Vertically extended Frenkel-Kontorova model: a real space renormalization group study

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A modification of the Frenkel-Kontorova model is presented in which particles are allowed to move in the vertical direction. This model is used to study the formation of islands for a monolayer of 1D interfaces and the corresponding roughness transition. Both analytical and numerical approaches are employed, and the numerical algorithm is based upon real space renormalization group techniques.

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I. INTRODUCTION

The Frenkel-Kontorova (FK) model\(^1\)\(^2\) was originally proposed by J. Frenkel and T. Kontorova in 1938 to study plastic deformations and twinning\(^3\). It was independently discovered by F.C. Frank and J.H. van der Merwe in 1949 to study 1D dislocations\(^4\). A rigid substrate is modelled by a sinusoidal potential, and film particles move within it making up a chain linked with harmonic springs of a given equilibrium length \(a_f\). The period of the sinusoidal potential is assumed to be \(a_s = 1\). Given the horizontal positions of the film particles \(\{x_i\}\), the system energy is

\[
E[x_i] = \sum_{i=1}^{N} J_s \cos(2\pi x_i) + \sum_{i=1}^{N-1} J_f (x_{i+1} - x_i - a_f)^2 \tag{1}
\]

At zero temperature this model presents a phase diagram in the variables \(J_f/J_s\) and \(a_f\) containing many tongues of commensurate phases separated by infinitesimal gaps of incommensurate structure\(^5\)\(^6\)\(^7\)\(^8\)\(^9\). These pathologies are removed at finite temperature\(^10\) but a continuous phase transition from a solid to a liquid-like structure remains with \(T_c > 0\).

The FK model has been extended both to finite-width stripes\(^11\) and truly 2D substrates\(^12\). More realistic interatomic potentials for the film interaction have been employed\(^13\), some of them with a phenomenological “temperature dependence” in order to study structural phase transitions\(^14\).

In this work the FK model is modified so as the film layer may curve, by allowing particles to displace vertically. Most methods of analysis of the classical FK model are not suitable in this case. Thus, we have resorted to a real space renormalization group (RG) numerical technique, inspired on the analysis of Griffiths and Chou\(^5\)\(^15\) and the Density Matrix Renormalization Group (DMRG) technique\(^16\). The extension of the DMRG concepts to a novel area of application may be of interest to practitioners.

Heteroepitaxial surface growth, i.e.: addition on a given crystalline substrate of particles of a different material with a given lattice mismatch, has attracted recently considerable technological interest\(^17\)\(^18\). When the lattice parameter is larger in the film than in the substrate, 3D islands may develop, making up quantum dots. There are three relevant growth modes: (a) Frank-van der Merwe (FvdM), consisting only of flat layers; (b) Stranski-Krastanov (SK), in which 3D islands grow on top of a flat wetting layer and (c) Volmer-Weber (VW), in which the 3D islands appear directly on the substrate.

Many theoretical models have been proposed, either within continuous elasticity theory\(^19\) and atomistic models\(^20\). We will focus on the semi-atomistic FK approach. It has been applied to study the mechanism of island formation both for 1D\(^21\) and 2D substrates with a realistic interatomic film potential\(^22\). For a given number of particles, if all monolayers cover completely the substrate, a FvdM growth mode is considered. If the particles are distributed in islands, leaving part of the substrate uncovered, a VW growth is assumed. Whenever a number of covering monolayers (i.e.: a wetting layer) appears with islands on top of them, the growth mode is SK. In these works, no vertical deformation of a layer is allowed: each island consists of a given number of completely flat layers. This assumption is questionable in the SK case for the reason exposed in the following paragraph.

Let \(a_s\) and \(a_f\) be the substrate and film equilibrium lattice parameters, with \(a_f > a_s\). Let us consider a wetting layer composed of flat monolayers with lattice parameters increasing upwards. The last monolayer, therefore, is less stressed than the first one. Thus, it is less likely to develop an islanding mechanism above it. The formation of a larger film surface has a certain energy cost, which would not have any counterpart. But this restriction disappears if all monolayers are allowed to bend. Consider a flat and a curved monolayer on the same substrate with the same number of atoms: the curved one must have larger atomic separation. Thus, the wetting layer height corresponds to the value where the extra energy needed to curve the film free surface is overcome by the reduction of the internal elastic energy provided by the effective stretching of all monolayers.

A first step in this direction is the analysis of the be-
haviour of a single monolayer of film which is allowed to curve. This single monolayer may provide a seed for the future formation of islands when more monolayers are deposited.

The rest of this article is organized as follows. Section II discusses the vertically extended FK model. Section III provides some analytical insight into the solutions. Section IV presents the RG-like technique we have employed to get the minimum energy states and section V discusses the numerical approach, along with the phase diagram for the model.

II. MODEL

The original FK model splits the energy for each configuration of the film particles into two parts: the interaction between each deposited film particle and the substrate is represented using a continuous sinusoidal substrate potential, and interaction between nearest-neighbor particles of the film is considered to be harmonic.

This splitting is preserved in our extension, but with some modifications. First, film particles are allowed to displace in the direction orthogonal to the substrate. These vertical displacements should be inhibited by an appropriate increase in the substrate potential energy. Thus, the sinusoidal substrate potential must be transformed into a realistic 1+1D potential. Also, the inter-particle film potential must be changed in accordance with the substrate in order to have the same long distance behaviour. A harmonic film potential is not realistic: when two neighbour film particles get sufficiently far away, the interaction should be negligible.

In our model the X axis shall be parallel to the substrate and the Z axis shall be orthogonal to it. Particle $i$ has coordinates $r_i = (x_i, z_i)$ and the configuration energy has the form:

$$E(\{r_i\}) = \sum_{i=1}^{N} V_s(r_i) + \sum_{i=1}^{N-1} V_f(|r_{i+1} - r_i|)$$

(2)

This model shall be referred to as Vertically Extended Frenkel-Kontorova (VEFK). Our target in this work is to find the ground states, i.e.: the global minimum energy configurations, and their properties.

A. Film potential

Anharmonic film potentials for the FK model have been studied for a long time. They must fulfill the following conditions: (a) as we get further away from the minimum, it should be harder to squeeze particles together than to separate them and (b) asymptotic freedom: particles should be free when their distance is large. There are many potentials fulfilling these conditions in the literature, and most details concerning them are irrelevant for the physics of our problem. We have chosen the Mie potential

$$V_f(d) = \frac{A_0}{\mu_f - v_f} \left[ \mu_f \left( \frac{a_f}{d} \right)^{\mu_f} - \mu_f \left( \frac{a_f}{d} \right)^{v_f} \right]$$

(3)

where $d \equiv |r_{i+1} - r_i|$ is the actual distance between neighbouring film particles, $a_f$ is their equilibrium distance, $A_0$ is a constant and $\mu_f > v_f$. In this work, $\mu_f = 12$ and $\nu_f = 6$, which correspond to a Lenard-Jones potential.

We define $K_f$ to be the spring constant of small oscillations around the equilibrium points of the film potential. In terms of $K_f$, we find $A_0 = K_f a_f^2 / \mu_f \nu_f$.

B. Substrate potential

The FK substrate potential is extended in the vertical (Z) direction in such a way that it reduces to its previous sinusoidal form when $z = z_{eq}$, a given equilibrium value. Away from it, the potential is modified so as it is energetically favourable to stay at the equilibrium height, but not compulsory. The equilibrium points of this potential must be arranged periodically at points $(x, z) = (na_s, z_{eq})$, where $n \in Z$ and $a_s$ is the substrate lattice parameter, which we shall assume to be $a_s = 1$ throughout this article.

The conditions on the height dependence of the substrate potential are similar to those for the film: (a) asymptotic freedom in the Z-axis, (b) very high barrier at the substrate height. We propose the following form

$$V_s(x, z) = \frac{B_0}{\mu_s - \nu_s} \left[ \nu_s \left( \frac{z_{eq}}{z} \right)^{\mu_s} - \mu_s \left( \frac{z_{eq}}{z} \right)^{\nu_s} \right] \frac{1}{2} \left( \cos \left( \frac{2\pi x}{a_s} \right) + 1 \right)$$

(4)

where $B_0$, $\mu_s$ and $\nu_s$ are constants. The +1 term by the cosine function makes the potential at $z = z_{eq}$ zero on average. For $z < z_{eq}$ this average value is positive, and it is negative, although tending to zero, for $z > z_{eq}$. This ensures that the ground state is always linked to the substrate. Figure 4 shows this potential for some typical values of the parameters. The potential may be seen to be large near the substrate and zero for large heights. There is an array of minima with their corresponding corridors, separated by potential barriers whose height decrease with $z$. The contour view, in the horizontal plane, depicts some ellipses whose centers correspond to these minima. We have chosen low values for the exponents: $\mu_s = 4$ and $\nu_s = 2$, so as to have deeper corridors and a clearer phase transition.

The substrate particles creating this potential are arranged at coordinate points $(x, z) = ((n + 1/2)a_s, 0)$, as is depicted in figure 2. From the figure it is obvious that $\theta_s = \arctan(2z_{eq}/a_s)$. 

This single monolayer may provide a seed for the future formation of islands when more monolayers are deposited.
Let us consider a film particle staying close to a minimum of the substrate potential. From the hessian matrix we may find the second derivative in the direction of \( \theta_s \), towards one of the substrate particles. If we relate this value to \( K_s \), a spring constant for the substrate-film interaction, we find that

\[
B_0 = K_s \frac{(\mu_s - \nu_s)(a_s^2 + 4z_{eq}^2)}{2\mu_s(\pi^2 + 2\mu_s\nu_s - 2\nu_s^2)}
\]  

(5)

In the rest of this paper we shall assume \( a_s = 1 \) and \( z_{eq} = 0.35 \). We define \( k \equiv K_f/K_s \). In order to define the energy scale we assume \( K_s + K_f = 1 \).

III. ANALYTICAL APPROACH

We are going to introduce an Ansatz which provides insight into the physics of the model. We shall consider all particles to have their \( x \)-coordinates in the equilibrium positions of the substrate potential. Furthermore, let us suppose that a fraction \( p \) of them leave the equilibrium plane \( z = z_{eq} \) and reach a new height value \( z_1 \). These particles shall be termed runaway particles and we shall assume them to be regularly spaced\(^{20}\). As a particular case, if \( p = 1/2 \) we get the zig-zag state, in which every other particle leaves the equilibrium plane as a way to relax the film springs.

Let us consider the function \( c(z_1) \) to be the energy per particle minus the value for the flat configuration within the Ansatz exposed in the text. The plots have different values of \( k \), but they all take \( a_f = 1.05 \) and \( p = 1/2 \). (Upper) The graphs illustrate the behaviour of the energy around \( k_1 \), where a second (rough) minimum appears, and \( k_1 \), where the two minima become equal. (Lower) The graphs show the situation around \( k_2 \), where the first (flat) minimum becomes unstable.

Let us consider the function \( c(z_1) \) to be the energy per particle minus the value for the flat configuration for given values of \( p \), \( k \) and \( a_f \). Figure 4 (upper) shows this function for five values of \( k \), with \( a_f = 1.05 \) and \( p = 1/2 \). The first two cases, \( k < k_1 \) and \( k = k_1 \approx 2.261 \), have a single minimum at \( z_1 = z_{eq} \). Therefore, the ground state is flat. At \( k > k_1 \) a second minimum appears at \( z_1 > z_{eq} \). The ground state for the third curve, with \( k_1 < k < k_t \approx 2.905 \), is flat, but there is also a metastable rough state. At \( k = k_t \approx 2.905 \) the two minima become equal. This point marks the rugosity transition. When \( k > k_t \) the ground state is rough, but the flat state is still metastable for some range in \( k \). Figure 5 (lower) shows that this situation extends up to \( k = k_3 \approx 8.128 \), when the flat minimum becomes a saddle point. Beyond that value, for \( k > k_2 \), the flat state becomes unstable, and a new metastable state appears, with \( z_1 < z_{eq} \). The true ground state is rough and has \( z_1 > z_{eq} \).
FIG. 4: Phase transition, $k$ vs $a_f$, for the VEFK model within the Ansatz exposed in section I. The full line labelled as $k_1$ denotes the phase transition. Above that line, the ground state is flat. Below the $k_1$ curve the ground state is rough. Between $k_1$ and $k_2$, although the true ground state is flat, there is also a metastable rough state. Between $k_1$ and $k_2$, the true ground state is rough, but the flat state is still metastable. Beyond $k_2$, the ground state is rough and the flat state is unstable.

Now let us consider the phase diagram, i.e.: for each value of $a_f$, the value of $k$ for which the two minima of the function $e(z_1)$, at $z = z_{eq}$ and $z_1 > z_{eq}$, take the same energy. This transition curve $k_1(a_f)$ is depicted in figure 4 with a full line. The lower curve shows $k_1(a_f)$, the values of $k$ for which a second local minimum appears at $z > z_{eq}$. Between these two curves, there is a metastable rough state. The upper curve shows $k_2(a_f)$, the points where the flat state becomes unstable. Therefore, in the region between the transition curve and this line, the flat state is metastable.

The energy $e(z_1)$ is proportional to $p$. Therefore, $p$ plays an irrelevant role in the determination of the transition point. This means that, within this Ansatz, the phase transition is not a truly collective phenomenon. Since $p = 1/2$ is the maximum possible value of $p$, this Ansatz predicts that beyond the transition point the rough states will always be zig-zag states.

The transition curve $k_1(a_f)$ follows with good approximation a power law $k_1 \sim (a_f - 1)^\beta$ with two different exponents. For low values of $a_f$ we have $\beta \approx -1.30\pm0.02$, and for high values $\beta \approx -1.94\pm0.02$. The exponents are not universal: they depend on the exponents of the substrate and film potentials. We shall compare these results with the numerical ones.

Although this Ansatz is quite crude, it provides certainly some insight into the physics of the model. The basic framework, with a transition curve and the metastability regions, shall remain valid in the more accurate approach of section IV. We shall see that $p = 1/2$ is not the preferred state after the transition. The fraction of runaway particles plays a more relevant role when the atoms are allowed to move in the X-axis.

IV. RENORMALIZATION GROUP PROCEDURE

A. Formulation

The main procedure involved by real space RG is to rewrite the system equations in terms of block variables without altering their form. As it has been stated, our RG technique is strongly inspired on the Griffiths and Chou approach and the Density Matrix Renormalization Group (DMRG).

A single particle moves within our 2D substrate potential, $V_s$, which we shall term $V^{(1)}$ from now on. The particle stays at position $r_1$, and the system energy is $V^{(1)}(r_1)$. Let us add a second particle on (e.g.) the right side, and link them with the “spring” $V_f(r_1, r_2)$. The second particle shall remain fixed at any point $r_2$ and we shall force the first particle to find its equilibrium position by minimizing $V^{(1)}(r_1) + V_f(r_1, r_2)$. Thus, we may write $r_1 = f_{1\rightarrow2}(r_2)$ for a known $f_{1\rightarrow2}$ function. The first particle will be said to be enslaved to the second one from now on, and function $f_{1\rightarrow2}$ shall be called a slaving mapping.

Now, the total energy of the system may be expressed as:

$$V^{(2)}(r_2) = V^{(1)}(r_1) + V_f(r_1, r_2) + V_s(r_2) = V^{(1)}(f_{1\rightarrow2}(r_2)) + V_f(f_{1\rightarrow2}(r_2), r_2) + V_s(r_2)$$

i.e.: the total energy of the two-particles block depends only on the position of the second particle. Thus, it may be considered as an effective or renormalized potential. The minimum value of $V^{(2)}$ is therefore the minimum possible energy for all the two-particles system. Minimizing for a single particle, we obtain the minimum for a two-particles chain.

The process may, of course, be iterated until a large chain is represented this way. If we have $V^{(n-1)}(r_{n-1})$, we may add a $n$-th particle and find the value of $r_{n-1}$ which minimizes $V^{(n-1)}(r_{n-1}) + V_f(r_{n-1}, r_n)$ for each value of $r_n$. This is again a slaving relation: $r_{n-1} = f_{n-1\rightarrow n}(r_n)$. The $(n-1)$-th particle is now enslaved to the $n$-th one. Now let us define $V^{(n)}(r_n)$ as

$$V^{(n)}(r_n) = V^{(n-1)}(r_{n-1}) + V_f(r_{n-1}, r_n) + V_s(r_n) = V^{(n-1)}(f_{n-1\rightarrow n}(r_n)) + V_f(f_{n-1\rightarrow n}(r_n), r_n) + V_s(r_n)$$

Using the same argument as before, the minimum value of $V^{(n)}$ is the minimum possible energy for the whole chain.
B. Reconstruction Procedure

Let us suppose that we have carried out the previous procedure up to a given value of $n$ and found the series of potentials $V^{(1)}, \ldots , V^{(n)}$. We may reconstruct the ground state in this way. The value $r_n^0$ which minimizes $V^{(n)}(r_n)$ is the position of the $n$-th particle in the ground state. When we have $r_n^0$, we may find $r_{n-1}$ by minimizing

$$V^{(n-1)}(r_{n-1}) + V_f(r_{n-1}, r_n^0) \tag{8}$$

Which is equivalent to the use of the enslaving function $r_{n-1} = f_n(r_{n-1}, r_n^0)$. Iterating backwards we can find the position of the first particle:

$$r_i^0 = f_{1+2}(f_{2+3}(\cdots (f_{n-1+n}(r_n^0)) \cdots )) \tag{9}$$

and, thus, obtain the exact solution $\{r_1^0, \ldots , r_n^0\}$.

Effectively, relation $\text{(9)}$ may be expanded backwards, substituting $V^{(n-1)}$ with its definition in terms of $V^{(n-2)}$, etc. Just as a check, we may evaluate $V^{(n)}(r_n^0)$ and find

$$V^{(n)}(r_n^0) = V_s(r_n^0) + V_f(r_{n-1}, r_n^0) + \sum_{i=1}^{n-1} V_s(r_i^0) + \sum_{i=1}^{n-2} V_f(r_i^0, r_{i+1}^0) \tag{10}$$

Which is, as it was already stated, the energy of the full chain in the ground state. Thus, the minimization equation for $r_n$ within potential $V^{(n)}$ solves the problem for the $n$-particles block, which is the essence of a real space RG method.

C. Renormalization Group Flow and Fixed Points

We may consider $V^{(i)}$ to be flowing under RG transformations in a certain functional space. Although the parameter space is infinite dimensional, this poses no special theoretical difficulties. All potentials are periodic in $x$ with period $a_s$, since a block displacement of the full chain of $a_s$ does not affect the energy, but they need not even be continuous. We will define a fixed point in this RG flow through the equation:

$$V^{(i)}(r) = V^{(i-1)}(r) + e \tag{11}$$

The parameter $e$ is just the energy per particle in the full chain. This fixed point equation may be rewritten as an eigenvalue equation within a minimax algebra for a target potential $R(r_i)$:

$$R(r_i) = V_s(r_i) + \min_{r_{i-1}} |V_f([r_i - r_{i-1}]) + R(r_{i-1})| + e \tag{12}$$

If the flow took place in a finite-dimensional vector space, this equation would be sure to have a solution. In our problem, despite the absence of a rigorous proof, we have found it to exist for a wide variety of cases. Solving equation $\text{(12)}$ is a hard problem unless the RG procedure, starting with $V^{(1)} = V_s$, converges. This convergence has always taken place in the cases we have tried.

If we are interested only in the thermodynamic limit, we may find the ground state from the fixed point potential $R$. The procedure is identical to the one described in the $\text{IV B}$ section, but using always the same potential. If finite-size effects are thought to be important, the full series of potentials should be used.

V. NUMERICAL APPROACH

The most straightforward strategy to obtain the ground state is to obtain the zero-force equations for each particle, solve them and choose the solution with lowest energy. The equation for $r_i$ depends both on $r_{i-1}$ and $r_{i+1}$. This yields a dynamical system which, for the original FK model, is related to the standard map. A minimization algorithm must be used to choose the orbit which corresponds to the minimum energy. In our case, this strategy is not appropriate, since it is not possible to solve analytically the $i$-th zero-force equation for $r_{i+1}$, as it is in the original FK model. Therefore, the numerical approach shall be based on global minimization techniques, whose problem is the existence of a complex landscape of local minima.

In order to obtain a good seed configuration to insert in a global numerical minimization routine, we have tried several different algorithms: (a) Simulated annealing; (b) Take a small chain and find its ground state; after that, add a site both at the left and the right borders and repeat the procedure until the desired length is reached; (c) A technique based on the Puncture Renormalization Group: start with any initial configuration, pick up a block of sites and minimize its energy while the left and right tails may only move as two solid blocks; afterwards, the chosen block moves rightwards and leftwards, sweeping the system, and (d) The RG method described in section $\text{IV B}$ whose implementation we are going to detail.

Method (d) has always provided the lowest energy minima, for reasons which will be discussed in the following paragraph. The other three methods give, in many cases, higher energy local minima. Method (b) is the second best, and its main handicap is that its solutions tend to have too much left-right symmetry. It is always convenient to optimize the solution found using a classical minimization algorithm.
A. Technical Details

The procedure described in section [IV] may not be carried out analytically. Our numerical implementation discretizes each $V^{(i)}$ into a regular grid of $N_x \times N_z$ points, typically 100 x 100 or 100 x 150 points. The discretization interval of the potential is an important issue. We have found the election $[-a_s/2, a_s/2] \times [z_{eq}/2, 5z_{eq}/2]$ to be appropriate. The $X$-interval is motivated by the $a_s$ periodicity of all potentials. In the $Z$-axis, the interval is designed to include all runaway particles.

In their seminal work, Griffiths and Chou obtain the minimum enthalpy state instead of the minimum energy one. This means that, in our case, the film potential would be changed into

$$V^*_f(r_1,r_2) \equiv \min_{m} V_f(|r_1 - r_2 + m \cdot e_x|)$$

where $e_x$ is the unit vector in the $X$-direction and $m$ is an integer. This change is made so as the search for the minimum in the construction of $V^{(n+1)}$ from $V^{(n)}$ has a solution in the $[-a_s,a_s]$ interval of the $X$-axis. Otherwise, the search should be extended to the whole real line. We have found an alternative approach to this problem. The search is carried out on two periods in the $X$-axis on the left side of the $(n+1)$-th particle. Since $a_f < 2a_s$ in all the studied cases, this procedure is sure to find the solution. Our solution is always optimal within the subspace of coarse-grained potentials on the given grid.

Our calculations are of two types: infinite systems, i.e.: systems in the thermodynamical limit, and finite-size systems. The differences between them shall be analyzed in the following sections.

For each value of $a_f$ and $k = K_f/K_s$ the ground state is found. For each ground state the following observables are considered: (a) energy per particle $e$, (b) average height $h \equiv \langle z \rangle$ and its standard deviation $\sigma_z$, known as roughness, and (c) effective lattice parameter $\alpha$, defined as the average of $|x_{i+1} - x_i|$, and its standard deviation $\sigma_\alpha$.

B. Roughness transition: infinite systems

For any given value of $a_f$, the value $k = K_f/K_s = 0$ always results in a flat configuration, with $h = z_{eq}$ and $\alpha = a_s$. If we increase $k$, all the observables increase smoothly up to a certain value $k_l(a_f)$, where an abrupt jump takes place.

The infinite system computation starts with the application of the RG flow on the substrate potential $V_0$ in order to find the fixed point potential $R(r)$. Typically, about 10 or 20 iterations were enough to get a maximum error of a part in $10^6$. This fixed point potential yields a unique enslaving function, $f$. We obtain the point where $R(r)$ takes its minimum value, $r_1^0$, and iterate the enslaving function on it so as to reconstruct the full ground state $\{r_1^0, r_2^0, \ldots, r_N^0\}$ for a large value of $N$. If, for a given tolerance, there is a value $N_0$ such that if $n > N_0$, $z_n \approx z_{eq}$, we shall assume that the ground state is flat. We have chosen a tolerance of $10^{-4}$.

The phase transition obtained with this criterion is shown in figure [5]. The first part, up to $a_f \approx 1.075$, may be fitted to $k_l(a_f) \sim (a_f - 1)^\beta$ with $\beta \approx -1.39$, in reasonable agreement with the value $-1.30 \pm 0.02$ obtained for the analytical Ansatz. For high values of $a_f$ the transition curve is more rough, and the fit is more difficult. Nonetheless, the exponent may be seen to increase in absolute value.

The transition always takes place at a higher value of $k$ than in the analytical Ansatz. This is due to the fact that particles were not allowed in that case to move in the equilibrium plane. This way to relax stress delays the transition in practice.

According to the results of section [III] for most points just above the transition the ground state is a zig-zag state, i.e.: the fraction of runaway particles is either $p = 1/2$ or $p = 1$.

C. Roughness transition: finite-size systems

Finite-size systems present interesting peculiarities. Whenever an island develops and new film particles are deposited on it, the size of the island renders the thermodynamical limit irrelevant. Therefore, finite-size effects might play an important role in practical applications. We have mapped and analyzed the roughness transition for a finite-size system with $N = 101$ particles.

In these calculations, the intermediate potentials of the RG flow are stored to disk so as they may be recovered during the reconstruction procedure. When convergence is attained, the program stops calculating any more potentials and assumes the rest to be equal to the last one in storage.

FIG. 5: The phase diagram for the VEFK model in the thermodynamical limit.
The positions of the particles always belong to the \( N_x \times N_z \) grid. Therefore, their precision is low. In the finite-size case the positions entered a standard minimization algorithm. Usually, this procedure only took a very short time, since the configuration was nearly optimal and its deviation was only due to the effect of the lattice. Checks were periodically made to ensure that the energy per particle in our results were lower than in the other approaches described at the beginning of this section.

Figure 6 shows three ground states with \( a_f = 1.03 \) and \( k = 3.04670, 3.04674 \) and 3.04678 for \( N = 101 \) particles. The first one is flat. In the second one, a single runaway particle appears. In the third one, two symmetrically placed particles leave the equilibrium plane \( z = z_{eq} \). The values of \( \sigma_h \) increase from \( 7 \cdot 10^{-4} \) to 0.032 and 0.045 respectively in a very small interval for \( k \). As we increase \( k \), new peaks appear steadily, in a slower way.

Figure 7 shows the behaviour of the energy per particle \( e \), roughness \( \sigma_h \) and deviation of the effective lattice parameter \( \sigma_k \) for \( a_f = 1.03 \) as we increase \( k \). The transition is clearly seen to coincide for the three observables.

For each value of \( k \) and \( a_f \) a certain flat domain-size \( D \) may be defined as the minimum distance between runaway particles, or between runaway particles and the extreme of the chain. Of course, a ground state is rough whenever \( D < N \).

Figure 8 shows the phase transition curve in the \( k - a_f \) plane for \( N = 101 \). This curve presents some jumps, e.g., at \( a_f = 1.0418 \) between \( k \approx 2.04 \) and 2.28, which are finite size effects. At this special jump, the domain size is \( D = 50 \), i.e.: half the system size. Thus, the first particle to leave the equilibrium plane is the central one. This behaviour is locked for a certain range of \( k \) values. The second jump in size is at \( a_f = 1.064 \), and there the domain size is \( D = 34 \), i.e.: very close to one third of the total lattice size. This locking is a collective phenomenon which does not appear in our analytical Ansatz.

This behaviour is clearly different from the one we have found for infinite systems. Border effects are clearly dominant in the phase transition for finite systems.

VI. CONCLUSIONS AND FURTHER WORK

A modification of the classical FK model, known as Vertically Extended Frenkel-Kontorova (VEFK), has been proposed in which particles may displace vertically, thus allowing the film layer to bend. Physical pathologies associated with the FK model, such as the sharp commensurate-incommensurate transition, disappear in this case. This modified model is used to study a roughness transition which might be the seed for island formation in surface growth phenomena, both with analytical and numerical approaches, at \( T = 0 \). The numerical technique is inspired on the effective potentials method of Chou and Griffiths and on real space renormalization group methods, specially on DMRG. The analytical approach shows both a transition curve and two broad metastability regions.

This roughness transition presents some general features: (a) it starts with some runaway particles which leave the equilibrium plane, (b) the size of the flat regions (domains) near the transition point depends on the parameters \( a_f \) and \( k \), and is rather sensitive to finite size
FIG. 8: The phase diagram for the VEFK model with \( N = 101 \) particles. Above the line, the ground states are always rough, and below they are flat. The phase border may be seen to have jumps at certain positions, as it is explained in the text.

As discussed at the introduction, rough configurations may be the origin of domains which make up the characteristic islands in SK and VW growth modes. The effect of many film monolayers is, of course, of great importance, and has been left for further work. A second monolayer may have a qualitative effect on the transition.

All the surface growth phenomena are, of course, 2+1D. The dimensional extension of our model involves some numerical difficulties, since there does not exist a straightforward extension of the RG approach. The performance of DMRG-like techniques decrease when the particle linking graph does not have a tree topology. Extensions of the DMRG algorithm to 2D and 3D problems are a field of active research\(^{26,27}\) and this problem might well pose a possible application for them.

This VEFK model may be studied at finite temperature with the transfer matrix formalism. The usual arguments against 1D phase transitions do not apply in this case, since the substrate potential imposes a long range order. Therefore, the roughness transition is likely to survive up to a finite value of \( T \). A positive result in this direction is the treatment of a finite temperature transition for FK.

In physical terms, there should be a second flatness transition at even higher values of \( k = K_f/K_s \), for which the film gets flat again, with the effective lattice parameter \( \alpha = a_f \). In our numerical analyses this second transition does not appear. The reason is the following: at very high values of \( k \) the substrate potential is almost inexistent, and the reference plane for the film disappears in practice. All configurations in which each particle is at a distance \( a_f \) from its neighbours, even if it is highly curved, have nearly the same energy.

Some relevant features, such as a slowly changing curvature or the second flatness transition, would be met if a three-body angular potential was included. This extension is physically plausible and may lead to a richer phase diagram.

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Other potentials with similar features, such as the Morse potential or the one proposed by Markov et al.\textsuperscript{11}, give the same qualitative physics.

The requirement of regular spacing for the runaway particles is not important within this Ansatz, i.e.: their distribution may be random as far as there are not neighbour. This is not true in the general case.

A conjugate gradient search with Polak-Ribiere modification\textsuperscript{25}.