a case $\kappa = 5$.

We look for a fixed point of the mapping next. The fixed point equations for each interval are found from Eq. 3.68 as,

$$\begin{aligned} \hat{x}^{*(k)} &= 2a\eta^{k-1} \quad , \quad \hat{\xi}_{-k-1} < \hat{x}_n < \hat{\xi}_{-k} \quad , \quad k = 2, \dots, \kappa \\ \hat{x}^{*(0)} &= 0 \quad , \quad \hat{\xi}_{-\kappa-3} < \hat{x}_n < \hat{\xi}_{-\kappa-1} \end{aligned} \quad (3.69)$$

Only one of the fixed points given by Eqs. 3.69 actually lie on the interval that its corresponding interval maps to. Intervals,

$$\hat{\xi}_{-k-1} < \hat{x}_n < \hat{\xi}_{-k} \quad , \quad k = 2, \dots, \kappa$$

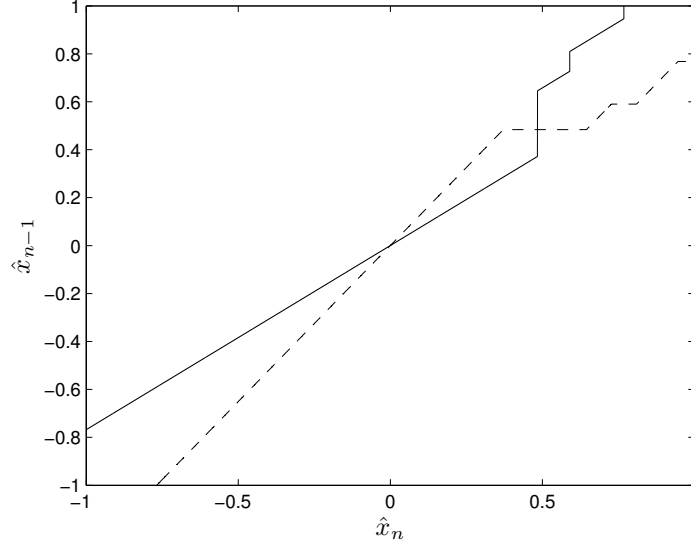


Figure 3.12. Numerically calculated mapping for a case with $\mu = 1.9$ and $\lambda_o = 0.07$. Dashed lines represent the mapping regarding the next pair of particles, with the axes swapped, so that the fixed point can be observed geometrically.

map to regions,

$$\hat{x}_{n-1}(\hat{\xi}_{-k-1}) < \hat{x}_{n-1} < \hat{x}_{n-1}(\hat{\xi}_{-k}) \quad , \quad k = 2, \dots, \kappa \quad .$$

We find the boundaries of these regions using Eq. 3.66 as,

$$\begin{aligned} \hat{x}_{n-1}(\hat{\xi}_{-k-1}) &= a\eta^{k-1}(\eta^2 - 2\eta + 2) \\ \hat{x}_{n-1}(\hat{\xi}_{-k}) &= a\eta^{k-1}(-\eta + 2) \quad . \end{aligned}$$

Recalling that $\eta < 1$ we have the inequality,

$$\hat{x}_{n-1}(\hat{\xi}_{-k-1}) < \hat{x}_{n-1}(\hat{\xi}_{-k}) < \hat{x}^{*(k)} \quad , \quad k = 2, \dots, \kappa \quad .$$

Therefore, only $\hat{x}^* = 0$ qualifies as a fixed point of the map⁹. Fig. 3.12 shows the numerically calculated mapping for a case with $\mu = 1.9$ and $\lambda_o = 0.07$. The fixed point of the map being 0 in the well coordinates means that, at whatever location

⁹Due to periodicity, all $\hat{x}^* = 2am$, $\hat{\xi}_{(m-1)\kappa-3} < \hat{x}^* < \hat{\xi}_{(m-1)\kappa-1}$ with integer m qualify as fixed points.

the end of the chain is, particles deeper in the chain sit right at the bottom of wells (see Fig. 3.13). Hence the ground state configuration for such a system is one where particles are located at well troughs, $2a$ apart, although μ is not exactly $2a$.

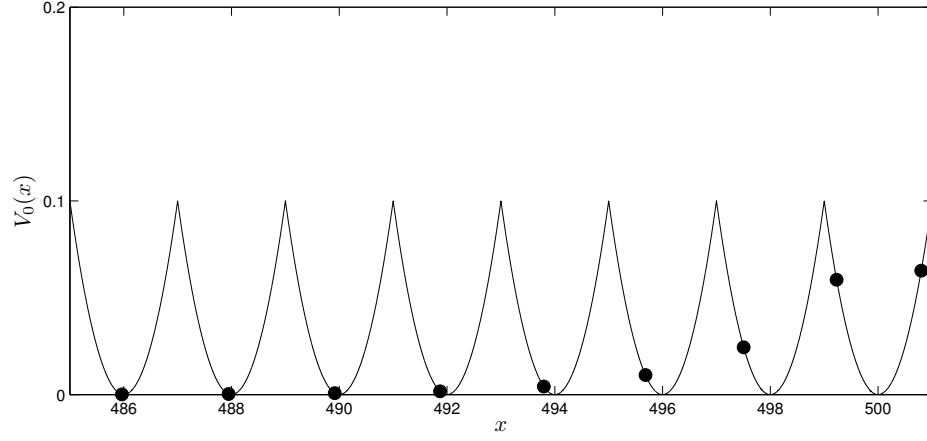


Figure 3.13. Configuration of particles in the ground state, generated by iteratively mapping starting from the rightmost particle.

4. CONCLUSION

We investigated the ground state configuration of a FK chain immersed in a scalloped potential, using the method of effective potentials. However we introduced a novel method of approach for the solution of the effective potentials. We were able to describe the evolution of the effective potential with respect to a continuous time parameter, corresponding to the growing chain length. This description reveals a deeper structure lying underneath the evolution of the effective potential, which will allow an analytical approach to determine the long-chain (steady state) behaviour of the effective potential, and hence the ground state configuration of particles.

We showed that with the lowest energy requirement, the derivative of the effective potential can be treated as a velocity field evolving according to Burgers' equation, where *time* is the reciprocal of the spring constant. This description allows a deeper understanding of how the effective potential evolves, as opposed to the method as proposed by Griffiths and Chou, where the effective potential evolves in discrete steps. By virtue of this continuous time description, the steady state behaviour of the effective potential is likely to be determined analytically, whereas the method of Griffiths and Chou is mostly numerical.

With the extension to the method of effective potentials, we investigated the steady state solution in the case of a scalloped potential, where the associated velocity fields are shock trains. We were able to determine analytically the steady state velocity field associated with the effective potential, when the equilibrium spacing is close to the period of the external potential. This, in turn, allowed us to determine the ground state configuration of particles analytically, which yielded the expected configuration of particles. The analytical solution to the problem of finding the long-chain effective potential and the particle configuration with an arbitrary spring length still remains unsolved.

However, in the last chapter we illustrated that the collision sequence in the evolution of the shock trains is subject to drastic change if the spring length is not within some bounds, giving rise to a phase transition that is verified by Aubry's exact results. We have reason to believe that more careful study of the shock dynamics will allow us to predict the steady state behaviour of the effective potential analytically, with an arbitrary value of the spring length.

If the evolution duration is large, an arbitrary velocity field will attain the shape of a shock train gradually. In other words, when the elastic interaction is relatively weaker than the potential strength, an arbitrary potential will effectively become a scalloped potential. Therefore the method has potential to be extended by a perturbation approach to cover a variety of external potentials other than scalloped potentials.

APPENDIX A: SOLUTION OF THE EXACT FORCE EQUILIBRIUM EQUATION USING FOURIER TRANSFORMS

The difference equation to solve is the force equilibrium equation, Eq. 2.4 of the exact solution:

$$(\lambda_o + 2k_o) u_i - k_o u_{i+1} - k_o u_{i-1} = 2m_i a \lambda_o \quad . \quad (\text{A.1})$$

Transforming Eq. A.1 to the dual variable Ω by the transformation

$$\mathcal{F}(\Omega) = \sum_n f_n e^{-i\Omega n} \quad ,$$

we find that

$$(\lambda_o + 2k_o) \mathcal{U}(\Omega) - k_o e^{i\Omega} \mathcal{U}(\Omega) - k_o e^{-i\Omega} \mathcal{U}(\Omega) = 2a \lambda_o \mathcal{M}(\Omega) \quad , \quad (\text{A.2})$$

which yields for $\mathcal{U}(\Omega)$,

$$\mathcal{U}(\Omega) = \mathcal{T}(\Omega) \mathcal{M}(\Omega) \quad (\text{A.3})$$

where

$$\mathcal{T}(\Omega) = \frac{2a \lambda_o}{\lambda_o + 2k_o - 2k_o \cos \Omega} \quad , \quad (\text{A.4})$$

so that u_i is given by the convolution

$$u_i = \sum_{n=-\infty}^{\infty} t_n m_{i-n} \quad , \quad (\text{A.5})$$

where t_n is the inverse fourier transform of $\mathcal{T}(\Omega)$.

We now note that $\mathcal{T}(\Omega)$ given by Eq. A.4 has the form of the Fourier transform of a discrete exponential function,

$$f_n = \eta^{|n|} \quad , \quad 0 < \eta < 1 \quad (\text{A.6})$$

whose Fourier transform is given as [17],

$$\mathcal{F}(\Omega) = \frac{1 - \eta^2}{1 + \eta^2 - 2\eta \cos \Omega} \quad . \quad (\text{A.7})$$

Hence, we conclude that the sequence t_n must also have a discrete exponential form as,

$$t_n = A\eta^{|n|} \quad . \quad (\text{A.8})$$

The constants η and A will be found by equating the right hand sides of Eqs. A.4 and A.7 which yields, after rearranging terms,

$$\left[A(1 - \eta^2)(\lambda_o + 2k_o) - 2a\lambda_o(1 + \eta^2) \right] + \left[4a\lambda_o\eta - 2Ak_o(1 - \eta^2) \right] \cos \Omega = 0 \quad . \quad (\text{A.9})$$

Since Eq. A.9 must hold for all Ω , the expressions inside square brackets must vanish identically, yielding the two equations:

$$\frac{A}{2a\lambda_o} = \frac{1 + \eta^2}{(1 - \eta^2)(\lambda_o + 2k_o)} \quad (\text{A.10})$$

$$\frac{A}{2a\lambda_o} = \frac{\eta}{k_o(1 - \eta^2)} \quad . \quad (\text{A.11})$$

The quadratic equation that η has to satisfy, keeping in mind that η is strictly smaller than one by definition (Eq. A.6), is immediately found by equating the right hand sides of Eqs. A.10 and A.11 as,

$$\eta^2 - \left(\frac{\lambda_o}{k_o} + 2 \right) + 1 = 0 \quad (\text{A.12})$$

with the solution,

$$\eta = 1 + \frac{1}{2} \frac{\lambda_{\circ}}{k_{\circ}} - \frac{1}{2} \frac{\lambda_{\circ}}{k_{\circ}} \sqrt{1 + 4 \frac{k_{\circ}}{\lambda_{\circ}}} \quad . \quad (\text{A.13})$$

Note that Eq. A.12 can be manipulated algebraically to yield a result that we will shortly use:

$$\frac{\lambda_{\circ}}{k_{\circ}} = \frac{(1 - \eta)^2}{\eta} \quad . \quad (\text{A.14})$$

The constant A can be found easily using Eq. A.11 as,

$$A = \frac{2a\lambda_{\circ}\eta}{k_{\circ}(1 - \eta^2)} \quad (\text{A.15})$$

which can then be simplified using Eq. A.14 to yield,

$$A = 2a \frac{1 - \eta}{1 + \eta} \quad . \quad (\text{A.16})$$

Finally, with the values computed for A and η , the solution to the difference equation Eq. A.1 follows:

$$u_i = A \sum_{n=-\infty}^{\infty} \eta^{|n|} m_{n+i} \quad (\text{A.17})$$

where we made use of the fact that

$$f_n = f_{-n}$$

by Eq. A.6.

APPENDIX B: THE COLE-HOPF TRANSFORMATION

Recall that we claimed that the diffusion equation, Eq. 2.61 of Section 2.3.2 reduced to the Burgers' equation with the Cole-Hopf transformation. We will rigorously derive the Burgers' equation from the diffusion equation in this appendix.

Consider the diffusion equation,

$$\psi_t = \frac{1}{2\beta} \psi_{xx} \quad (\text{B.1})$$

where subscripts denote differentiation with respect to the associated variable. Now define two functions, $\epsilon(x, t)$ and $v(x, t)$ as,

$$\epsilon(x, t) = \frac{1}{\beta} \log \psi(x, t) \quad (\text{B.2})$$

$$v(x, t) = \epsilon_x(x, t) \quad (\text{B.3})$$

We will need the derivatives of ψ with respect to t and x in order to write Eq. B.1 in terms of v . The derivatives can easily be found in terms of ϵ as,

$$\psi_t = -\beta \epsilon_t e^{-\beta \epsilon} \quad (\text{B.4})$$

$$\psi_x = -\beta \epsilon_x e^{-\beta \epsilon} \quad (\text{B.5})$$

$$\psi_{xx} = (-\beta \epsilon_{xx} + \beta^2 \epsilon_x^2) e^{-\beta \epsilon} \quad (\text{B.6})$$

Using these derivatives, Eq. B.1 becomes,

$$\epsilon_t + \frac{\epsilon_x^2}{2} = \frac{\epsilon_{xx}}{2\beta} \quad (\text{B.7})$$

Differentiating Eq. B.7 with respect to x yields,

$$\epsilon_{xt} + \epsilon_x \epsilon_{xx} = \frac{\epsilon_{xxx}}{2\beta} \quad (\text{B.8})$$

Using the definition Eq. B.3 of v , we finally obtain the general form of Burgers' equation:

$$v_t + vv_x = \frac{v_{xx}}{2\beta} \quad . \quad (\text{B.9})$$

APPENDIX C: AREA CONSERVATION OF SHOCK TRAINS

Recall that Burgers evolution preserves the area under the velocity field. Since the velocity field associated with the scalloped potential is a series of ramps with zero area, the shock trains that appear in the discussion of the evolution of effective potentials also have zero area beneath them at all times.

The area under each segment i of a shock train with n shocks is a trapezoid with area:

$$\frac{v(\xi_i^-) + v(\xi_{i-1}^+)}{2}(\xi_i - \xi_{i-1}) \quad , \quad (\text{C.1})$$

so the area under the profile is equal to zero as,

$$0 = \sum_{i=1}^n \frac{v(\xi_i^-) + v(\xi_{i-1}^+)}{2}(\xi_i - \xi_{i-1}) \quad . \quad (\text{C.2})$$

The value of the velocity field at the edges of a segment, namely $v(\xi_i^-)$ and $v(\xi_i^+)$ are readily found as,

$$\begin{aligned} v(\xi_i^-) &= \lambda(\xi_i - \nu_{i-1}) \\ v(\xi_i^+) &= \lambda(\xi_i - \nu_i) \quad . \end{aligned} \quad (\text{C.3})$$

Using Eqs. C, the area condition in Eq. C.2 can be rewritten as,

$$\begin{aligned} 0 &= \sum_{i=1}^n \frac{\lambda}{2} (\xi_i + \xi_{i-1} - 2\nu_i) (\xi_i - \xi_{i-1}) \\ &= \sum_{i=1}^n (\xi_i^2 - \xi_{i-1}^2) - 2 \sum_{i=1}^n \nu_i (\xi_i - \xi_{i-1}) \\ &= \xi_n^2 - \xi_0^2 - 2 \sum_{i=1}^n (\nu_i \xi_i - \nu_i \xi_{i-1}) \quad . \end{aligned} \quad (\text{C.4})$$

Because of periodicity, the profile parameters have the property that,

$$\begin{aligned}\nu_{i+n} &= \nu_i + 2a \quad , \\ \xi_{i+n} &= \xi_i + 2a \quad .\end{aligned}\tag{C.5}$$

Exploiting this property to rewrite the ξ_0 's on the right hand side of Eq. C.4 both inside and outside the summation, and then grouping similar terms, we have

$$\sum_{i=1}^n \xi_i (\nu_{i+1} - \nu_i) = 2a(a + \nu_1) \quad ,\tag{C.6}$$

which is the area constraint on a shock train written in terms of the profile parameters.

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