

Heterogeneous versus discrete mapping problem

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We propose a method for mapping a spatially discrete problem, stemming from the spatial discretization of a parabolic or hyperbolic partial differential equation of gradient type, to a heterogeneous one with certain comparable dynamical features pertaining, in particular, to coherent structures. We focus the analysis on a $(1+1)$ -dimensional ϕ^4 model and confirm the theoretical predictions numerically. We also discuss possible generalizations of the method and the ensuing qualitative analogies between heterogeneous and discrete systems and their dynamics.

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I. INTRODUCTION

In the past two decades, the effects of discreteness in the waves of parabolic and hyperbolic nonlinear partial differential equations (PDE's) have been shown to be important in a variety of physical settings. From the behavior of calcium waves in living cells [1] to the discontinuous propagation of action potentials in the heart [2] or chains of neurons [3] and from chains of chemical reactors [4] or arrays of Josephson junctions [5,6] to optical waveguides [7], dislocations [8], and the DNA double strand [9], the relevant models of physical reality are inherently discrete. This realization has led to the acknowledgment of discreteness as a factor that can quite dramatically modify the continuum picture and enrich its phenomenology with effects such as resonant energy transfer to extended waves [10], braking [11], and eventual failure of propagation [12] of coherent structures.

An alternative factor that can change the homogeneous continuum picture is the presence of heterogeneities in a genuinely continuous medium [13]. Heterogeneity is also relevant in a variety of physical settings ranging from the behavior of chemical reactions on composite catalyst surfaces [14,15] to the diffusion of flame fronts [13] or the migration of populations in population dynamics [16].

Our aim in this work is to show that these two types of variation of the continuum behavior can be related to each other.

The existence and motion of coherent structures constitutes the backbone of spatiotemporal pattern formation and dynamics in all three types (homogeneous continuum, discrete, heterogeneous continuum) of systems. We intend to demonstrate that a discrete problem derived from the "natural" semidiscretization of a parabolic reaction-diffusion (RD) or hyperbolic nonlinear wave PDE of gradient type can

be mapped into a heterogeneous continuum problem with comparable coherent structure dynamic features. In a sense, this mapping is not very surprising: one of the main features of discrete systems which is, at least partially, responsible for the new phenomena observed therein, is the breaking of translational invariance. This also occurs in heterogeneous systems. The way in which this statement is translated into mathematical terms and in which it affects the behavior of the coherent structures will become evident later in this exposition. In spatially discrete systems, the discrete integer translational shift invariance that results from the breakup of translational invariance prompts one to think that it could be matched by a heterogeneous medium with a natural period of variation due to heterogeneity equal to the intersite distance (the lattice spacing). Even though our method will be applied to systems of gradient type and hence will not be completely general, we will present below an extended discussion of the more general aspects of the analogy between heterogeneous and discrete systems.

We present our results as follows. In Sec. II, we give the general setup of the models of interest to this study. In Sec. III, we will present a methodology of how to "construct," given a discrete system of gradient type, a corresponding heterogeneous system; the correspondence, based on respective coherent structure dynamics, will be discussed. The methodology will be illustrated in the specific example of a ϕ^4 , $(1+1)$ -dimensional field theory and will subsequently be numerically tested. Section IV presents an extended discussion of the analogies between heterogeneous and discrete systems that goes beyond our particular method. In Sec. V, we analyze the relevance and usefulness of a transformation that maps a discrete system to a heterogeneous one for a number of physical problems of recent interest. Finally, in Sec. VI, we summarize our findings and conclude.

II. GENERAL SETUP

The mathematical models of interest to this study will be of the form

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$$\{u_t, u_{tt}\} = -\frac{\delta V}{\delta u} \quad (1)$$

with a potential energy functional $V[u]$,

$$V[u] = \int dx \left(F(u) + \frac{u_x^2}{2} \right). \quad (2)$$

Equation (1) with one temporal derivative corresponds to a scalar equation of the RD type, while with two it represents a nonlinear Klein-Gordon wave equation. We will use equations of this form for illustration purposes, but we should note that the methodology can naturally be generalized to *any parabolic or hyperbolic* (also possibly vector) *system of gradient type*. The gradient nature of the system, expressed through the form of potential energy given by Eq. (2), is quite crucial to the considerations that follow. Note that such a structure will generically be present for Hamiltonian systems as well as for scalar RD equations, but not necessarily so, for instance, for systems of dissipative PDE's.

The equation of motion for (1), using (2), reads

$$\{u_t, u_{tt}\} = f(u) + u_{xx} \quad (3)$$

with $f(u) = -F'(u)$. The corresponding heterogeneous problem of Eq. (3) is

$$\{u_t, u_{tt}\} = f(u, b(x)) + [a(x)u_x]_x \quad (4)$$

with at least one of $a(x), b(x)$ explicitly dependent on the spatial variable x .

The discrete counterpart problem has a potential energy functional

$$V_d = \sum_n \frac{(u_{n+1} - u_n)^2}{2h^2} + F(u_n) \quad (5)$$

for a lattice of spacing h , i.e., $u_n = u(x = nh)$.

III. TRANSFORMATION OF A DISCRETE INTO A HETEROGENEOUS SYSTEM

Suppose that we have a discrete system with lattice spacing h and we calculate its potential energy V_d . This potential energy determines, among other things, the existence and motion of coherent structures for the model. If we wish to approximate the discrete system's dynamic behavior and, in particular, the average shape and dynamics of its coherent structures with a heterogeneous system of, say, variable diffusivity $a(x; h)$, we can require that the two systems have the same energy:

$$\int dx \left(a(x; h) \frac{u_x^2}{2} + V(u) \right) = V_d(h). \quad (6)$$

This, however, given $u(x)$, can be treated as an inverse problem for $a(x; h)$. In particular, if we use an *Ansatz* solution—which below will be a coherent structure $u(x)$ such as a

constant shape front— $\int V(u) dx = p$ is just a number or, at most, a function of h and hence the problem can be translated into

$$\int dx a(x; h) s(x) = E(h) = V_d - p. \quad (7)$$

$E(h)$ is now explicitly known, and so is $s(x) = u_x^2/2$ upon substitution of the chosen *Ansatz*, and the inverse problem needs to be solved to determine $a(x; h)$.

We should highlight at the outset that there are two levels of approximation in this approach.

(1) The first approximation lies in the choice of the *Ansatz*. Since we concentrate on the nature and dynamics of coherent structures, we will use as our *Ansatz* the uniform continuum problem coherent structure solution, in order to illustrate the method. More sophisticated *Ansätze* can also be used [12]. A more refined methodology would entail finding the exact discrete solution, and substituting it in the expression for the discrete energy; and also appropriately correcting the coherent structure and its asymptotic tails before inserting it in the continuum left-hand side (LHS) of Eq. (6). However, since the leading order effects can be captured by a homogeneous continuum problem coherent structure, in this approach we will, for illustration purposes, implement only the simplest possible *Ansatz*. It should be noted once again that it will be implicitly assumed in the exposition that we are interested in the coherent structure dynamics of the models under study.

(2) The second ‘‘approximation’’ lies in the fact that the behavior of the constructed system should *not* be expected to be in detail the same as the one of the continuum. Instead, one should expect only the corresponding coherent structures to be close, as sets, in a meaningful norm, and the nature and time scales of their dynamics to be close to each other. One thus expects only ‘‘coarse,’’ or ‘‘average,’’ properties of the two systems under study to match.

As is well known [17], discreteness introduces a potential energy barrier in which the coherent structure can be considered as a particle at the mean field level. The aim of this exercise is, then, to suitably pick $a(x; h)$ so that the (quasi)harmonic modulation of exponentially small width as imposed by the ‘‘just-right’’ heterogeneity is the same as the one imposed by discreteness. To solve this problem, we Fourier decompose $a(x; h)$,

$$a(x; h) = \sum a_m(h) \exp\left(\frac{im\pi x}{h}\right), \quad (8)$$

substitute the *Ansatz* for $u(x)$, and solve the ensuing equations for the Fourier components $a_m(h)$.

To illustrate the methodology, we pick as a specific example of a $(1+1)$ -dimensional field theoretic model the ϕ^4 problem; the discrete and the heterogeneous versions are compared to each other with the help of the homogeneous continuum problem as a reference point. The equation of motion reads

$$\{u_t, u_{tt}\} = u_{xx} + 2(u - u^3). \quad (9)$$

The continuum potential energy is

$$V_c = \int dx \left(\frac{u_x^2}{2} + F(u) \right), \quad (10)$$

where $F(u) = (u^2 - 1)^2/2$, while the discrete potential energy is

$$V_d = \sum_n \left(\frac{(u_{n+1} - u_n)^2}{2h^2} + F(u_n) \right), \quad (11)$$

and the heterogeneous potential energy we try to match with it is given by

$$V_{het} = \int dx \left(a(x;h) \frac{u_x^2}{2} + F(u) \right). \quad (12)$$

As per our remarks above, for small h , we will use in both perturbed problems the continuum front *Ansatz* $u(x) = \tanh(x)$. Setting Eq. (12) equal to Eq. (10), we obtain

$$\begin{aligned} & \int dx a(x;h) \frac{1}{2 \cosh^4(x)} + \int F(\tanh(x)) dx \\ &= h \sum_n \left(\frac{\{\tanh[(n+1)h] - \tanh(nh)\}^2}{2h^2} + F(\tanh(nh)) \right). \end{aligned} \quad (13)$$

Notice the h factor in front of the sum, placed there for convenience. We now use the Poisson summation formula (see, e.g., [17,18])

$$\sum_{n=-\infty}^{\infty} f(nh)h = \int_{-\infty}^{\infty} dx f(x) \left[1 + 2 \sum_{s=1}^{\infty} \cos\left(\frac{2\pi s x}{h}\right) \right] \quad (14)$$

to convert the sums into integrals. We thus have

$$\begin{aligned} & \int dx a(x;h) \frac{1}{2 \cosh^4(x)} + \int F(\tanh(x)) dx \\ &= \int dx \left(\frac{[\tanh(x+h) - \tanh(x)]^2}{2h^2} + F(\tanh(x)) \right) \\ & \times \left[1 + \sum_{s=1}^{\infty} \left[\cos\left(\frac{2\pi s x}{h}\right) \right] \right]. \end{aligned} \quad (15)$$

Hence, after some simplification,

$$\begin{aligned} \int dx a(x;h) \frac{1}{\cosh^4(x)} &= \int dx \frac{[\tanh(x+h) - \tanh(x)]^2}{2h^2} \\ &+ \left(\frac{[\tanh(x+h) - \tanh(x)]^2}{2h^2} \right. \\ & \left. + F(\tanh(x)) \right) \sum_{s=1}^{\infty} \left[\cos\left(\frac{2\pi s x}{h}\right) \right]. \end{aligned} \quad (16)$$

We now expand

$$a(x;h) = a_0 + \sum_{m=-\infty, m \in N^*}^{\infty} a_m(h) \exp\left(\frac{i\pi m x}{h}\right), \quad (17)$$

keeping, in this case, only the cosine terms, having in mind to match the Poisson formula coefficients. However, as will be clear below, this is not necessary. Performing the integrals of the left- and the right-hand sides, we can equate the zeroth order terms (the ones independent of m, s) to obtain

$$a_0 = \frac{3[h \coth(h) - 1]}{h^2}. \quad (18)$$

Notice that the correct limit is retrieved from the heterogeneous model for $h \rightarrow 0$. Equating the remaining terms, we have

$$\begin{aligned} & \sum_{m=1}^{\infty} a_m \frac{(\pi^2 m)(h^2 + \pi^2 m^2/4)}{3h^3 \sinh(\pi^2 m/4h) \cosh^2(\pi^2 m/4h)} \\ &= \sum_{s=1}^{\infty} \left[\frac{(2\pi^2 s)(h^2 + \pi^2 s^2)}{3h^3 \sinh(\pi^2 s/2h) \cosh^2(\pi^2 s/2h)} \right. \\ & \left. - \frac{4\pi^2 s}{h^3} \exp\left(-\frac{\pi^2 s}{h}\right) \right]. \end{aligned} \quad (19)$$

Equation (19) is a key result for our methodology. It illustrates how the Fourier components of the heterogeneity have to be chosen in order for it to match the average effects of discreteness.

Some remarks are in order here.

(1) One could equilibrate the series of the LHS and the RHS of Eq. (19) term by term as is done when one has—orthogonal—Fourier components, i.e., the $m=i$ with the $s=i$ terms of the series. We notice that in this case this is not necessary; one can just use a single term of the LHS series to compensate for the effects of the sum of terms in the RHS exactly, because the matching is performed at the average level. In particular, for simplicity, we use only the $m=1$ term, choosing

$$a_1 = \frac{3h^3 \sinh(\pi^2/4h) \cosh^2(\pi^2/4h)}{(\pi^2)(h^2 + \pi^2/4)} \sum_{s=1}^{\infty} \left[\frac{(2\pi^2 s)(h^2 + \pi^2 s^2)}{3h^3 \sinh(\pi^2 s/2h) \cosh^2(\pi^2 s/2h)} - \frac{4\pi^2 s}{h^3} \exp\left(-\frac{\pi^2 s}{h}\right) \right]. \quad (20)$$

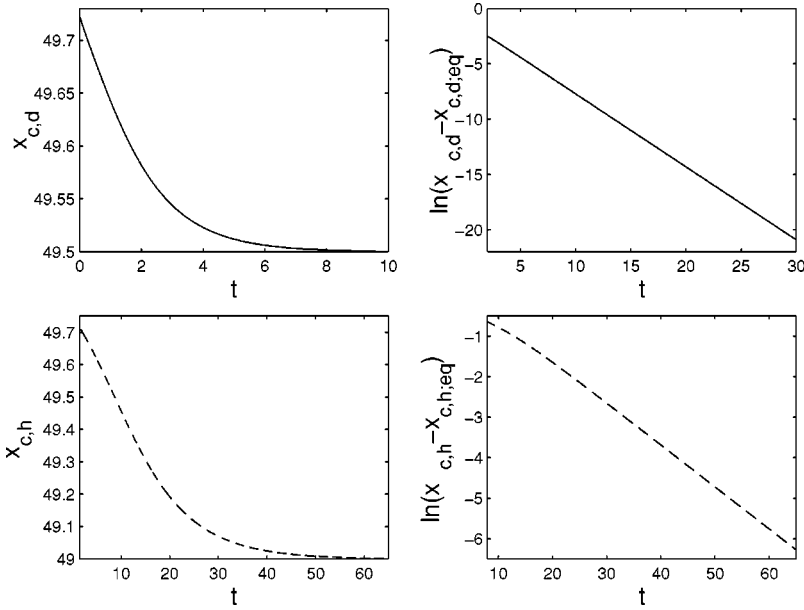


FIG. 1. The dynamical time evolution of the front solution center toward its equilibrium position in the discrete medium (top panels) as well as the (“equivalent”) heterogeneous medium (bottom panels). The left panel shows, in both cases, the time evolution of the center ($h=1$) whereas the right panels demonstrate in a semi-logarithmic scale the exponential nature of the convergence toward the equilibrium static minimum potential energy configuration (see text also).

(2) As the careful reader will have noted, in the expansion for the heterogeneity we have used wave numbers $k=k'/2$ where k' are the corresponding wave numbers “of discreteness” as imposed by the Poisson formula. In general, at the level of matching we perform, the above choice is not necessary; however, a choice of $k < k'$ will be needed since for $k=k'$ the inverse of the first fraction in the RHS of Eq. (20) goes to 0 faster than the second term in the series summation as $h \rightarrow 0$. Hence, the limit becomes ill defined. For the choice made here, an interval of $2h$ of the heterogeneous medium simply corresponds to a lattice spacing distance for the discrete medium.

(3) It is also worth noting that, modulo the above mentioned difference, the terms in the series of the LHS are the same as the first terms of the series of the RHS in Eq. (19). Retracing this coincidence back to Eq. (13), we can observe that it is due to the Bogomol’nyi bound (see, e.g., [19]). The latter necessitates, in models similar to the one studied here that the static solution saturates the lower bound of the continuum potential energy, rendering the coupling, i.e., the one coming from the first term in the integral of Eq. (6), and the substrate, i.e., stemming from the second term in the integral of Eq. (6), potential energies equal.

We now proceed to examine numerically the results of our approach. If we used a trial *Ansatz* of the form $\tanh(x - x_0)$ to map the potential energy landscape as a function of the variable x_0 , we could easily [18,20] generalize the result of Eq. (19) to see that a $\cos(2\pi s x_0/h)$ term would be present, giving rise to a (roughly, since the higher order terms are exponentially weaker with respect to $s=1$) harmonic potential which for the discrete problem has minima at $x_0 = nh/2, n \in N$, and maxima at $x_0 = nh$. This picture for the heterogeneous problem would be translated to a harmonic $\sim \cos(\pi x_0/h)$ potential with minima at $x_0 = (2n+1)h$ (“black” sites) and maxima at $x_0 = 2nh$ (“white” sites). In [18,20], a constant external field was used to washboard the harmonic potential. As a result of the tilting, the maxima and minima can collide and disappear for a finite value of the

field in saddle-node bifurcations that will result in the appearance of burst waves. For such problems one would expect the traveling of the coherent structures to match between discrete and heterogeneous problems. However, in our case, the presence of static solutions renders them stable for the dynamics for the Hamiltonian as well as for the dissipative—as the maximum principle dictates [13]—systems. Hence, in our numerical computations, we observe the relaxation to the prescribed steady states of a perturbed original front like solution; the results for the dissipative system are shown here.

In Fig. 1, we initialize the discrete as well as the corresponding heterogeneous system for various values of h —specifically here the case of $h=1$ is shown—with a perturbed front with $x_0=49.75$. As we expect the discrete system relaxes to the equilibrium position of $x_0=49.5$, while the heterogeneous system relaxes to the “black” site with $x_0=49$. Notice that the picture reports the position of the front’s center following the method used in [21]. The time evolution of the relaxation to equilibrium follows a clearly exponential decay in each case, according to

$$\frac{dx_0}{dt} = - \frac{dV_{eff}(x_0)}{dx_0} \approx - \omega(h)x_0. \quad (21)$$

This “effective particle evolution” equation can be extracted by using the *Ansatz* with $x_0(t)$ for the potential energy and considering x_0 as a collective coordinate. The corresponding relaxation rate $\omega(h)$ can be theoretically predicted by expanding $\cos(2\pi s x_0/h)$ or $\cos(\pi x_0/h)$ close to the equilibrium position. It can thus be derived from Eq. (19) that $h^5 \omega$ (where ω is the associated rate of decay) will behave as $\exp(-\pi^2/h)$, with exponentially small corrections. In fact, from the semilogarithmic plot of $h^5 \omega$ as a function of h^{-1} in Fig. 2, we deduce that the solid curve corresponding to the discrete medium is within 4.01% of the theoretical prediction ($-\pi^2$) for the slope, while the dashed line of the heterogeneous medium is within 2% of the same prediction. Notice

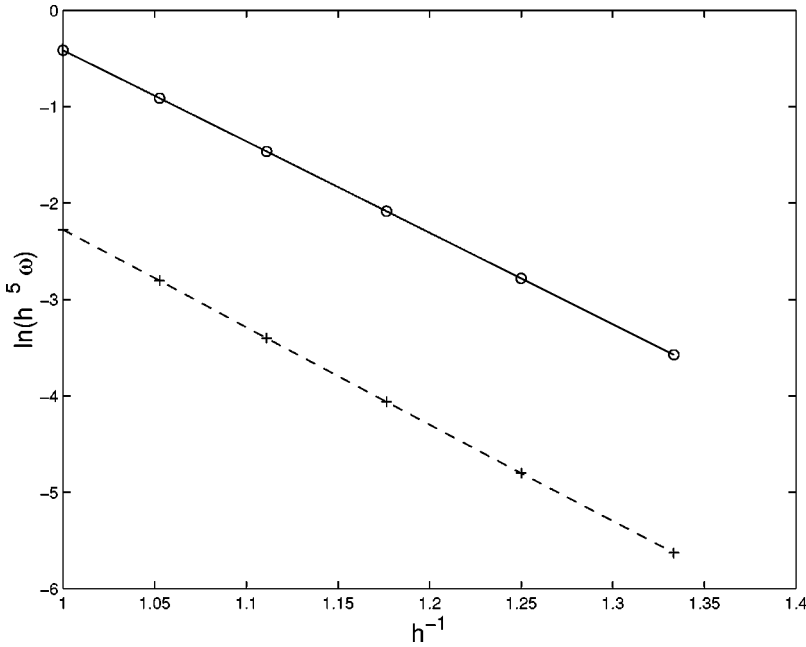


FIG. 2. The behavior of the (appropriately rescaled) rate ω of the approach [according to $\exp(-\omega t)$] to equilibrium is shown in a semilogarithmic plot as a function of h^{-1} . The solid line is the best fit to the data for the discrete system (circles) while the dashed line is that for the corresponding heterogeneous system (crosses). See text also.

that the only slightly higher deviation of the discrete problem is more than well justified as all terms with $s \geq 2$ in Eq. (19) have, in essence, been neglected in such a prediction. The very good agreement of this “average” picture with the theoretical result indicates the validity of the description set forth for the effective correspondence of discrete and appropriately “crafted” heterogeneous systems.

IV. TOWARD A GENERAL TRANSFORMATION OF DISCRETE TO HETEROGENEOUS SYSTEMS

In the previous section we saw that a particular discrete system could be mapped into a heterogeneous one with comparable coherent structure and coherent structure relaxation features. The mapping was based on matching the potential energies of the particular discrete system and of the corresponding heterogeneous one. We will now show that, formally, the potential energy of *any* discrete problem of the type mentioned in Sec. II can be mapped into the potential energy of a heterogeneous continuum system.

The basic tool for the exposition will be once again the Poisson summation formula (14), a useful special case result of which is

$$\sum_{n=-\infty}^{\infty} \exp(ian) = 2\pi \sum_{m=-\infty}^{\infty} \delta(a - 2\pi m). \quad (22)$$

If we now use V_d from Eq. (5) and write it according to Eq. (14), we obtain

$$V_d = \frac{V_{sc}}{h} + \frac{2}{h} \sum_{s=1}^{\infty} \int_{-\infty}^{\infty} \left(\frac{[u(x+h) - u(x)]^2}{2h^2} + F(x) \right) \times \cos\left(\frac{2\pi s x}{h}\right). \quad (23)$$

In what follows, for simplicity, we will rescale V_d in Eq. (23) by a factor of h as we are always allowed to. V_{sc} —the subscript indicating semicontinuum for reasons that will be obvious below—in the above equation reads

$$V_{sc} = \int dx \left(\frac{[u(x+h) - u(x)]^2}{2h^2} + F(x) \right) \approx V[u] + h^2 \int dx \left(\frac{u_{xx}^2}{4} + \frac{u_x u_{xxx}}{3} \right) \quad (24)$$

and yields the continuum potential energy functional up to $O(h^2)$; notice that the functional derivative of the $O(h^2)$ term yields the $O(h^2)$ correction ($=h^2 u_{xxx}/12$) in the Taylor expansion of the second order difference $[u(x+h) + u(x-h) - 2u(x)]/h^2 \approx u_{xx} + h^2 u_{xxx}/12 + O(h^4)$.

For the second part of the RHS of Eq. (23), we will use the semicontinuum approximation

$$2 \sum_{s=1}^{\infty} \int_{-\infty}^{\infty} \left(\frac{[u(x+h) - u(x)]^2}{2h^2} + F(x) \right) \cos\left(\frac{2\pi s x}{h}\right) \approx 2 \sum_{s=1}^{\infty} \int_{-\infty}^{\infty} \left(\frac{u_x^2}{2} + F(x) \right) \cos\left(\frac{2\pi s x}{h}\right), \quad (25)$$

since as we will show the continuum part of Eq. (25) is $O(C(h)\exp(-s\pi^2/h))$ and hence the rest will be $O(h^2)$ smaller and can consequently be ignored, as we are interested in the leading order, power-law as well as exponential, effects. We should note that the above estimate of exponential smallness holds true for the dynamics of coherent structures, which are implicitly of interest in this work, as has been highlighted also in the previous section.

Combining the results of Eqs. (24) and (25), we have that the potential energy of the discrete system is

$$V_d \approx \int_{-\infty}^{\infty} D(x) \left(\frac{u_x^2}{2} + F(x) \right) dx + h^2 \int dx \left(\frac{u_{xx}^2}{4} + \frac{u_x u_{xxx}}{3} \right) \quad (26)$$

where the corrections are $O(h^4)$ for the power-law terms and $O(h^{2+\alpha} \exp(-s\pi^2/h))$ [where α is of the order of $C(h)$] for the exponentially small terms. $D(x) = 1 + 2 \sum_s \cos(2\pi s x/h)$ is the variable diffusivity of the corresponding heterogeneous problem.

We will now present the argument about ‘‘exponential smallness’’ of the ‘‘effective’’ contributions of the variable diffusivity. Returning to the second term of the RHS of Eq. (23), we observe that the integrals within this expression contain rapidly oscillating integrands. Using the method of residues for integrals of the form $f(z) \exp(iaz)$ [22], we can see that they are equal to $\text{Re}[2\pi i \text{Res}_{z \rightarrow z_{pole}} f(z) \exp(iaz)]$ with $a = 2\pi s/h$. Typically, for the patterns of interest in such problems, such as kinks in the sine-Gordon equation $u(x) = 4 \tan^{-1} \exp(x)$, or the ϕ^4 model $u(x) = \tanh(x)$, and/or for pulses of the nonlinear Schrödinger equation $u(x) = 1/\cosh(x)$, the first pole of the coherent structure lies at $x = i\pi/2$. Generically, $f(z)$ will have exponential tails and analytic behavior on the real axis but will have poles at $x = iy, y \in R^*$, on the imaginary axis. Suppose, for simplicity, that the pole is at $x = i\pi/2$. Then,

$$V_d = V_{sc} + C(h) \exp\left(-\frac{\pi^2 s}{h}\right) \quad (27)$$

with $C(h) \approx \text{Re}[2\pi i \text{Res}_{z=i\pi/2} f(z)]$.

We have thus shown that the potential energy of any discrete system of the form of Eq. (1) can be approximated up to controllable higher order terms by that of an appropriately chosen heterogeneous system where both the coupling and the reaction terms are modulated by a special form of heterogeneity which on the average mirrors the exponentially small effects of discreteness, and a quartic derivative which mirrors its power-law effects. The higher order power-law effects can be captured by the Taylor series

$$\sum_{j=1}^{\infty} \frac{2h^{2j-2}}{(2j)!} \frac{d^{2j}u}{dx^{2j}}. \quad (28)$$

Some remarks are now in order.

(1) Since the effects of the variable part of the ‘‘diffusion coefficient’’ $D(x)$ are, on the ‘‘average’’ in the sense given above, $O(\exp(-\pi^2 s/h))$, it is worth noting that we will not need more than the first few terms in the series for $D(x)$.

(2) Exponentially small effects are generically observable in discrete systems, mirroring the exponentially small splitting of the heteroclinic or homoclinic orbits introduced by discreteness [23].

(3) Also, generically at the functional level, i.e., on the average, exponentially small phenomena will be present for any heterogeneous problem because of the nature of the in-

tegrals of the form $\int \exp(iaz) f(z) dz$, when f is reasonably well behaved on the real axis as is expected to be the case for the problems of interest here. Due to the residue theorem, generically such integrands will give rise to transcendental corrections in observable quantities such as, e.g., the coherent structure speed. As a particular form of heterogeneity imposed essentially by the Poisson formula and illustrated through Eq. (26), discreteness gives rise to an almost harmonic potential energy barrier of exponentially small width, which explains the exponentially small separation of the extrema of such a barrier observed in discrete systems [11,23,18].

(4) In the continuum limit, the $O(h^2)$ terms naturally disappear as $h \rightarrow 0$, but also the limit of the integrals with the rapidly oscillating integrands is well defined according to the Riemann-Lebesgue lemma: when $x \rightarrow \infty$ and if $\int f(z) dz$ exists, the limit of the definite integral $\int [f(z) \exp(ixz)] dz$ is always equal to zero.

(5) It should also be noted that, even though we have tried to keep the calculations as general as possible, it has been implicit and important in some points, such as the exponential smallness estimates, that we are interested in the dynamics of patterns or coherent structures in discrete and/or heterogeneous environments.

(6) Finally, a more general remark: The formal proof of the equivalence of the discrete potential energy with an appropriately chosen heterogeneous one predisposes us to accept the similarity of the relaxational or conservative dynamics driven by such a potential energy functional. Furthermore, the methodology of Sec. III and its successful numerical tests add to that belief. However, a note of caution is in order. The method of Sec. III is approximate. Were we to formally transform the dynamics, i.e., the time evolution of the discrete system, into that ones of a heterogeneous continuum system, a process similar to that carried out for V_d should also be performed for the LHS of Eq. (1). This would result in the presence of a $D(x)$ in the LHS, i.e., $D(x)$ would also multiply the temporal derivatives of the LHS. This means that the discrete system can be thought of as a continuum system where, by construction, in all of the terms of both LHS and RHS infinite weight has been placed on the lattice sites $x = nh$, as opposed to 0 weight on the rest of the line. This interpretation follows directly from the functional form of $D(x)$ and Eq. (22). Hence, this is not a conventional heterogeneous system. However, the analogy of the potential energies had as its scope to reveal the nature of the dominant power law as well as exponentially small terms in the functional; it also aimed to justify, *a posteriori*, the success of methods such as the one used in the previous section and to illustrate the similarities between heterogeneity and discreteness.

V. RELEVANCE AND USEFULNESS OF A DISCRETE TO HETEROGENEOUS TRANSFORMATION

In the previous sections, we have attempted to construct a transformation from a discrete to a heterogeneous system

that has the same “average” coherent structure dynamics. We have also attempted to give the general analogies between discrete and heterogeneous systems. One may naturally, however, enquire about the usefulness of such a transformation in relevant physical applications.

It is clear that the gain in using such a mapping is not a numerical one. In particular, to resolve a continuum but heterogeneous system, a finer computational grid is required that takes into account the details of the periodic functions $a(x;h), b(x;h)$ at a scale finer than h . In a discrete system, the periodicity is “encoded” in the integer shift translational invariance and hence no length scales finer than h need to be resolved.

On the other hand, however, there can be a significant gain in tackling the dynamics of a heterogeneous system rather than that of a discrete one by means of analytical calculations. In particular, the mathematical techniques that are much more well developed for heterogeneous rather than discrete systems include among others homogenization [24,13] which converts the heterogeneous system into a homogeneous one with appropriately “averaged” coefficients, and hence whose dynamics are much simpler to study; asymptotic expansions [12,25] and multiscale analysis [12,13] which can be used to determine the effective speed of coherent structures in heterogeneous media and hence predict, by comparing it to zero, approximately when propagation will fail in heterogeneous and hence also in discrete media; use of the degree theory approach of [26] and the continuation method of [27] in proving the existence and constructing coherent structure solutions of the heterogeneous periodic media [27,28] (see also [13]); use of general operator theoretic notions [29] to address the asymptotic stability of fronts or pulses in periodic media [13].

Notice that many of the above references and hence the corresponding techniques have been developed quite recently and thus it would be of considerable interest to use the mapping proposed here to “translate” our understanding of the heterogeneous systems’ dynamics into an understanding of discrete systems proper. This program can be carried out for the many applications of discrete systems mentioned in the Introduction and can potentially impact our understanding of areas as important and diverse as heart dynamics, chemical reactions, optical fibers, dislocations, or neuronal activity.

Another direction in which this mapping may be useful is the experimental one. Very recently, it has been appreciated that many systems amenable to experiments and as diverse as optical lattices in Bose-Einstein condensates (BEC’s) [30], quadratic nonlinear photonic crystals [31], calcium waves in the T tubules of cardiac cells [12], or chemical reactions in heterogeneous catalytic surfaces [32] are heterogeneous systems that through the appropriate transformation can be mapped into discrete systems. In particular, such mappings of heterogeneous to discrete systems, i.e., the inverse of the transformation performed here, involve either an amplitude expansion of the field [31] or a tight-binding approximation [30], both of which result in differential-difference equations for the discrete amplitude coefficients of the expansion. It should be noted that, at least in some of the

experiments, such as the optical lattices in BEC’s where one can modify the properties of the lasers forming the lattice, or in chemical reactions where one can construct different masks with different percentages of each catalyst or with various different catalysts, the properties of the heterogeneity are, in a sense, “tunable.” The realization that periodic heterogeneity of a tunable form can be mapped into discreteness can be very useful in studying the dynamics of various discrete systems through our “inverse” transformation. In particular, considering an intrinsically discrete system stemming from the physical application of interest, by performing the above transformation and using some of the freedom that it allows—see, e.g., the discussion below Eq. (19)—one can map the discrete system into a heterogeneous one relevant to one of the above experiments; then it will be possible to use the available continuum heterogeneous experimental data to understand the features of the discrete system or to motivate new experiments that, by tuning the heterogeneity appropriately, could provide results and conclusions relevant to the discrete system.

VI. CONCLUSIONS AND FUTURE CHALLENGES

In this work, we have used the Poisson formula to explicitly construct heterogeneous (and thus not translationally invariant) continuum systems that possess comparable leading order coherent structure dynamical effects to those in discrete systems. This is a program that can be generally carried out for systems of gradient type and that aims to capture, on the average, the behavior of the patterns of the discrete system. This program can equally well be carried out for modified (heterogeneous) diffusivity or modified (heterogeneous) substrate nonlinearity.

The ensuing inverse problem was solved by means of Fourier decomposition and appropriate selection of the Fourier components. The method was shown to work very well and in full agreement with the theoretical predictions for the specific example of a ϕ^4 field theory. Following that, a more general discussion was presented at the level of potential energies showing that the discrete system potential energy can always be converted to a continuum one on a heterogeneous substrate. The relevant power-law as well as exponentially small contributions to the functional were also revealed. The potential of application of such a transformation in understanding the dynamics of systems recently studied theoretically as well as experimentally has also been highlighted.

In all of the program presented here, the focus has been on the “average” properties of the patterns or nonlinear waves present in the PDE’s. On the other hand, one may imagine situations (see, e.g., [6] for an example) where discreteness and/or heterogeneity may have very delicate effects (such as the resonances observed in [6]). In such cases one may expect that a detailed dynamic picture of the attractors will be more necessary and that this “quick” effective description may miss some of the relevant phenomenology. Such a careful study of the limits of this and possibly more refined methodologies (such as ones based on the use of

more “informed” selection of *Ansätze* [12]) would clearly be desirable. In this spirit, we mention the recent work of Fiedler and Vishik on the quantitative homogenization of global attractors in near-gradient reaction-diffusion systems [33]. Such efforts are in progress and will be reported in future studies.

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- [1] S.P. Dawson, J. Keizer, and J.E. Pearson, Proc. Natl. Acad. Sci. U.S.A. **96**, 6060 (1999).
- [2] J.P. Keener, J. Theor. Biol. **148**, 49 (1991).
- [3] D.W. McLaughlin, R. Shapley, M. Shelley, and D.J. Wielaard, Proc. Natl. Acad. Sci. U.S.A. **97**, 8087 (2000); J. Rinzel, D. Terman, X.-J. Wang, and B. Ermentrout, Science **279**, 1351 (1998).
- [4] J.P. Laplante and T. Erneux, J. Phys. Chem. **96**, 4931 (1992).
- [5] A.V. Ustinov, T. Doderer, I.V. Vernik, N.F. Pedersen, R.P. Huebener and V.A. Oboznov, Physica D **68**, 41 (1994).
- [6] H.S.J. van der Zant, T.P. Orlando, S. Watanabe, and S.H. Strogatz, Phys. Rev. Lett. **74**, 174 (1995).
- [7] J. Kutz, C. Hile, W. Kath, R.-D. Li, and P. Kummar, J. Opt. Soc. Am. B **11**, 2112 (1994).
- [8] J.P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982).
- [9] M. Peyrard and A.R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989).
- [10] P.G. Kevrekidis and M.I. Weinstein, Physica D **142**, 113 (2000).
- [11] M. Peyrard and M.D. Kruskal, Physica D **14**, 88 (1984).
- [12] J.P. Keener, Physica D **136**, 1 (2000); SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. **61**, 317 (2000).
- [13] J. Xin, SIAM Rev. **42**, 161 (2000).
- [14] S.Y. Shvartsman, E. Schuetz, R. Imbihl, and I.G. Kevrekidis, Phys. Rev. Lett. **83**, 2857 (2000).
- [15] A.K. Bangia, M. Baer, M.D. Graham, I.G. Kevrekidis, H.-H. Rotermund, and G. Ertl, Chem. Eng. Sci. **51**, 1757 (1996).
- [16] N. Shigesada, K. Kawasaki, and E. Teramoto, Theor. Population Biol. **30**, 143 (1986).
- [17] T. Munakata and Y. Ishimori, Physica B & C **98B**, 68 (1979); J. Phys. Soc. Jpn. **51**, 3367 (1982).
- [18] K. Kladko, I. Mitkov, and A.R. Bishop, Phys. Rev. Lett. **84**, 4505 (2000).
- [19] See, e.g., J.M. Speight and R.S. Ward, Nonlinearity **7**, 475 (1994).
- [20] P.G. Kevrekidis, I.G. Kevrekidis, and A.R. Bishop, Phys. Lett. A **279**, 361 (2001).
- [21] R. Boesch, C.R. Willis, and M. El-Batanouny, Phys. Rev. B **40**, 2284 (1989).
- [22] R.V. Churchill and J.W. Brown, *Complex Variables and Applications* (McGraw-Hill, New York, 1996).
- [23] P.G. Kevrekidis, C.K.R.T. Jones, and T. Kapitula, Phys. Lett. A **269**, 120 (2000).
- [24] A. Bensoussan, J.L. Lions, and G. Papanicolaou, *Asymptotic Analysis for Periodic Structures*, Vol. 5 of Studies in Applied Mathematics (North-Holland, Amsterdam, 1978).
- [25] T.J. Lewis and J.P. Keener, SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. **61**, 293 (2000).
- [26] H. Berestycki, B. Nicolaenko, and B. Scheurer, SIAM (Soc. Ind. Appl. Math.) J. Math. Anal. **16**, 1207 (1985).
- [27] J.X. Xin, Arch. Ration. Mech. Anal. **121**, 205 (1992).
- [28] J.X. Xin, J. Stat. Phys. **73**, 893 (1993); Arch. Ration. Mech. Anal. **128**, 75 (1994).
- [29] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, New York, 1966).
- [30] A. Trombettoni and A. Smerzi, Phys. Rev. Lett. **86**, 2353 (2001).
- [31] A. Sukhorukov, Yu.S. Kivshar, O. Bang, and C.M. Soukoulis, Phys. Rev. E **63**, 016615 (2001).
- [32] S. Shvartsman, E. Schuetz, R. Imbihl, and I.G. Kevrekidis, Catal. Today (to be published); O. Runborg, C. Theodoropoulos, and I.G. Kevrekidis (unpublished).
- [33] B. Fiedler and M. I. Vishik, Fachbereich Mathematik und Informatik, FU Berlin, Reports No. A-11-2000 and No. A-18-2000, 2000 (unpublished).