General Non-Existence Theorem for Phase Transitions in One-Dimensional Systems with Short Range Interactions, and Physical Examples of Such Transitions

José A. Cuesta[1] **and Angel Sánchez**[1]

We examine critically the issue of phase transitions in one-dimensional systems with short range interactions. We begin by reviewing in detail the most famous non-existence result, namely van Hove's theorem, emphasizing its hypothesis and subsequently its limited range of applicability. To further underscore this point, we present several examples of one-dimensional short ranged models that exhibit true, thermodynamic phase transitions, with increasing level of complexity and closeness to reality. Thus having made clear the necessity for a result broader than van Hove's theorem, we set out to prove such a general non-existence theorem, widening largely the class of models known to be free of phase transitions. The theorem is presented from a rigorous mathematical point of view although examples of the framework corresponding to usual physical systems are given along the way. We close the paper with a discussion in more physical terms of the implications of this non-existence theorem.

KEY WORDS: Phase transitions; one-dimensional systems; short-range interactions; transfer operators; rigorous results.

1. INTRODUCTION

One-dimensional (1D) systems are among the most important and fruitful areas of research in Physics. This is due to the fact that such models are generally much more amenable to analytical calculations than higher-dimensional ones, while describing to a certain degree many problems of actual physical relevance. Indeed, exact results for 1D systems have offered

[1] Grupo Interdisciplinar de Sistemas Complejos (GISC), and Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Madrid, Spain; e-mail: {cuesta, anxo}@math.uc3m.es

deep insights about very many phenomena which subsequently have led to advances in much broader contexts. Remarkably, in spite of the large body of knowledge already available about this class of problems, 1D systems still are a continuous source of exciting new physics.[1, 2] This is so in spite of the unjustifiable prejudices or careless generalizations that prevent researchers from considering many 1D problems on the grounds of their lack of interest. This has been the case, for instance, with Anderson localization in 1D disordered systems: although all proofs in the literature are model dependent, for almost thirty years it has been regarded as a general dictum that any kind and amount of disorder will localize all electronic states in 1D. During this time, almost no researchers have studied localization in 1D as the previous statement amount to consider it a case closed. However, thanks to a few works carried out with critical attitude, we now know that in the presence of short-ranged[3] or long-ranged *correlated* disorder[4] bands of extended states do exist. Subsequently, the breakdown of the belief on the generality of 1D localization phenomena has paved the way to most relevant results, such as, e.g., the dependence of the transport properties of DNA on their information content (ref. 5; see also a partial retraction that does not affect the DNA part of the paper in ref. 6).

In this paper, we undertake the critique of another famous general statement, namely that there cannot be phase transitions in 1D systems with short range interactions. This assertion is practically never questioned (see ref. 7 for a recent exception), even though no general proof of it has ever been provided, an impossible task in view that counterexamples have been given more than thirty years ago as we will see below. The influence of this piece of received wisdom cannot be underestimated, and for the past fifty years has become an almost unsurmountable barrier for any research on 1D phase transitions. It is important then to remind the physics community of the limits of applicability of this result. To this end, we need to make the statement rigorous for the widest possible class of models. In doing so, (quasi) 1D physical systems exhibiting phase transitions will be again available for a host of applications; in addition, the possibility of using 1D models, often exactly solvable ones, to advantageously study phase transitions will be reopened.

To carry out this program, we proceed along two complementary directions. First, we review the existing results about non existence of phase transitions in short-ranged 1D systems. To our knowledge, these amount to a theorem proven by van Hove[8] for homogeneous fluid-like models, with pairwise interactions with a hard core and a cutoff, and in the absence of an external field, which was later generalized by Ruelle[9] to lattice models. We note that the well known argument by Landau[10] about domain walls

is heuristic and relies on approximate calculations; we will also comment briefly on this below. We then discuss several 1D models proposed in the past which exhibit true thermodynamic phase transitions; these models have different degrees of complexity and closeness to physical situations, and we will pay special attention to the specific reasons why each of them is not included in the existing theorems. Having thus established clearly the existence of phase transitions in 1D systems with short range interactions, we move to our second contribution, introducing rigorously a very general theorem on the impossibility of phase transitions in such models. As we will see, the theorem, which includes van Hove's and Ruelle's results as particular cases, gives sufficient but not necessary conditions to forbid phase transitions. We will also show how models not fulfilling one of the hypotheses exist which do have phase transitions and comment on the ways to violate those hypotheses. Finally, we conclude the paper with a discussion focused on the physics underlying the mathematical results presented.

2. VAN HOVE'S THEOREM

When one encounters the sentence "1D systems with short range interactions can not have phase transitions" in the literature, it is either considered public knowledge and not supported by a quotation, or else is directly or indirectly referred to a 1950 paper by van Hove, written in French.[8] Indeed, the above statement often receives the name "van Hove's theorem." However, there is nothing that general in the excellent work by van Hove, nor does he intend to mean it in his writing. It is very illuminating to quote the English abstract here:

> "The free energy of a one-dimensional system of particles is calculated for the case of non-vanishing incompressibility radius of the particles and a finite range of the forces. It is shown quite generally that no phase transition phenomena can occur under these circumstances. The method used is the reduction of the problem to an eigenvalue problem."

Let us expand some more on the abstract, in order to understand exactly what van Hove proved. He considered a system of N identical particles, lying on a segment of length L on positions x_i, $i = 1,\ldots, N$, $0 \leqslant x_i \leqslant L$. The potential energy of the system is given by

$$V = \sum_{i=1,\, i<j}^{N} U(|x_i - x_j|), \tag{1}$$

with

$$U(\xi) = \begin{cases} +\infty, & \text{if} \quad 0 \leqslant \xi \leqslant d_0, \\ 0, & \text{if} \quad \xi \geqslant d_1, \end{cases} \tag{2}$$

and $0 < d_0 < d_1$. We are thus faced with a system of hard-core segments of diameter d_0, that interact only at distances smaller than d_1; van Hove's remaining assumption about the interaction is that U is a continuous, bounded below function.

The way he proves this result is, as he himself says, by reducing the problem to an eigenvalue problem. He is able to write the partition function of the system in terms of a transfer operator, whose largest eigenvalue gives the only relevant contribution to the free energy in the thermodynamic limit. After transforming the operator into a more useful form, van Hove resorts to the theory of Fredholm integral operators and other theorems of functional analysis to show that this eigenvalue is an analytic function of temperature and, consequently, that the system can not have phase transitions, understood rigorously as nonanalyticities of the free energy. The mathematical basis of this result will be made clear by the theorem we will present later in this article, and therefore we do not need to go into further detail at this point (other than enthusiastically referring the interested reader to the original paper[8]). For the time being, suffice it to say that the basic idea is an extension of the well-known Perron–Frobenius theorem for non-negative matrices;[11, 12] we will come back to this theorem when discussing our first example in the next section.

The key point we want to make here relates to the *hypotheses needed to prove van Hove's theorem, i.e., to the class of systems to which it applies*. Let us consider them separately:

Homogeneity. First of all, the system has to be perfectly homogeneous, made up of *identical* particles. This automatically excludes any inhomogeneous model, where inhomogeneous means either aperiodic or disordered. Periodic systems could in principle be included in the frame of van Hove's theorem by analyzing the transfer operator for a unit cell. This is a very strong restriction, and it should be very clear that any degree of inhomogeneity in the system makes it impossible to exclude phase transitions on the ground of van Hove's result.

No External Fields. van Hove's choice for the potential energy does not include terms depending on the position of the particles x_i alone, i.e., they only depend on relative interparticle distances. The simplest way to have those terms in the potential is by introducing external fields. With such an addition the model does not satisfy the hypothesis of van Hove's theorem and might therefore have phase transitions.

Hard-core Particles. We do not need to insist much on the finite range of the interaction potential, as this is almost always included in any

statement about the impossibility of phase transitions in 1D systems. It is much less known, however, that the validity of van Hove's result requires a hard core potential as well, meaning that it does not apply to point-like or soft particles.

Of these three conditions, the theorem we will introduce below will relax very much the second and third restrictions, although we will also present counterexamples showing that the theorem cannot be extended to include any external field. Our work leaves open the question as to the types of external fields that may give rise to a phase transition. As for the first condition, however, we will say nothing about the inhomogeneous case. This is a much more complicated question, far beyond the scope of the present work, and that is why we want to stress here that there is no known theorem forbidding phase transitions in 1D inhomogeneous systems. As a matter of fact, their existence is largely acknowledged within the community working on the so called "2D wetting" on disordered substrates,[13] a phenomenon described by inhomogeneous 1D models.

To conclude this section, a comment is in order about extensions and generalizations of van Hove's theorem. The most relevant one is due to Ruelle,[9, 14] who proved the lattice version of the theorem under the same basic hypotheses (earlier, Rushbrooke and Ursell proved it for the lattice gas with finite neighbor interaction[15]). As for the finite range of the interactions, the work of Ruelle[14] and Dyson[16] proved that pair interactions decaying as $1/r^2$ (r being the distance between variables) represent the boundary between models with and without phase transitions. Subsequently, Fröhlich and Spencer[17] showed that case $1/r^2$ was to be included in those with phase transitions. We do not know of further results in this direction, and therefore this is as much as can be safely said about systems having or not having phase transitions in 1D.

3. EXAMPLES OF 1D MODELS WITH PHASE TRANSITIONS

After reviewing the available results about non-existence of phase transitions in 1D systems with short-range interactions, we now present some selected examples where there indeed are true thermodynamic phase transitions in spite of their 1D character and the range of their interactions. We proceed in order of difficulty, and try to cover the three main levels of transfer operators: finite matrices, infinite matrices and integral operators. Our first example is actually very simple, and will allow us to review the transfer matrix formalism. Both this one and the second model are exactly solvable, and will make it clear that phase transitions are certainly possible. The third model can be written in terms of a transfer operator as well, but the corresponding eigenvalue problem can only be solved numerically.

3.1. Kittel's Model

3.1.1. Model Definition

The first system we consider was proposed by Kittel in 1969,[18] and is closely related to another one introduced by Nagle a year earlier[19] as a simple model of KH_2PO_4 (usually known as KDP), which exhibits a first-order phase transition as well. Incidentally, both papers were published in *American Journal of Physics*, which points to the very pedagogical character of these models. Kittel's model is in fact a single-ended zipper model, discussed "as a good way to introduce a biophysics example into a course on statistical physics," and inspired in double-ended zipper models of polypeptide or DNA molecules.

Kittel's model is as follows. Let us consider a zipper of N links that can be opened *only from one end*. If links 1, 2,..., n are all open, the energy required to open link $n+1$ is ϵ; however, if not all the preceding links are open, the energy required to open link $n+1$ is infinite. Link N cannot be opened, and the zipper is said to be open when the first $N-1$ links are. Further, we suppose that there are G orientations which each open link can assume, i.e., the open state of a link is G-fold degenerated. As we will see below, there is no phase transition if $G=1$, whereas for larger degeneracy a phase transition arises. In ref. 18 the partition function is expressed as a geometric sum which can be immediately obtained, and subsequently all the magnitudes of interest can be calculated as well. Nevertheless, in order to introduce the context of this work, namely the transfer operator formalism, we will solve Kittel's model in terms of a transfer matrix (Kittel's way is much simpler, see ref. 18, but it is not a general procedure). To this end, let us write the model Hamiltonian as

$$\mathscr{H}_N = \epsilon(1-\delta_{s_1,0}) + \sum_{i=2}^{N-1} (\epsilon + V_0\delta_{s_{i-1},0})(1-\delta_{s_i,0}) \tag{3}$$

where $s_i = 0$ means that link i is closed, $s_i = 1, 2,..., G$ means that the link is open in one of the possible G states, and $\delta_{s,s'}$ is the Kronecker symbol. Note that Kittel's constraint on the zipper corresponds to the choice $V_0 = \infty$, and that we have also imposed the boundary condition $s_N = 0$ (the rightmost end of the zipper is always closed). The partition function will then be given by

$$\mathscr{Z}_N = \sum_{\text{config.}} \exp(-\beta\mathscr{H}_N), \tag{4}$$

with $\beta = 1/k_BT$ being the inverse temperature and where the sum is to be understood over all configurations of the variables s_i, $i = 1,..., N-1$.

3.1.2. Transfer Matrix Solution

The transfer matrix formalism to compute the partition function is a well-known technique in equilibrium Statistical Mechanics that can be found in most textbooks (see, e.g., refs. 20–22). To implement this procedure, we rewrite the partition function as

$$\mathscr{Z}_N = \sum_{\text{config.}} e^{-\beta\epsilon(1-\delta_{s_1,0})} \prod_{i=1}^{N-2} e^{-\beta\epsilon(1-\delta_{s_{i+1},0})}[1+(e^{-\beta V_0}-1)\,\delta_{s_i,0}(1-\delta_{s_{i+1},0})]. \quad (5)$$

From now on, we follow Kittel and let $V_0 = \infty$, which implies that $e^{-\beta V_0} = 0$. We introduce the transfer matrix $\mathbf{T} = (t_{s,s'})$, defined as

$$t_{s,s'} = e^{-\beta\epsilon(1-\delta_{s',0})}[1-\delta_{s,0}(1-\delta_{s',0})], \quad (6)$$

or in $(G+1)\times(G+1)$ matrix form

$$\mathbf{T} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & a & \cdots & a \\ \vdots & \vdots & & \vdots \\ 1 & a & \cdots & a \end{pmatrix}, \quad (7)$$

where $a \equiv e^{-\beta\epsilon}$. It is very important to realize that the constraint that link s_{i+1} cannot be open (cannot take the values 1, 2,..., 6) if link s_i is closed ($s_i = 0$) yields the null entries in the first row of $\mathbf{T}$.

The partition function can thus be recast in the form

$$\mathscr{Z}_N = (1 \quad a \quad \cdots \quad a)\,\mathbf{T}^{N-2} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \quad (8)$$

Matrix $\mathbf{T}$ has three different eigenvalues, namely $\lambda_1 = Ga$, $\lambda_2 = 1$, and $\lambda_3 = 0$ (with multiplicity $G-1$). The eigenvectors of the two nonzero eigenvalues are, respectively,

$$\mathbf{v}_1 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \qquad \mathbf{v}_2 = \begin{pmatrix} 1-Ga \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \quad (9)$$

so, if we express

$$\begin{pmatrix} 1 \\ a \\ \vdots \\ a \end{pmatrix} = \frac{a(1-Ga)-1}{1-Ga}\,\mathbf{v}_1 + \frac{1}{1-Ga}\,\mathbf{v}_2, \qquad \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = \frac{-Ga}{1-Ga}\,\mathbf{v}_1 + \frac{1}{1-Ga}\,\mathbf{v}_2, \quad (10)$$

we arrive finally at

$$\mathscr{Z}_N = \frac{1-(Ga)^N}{1-Ga} = \frac{1-(Ge^{-\beta\epsilon})^N}{1-Ge^{-\beta\epsilon}} \quad (11)$$

in agreement with Kittel's result[18] or, alternatively,

$$\mathscr{Z}_N = \frac{1}{1-Ge^{-\beta\epsilon}}\,(-\lambda_1^N + \lambda_2^N) \quad (12)$$

which is more suitable to our purposes, and shows the general structure of transfer matrix results: the partition function is expressed as a linear combination of Nth powers of the transfer matrix eigenvalues. In the thermodynamic limit, only the contribution of the largest eigenvalue remains, and we have, as $N \to \infty$, that the free energy is given by

$$f \equiv \frac{1}{N}\mathscr{F} \equiv -\frac{1}{\beta N}\ln \mathscr{Z}_N = -\frac{1}{\beta}\ln \max(\lambda_1, \lambda_2). \quad (13)$$

We are thus faced with the crux of the matter: in order to have a phase transition, meaning a nonanalyticity of the free energy—given that the eigenvalues are positive, analytic functions of β—we need two eigenvalues to cross at a certain β_c. In our problem, we only have to compare λ_1 and λ_2 to find that they cross at a temperature given by $\beta_c = \ln G/\epsilon$, or, equivalently, $T_c = k_B\epsilon/\ln G$; above (below) T_c, λ_1 (λ_2) is the largest eigenvalue (see Fig. 1). At T_c, the derivative of the free energy is discontinuous marking the existence of a phase transition. It is interesting to note that $T_c = k_B\epsilon/\ln G$ is finite as long as $G > 1$; for the non-degenerate case $G = 1$ (only one open state) the transition takes place at $T = \infty$ or, in other words, there is no phase transition.

3.1.3. Discussion

We are now in a position to explain in more detail the mathematical reasons underlying these results as well as, generally speaking, van Hove's theorem on the absence of phase transitions. In the preceding section we

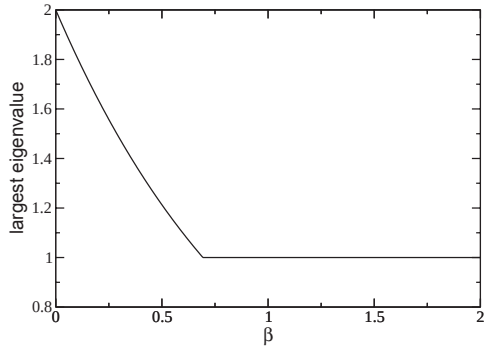

Fig. 1. Largest eigenvalue of the transfer matrix for Kittel's model with $G = 2$ vs inverse temperature, with $\epsilon = 1$. Note the nonanalyticity at $\beta = 1/\ln 2$.

mentioned that van Hove's theorem relies on an extension of the Perron–Frobenius theorem for matrices to integral operators; however, for our discussion of Kittel's model, we need only the original result by Perron and Frobenius:[11, 12]

Theorem 1 (Perron–Frobenius). Let $\mathbf{A}$ be a non-negative (all its elements are non-negative), irreducible matrix; then its spectral radius (maximum eigenvalue) $\rho(\mathbf{A}) > 0$ is an eigenvalue of algebraic multiplicity one.

A matrix $\mathbf{A}$ is *irreducible* if there does not exist a permutation matrix $\mathbf{P}$ such that

$$\mathbf{P}^t\mathbf{A}\mathbf{P} = \begin{pmatrix} \mathbf{X} & \mathbf{Y} \\ \mathbf{0} & \mathbf{Z} \end{pmatrix} \tag{14}$$

with both $\mathbf{X}$ and $\mathbf{Z}$ being square submatrices.

Let us note that this theorem is not enough for our purposes, because we are not dealing with a specific matrix; instead, we are considering a family of matrices depending on temperature, $\mathbf{T}(\beta)$. We also need the following result (see ref. 23, Section II.1.8), valid for matrices analytic in β (all their elements are analytic functions of β):

Theorem 2. For every β in a simply connected set $D \subset \mathbb{C}$, let $\mathbf{T}(\beta)$ be a linear operator on an n-dimensional vector space X (i.e., $\mathbf{T}(\beta)$ is an $n \times n$ complex matrix). Assume that $\mathbf{T}(\beta)$ is analytic in D. Let Σ be a subset of eigenvalues of $\mathbf{T}(\beta)$ whose number, s, remains constant for all $\beta \in D$ (i.e., eigenvalue splitting does not occur). Then each eigenvalue of Σ has

constant multiplicity and can be expressed as an analytic function in D, $\lambda_j(\beta)$ ($j = 1,\ldots, s$).

So for a non-negative, irreducible transfer matrix $\mathbf{T}(\beta)$ whose elements are analytic functions in a neighborhood of the positive real axis, $\beta > 0$, Theorems 1 and 2 imply that the maximum eigenvalue (hence the free energy) is an analytic function of β, for all $\beta > 0$.

We can now turn to the reasons as to why there is a phase transition in Kittel's model. We stress that transfer matrices, made up from Boltzmann factors, i.e., exponentials, are always strictly positive and, consequently, irreducible and analytic in β. Under these conditions there cannot be a phase transition for any finite $\beta > 0$. Therefore, the only way we can escape the hypothesis of the Perron–Frobenius theorem is by assigning an infinite energy to some configurations, thus giving rise to null entries in the matrix, which may or not then be irreducible. This is exactly the case in Kittel's model. It is important to realize that breaking the irreducibility hypothesis does not ensure eigenvalue crossing: Kittel's model transfer matrix for the non-degenerate case, $G = 1$, is also reducible, and the eigenvalue crossing takes place only at $\beta = 0$, as we have already explained, yielding the analyticity of the maximum eigenvalue (hence of the free energy) for any finite temperature.

Summarizing, Kittel's model has allowed us to show how phase transitions can take place in 1D models whose statistical mechanics can be computed with $n \times n$ matrices or, equivalently, in 1D lattice models with a finite number of states per node and finite range of interactions. Due to the nature of the transfer matrix and the theorems that apply to it, phase transitions are impossible (with the caveat about boundary conditions discussed in Section 4.3.1) unless there are forbidden (infinite energy) configurations, but fulfilling this condition does not necessarily induce a phase transition. As we will now see, this clear-cut conclusion will become more and more complicated as transfer matrices of infinite size or integral transfer operators are considered. The next two subsections will discuss briefly two such examples before proceeding to the detailed, rigorous discussion of the corresponding theorems.

3.2. Chui–Weeks's Model

We now proceed in order of increasing mathematical complexity and consider a model in which the transfer matrix has infinite size. The specific example we consider was proposed by Chui and Weeks[24] and is given by the following Hamiltonian:

$$\mathscr{H}_N = J \sum_{i=1}^{N} |h_i - h_{i+1}| - K \sum_{i=1}^{N} \delta_{h_i, 0}. \tag{15}$$

This is a typical instance of the family of models called solid-on-solid (SOS) for surface growth, in which h_i stands for the height above site i of the lattice; the reason for the name SOS is that overhangs are not allowed, i.e., the surface profile is single-valued. We will consider that heights can take on only integer values and that there is an impenetrable substrate, imposing $h_i \geqslant 0$. In this context, the first term represents the contribution of surface tension to the total energy, and the second one introduces an energy binding the surface to the substrate. As we will comment below, this is crucial for the model to exhibit a phase transition. Interestingly, these systems have often been considered as two-dimensional ones because of the fact that they represent interfacial phenomena on a plane, and therefore they have been considered not relevant for the 1D phase transition issue. We stress here that the fact that h_i stands for a height does not change the 1D nature of the model, as it could equally well represent any other magnitude or internal degree of freedom, not associated to a physical dimension.

Instead of following Chui and Weeks's presentation, which is very simple but does not lead to explicit results, we resort to an alternative derivation proposed as Exercise 5.7 in Yeomans's textbook.[25] We will not go here into the details of the derivation and quote only its main steps. A transfer matrix for the model is evidently

$$(\mathbf{T})_{ij} \equiv e^{-\beta J\,|i-j|}[1+(e^{-\beta K}-1)\,\delta_{i,0}], \qquad i, j = 1, 2, \ldots . \tag{16}$$

Note that the matrix dimension is actually infinite, as announced, and stems from the fact that the amount of possible states (heights) at any site of the lattice is infinite. It is also important to realize that in this case none of the entries in the matrix is zero, so we have a strictly positive matrix, although out of the scope of the theorems discussed above because of its infinite dimension.

For simplicity, we introduce the notation $\omega \equiv e^{-\beta J}$, $\kappa \equiv e^{-\beta K}$. Then, by considering eigenvectors of the form

$$\mathbf{v}_q \equiv (\psi_0, \cos(q+\theta), \cos(2q+\theta), \ldots), \tag{17}$$

it is a matter of algebra to show that there is a continuous spectrum of eigenvalues,

$$\sigma(\mathbf{T}) = \left[\frac{1-\omega}{1+\omega}, \frac{1+\omega}{1-\omega}\right]. \tag{18}$$

The phase transition arises because, in the range of temperatures such that $\kappa > 1/(1-\omega)$, there is an additional eigenvector,

$$\mathbf{v}_0 \equiv (\psi_0, e^{-\mu}, e^{-2\mu}, \ldots) \tag{19}$$

with eigenvalue

$$\lambda_0 = \frac{\kappa(1-\omega^2)(\kappa-1)}{\kappa(1-\omega^2)-1}, \tag{20}$$

which, when it exists, is the largest eigenvalue. Thus, we have found again another case of eigenvalue crossing in the transfer matrix, which indicates the existence of a phase transition. The physics of the transition is that, for temperatures below T_c, the temperature at which $\kappa = 1/(1-\omega)$, the surface is bound to the substrate and henceforth is macroscopically flat; on the contrary, above T_c the surface becomes free and its width is unbounded. This is an example of the so called roughening (or wetting, depending on the context) transitions.

It is interesting to observe that, if the substrate is not impenetrable and all integer values from $-\infty$ to ∞ are allowed for the variables h_i, the transition disappears, and the surface is always pinned to the line $h_i = 0$,[24] meaning that it is flat at all temperatures. As discussed by Chui and Weeks, this is closely related to the fact that, in Quantum Mechanics, a potential well always has a bound state if it is located within the infinite line $[-\infty, \infty]$, while it needs special parameters to have a bound state if the well is at the left side of the semi-infinite line $[0, \infty]$. This comment will be in order later, when discussing the general theorem on the absence of phase transitions, because we will point out that the range of definition of the transfer operator can be crucial to suppress or to allow phase transitions.

3.3. Dauxois–Peyrard's Model

We conclude this section on examples of phase transitions in 1D systems with short range interactions by considering the situation in which the model is still defined on a lattice, but the variables at the lattice sites are real valued. In this case, the infinite transfer matrix of the previous subsection becomes an integral transfer operator, as we will see below. A good instance of this class of problems is the extension of the model we have just discussed to real-valued heights, studied by Burkhardt.[26] A transfer operator for Burkhardt's model is

$$\mathbf{T}\phi(h) = \int_0^\infty dh' \exp[-\beta(J\,|h-h'| + \tfrac{1}{2}(U(h)+U(h')))]\,\phi(h'), \tag{21}$$

where $U(h)$ is the potential well binding the surface to the substrate, generalizing the Kronecker delta in Chui–Weeks's model. We will not discuss Burkhardt's results in detail as they are qualitatively the same as in the discrete height version, including the suppression of the phase transition by considering a doubly infinite range for h. Let us simply point out that, in this case, the analogy with the quantum-mechanical problem, mentioned at the end of the previous subsection, of the existence of bound states in a 1D well becomes exact, as the statistical mechanical problem can be mapped to a Schrödinger equation. We refer the interested reader to ref. 26 for details.

In order to include examples taken from different contexts, we want to discuss in this section a model for DNA denaturation, that, in addition, is a much more realistic model than the toy model introduced by Kittel and discussed in detail above. The model was proposed in ref. 27 (see ref. 28 for recent results; see ref. 29 for a brief review on DNA denaturation models), and we will refer to it as Dauxois–Peyrard's model. The corresponding Hamiltonian is

$$\mathscr{H}_N = \sum_{i=1}^{N} [\tfrac{1}{2} m\dot{y}_n^2 + D(e^{-\alpha y_n} - 1)^2 + W(y_n, y_{n-1})], \tag{22}$$

where the variable y_n represents the transverse stretching of the hydrogen bonds connecting the two base pairs at site n of the double helix of DNA (note that the molecule is supposed to be homogeneous). The first term in the Hamiltonian is the kinetic energy, with m being the mass of the base pairs; the second term, a Morse potential, represents not only the hydrogen bonds between base pairs but also the repulsion between phosphate groups and solvent effects; finally, the stacking energy between neighboring base pairs along each of the two strands is described by the anharmonic potential

$$W(y_n, y_{n-1}) = \frac{K}{2} [1 + \rho e^{-\alpha(y_n + y_{n-1})}](y_n - y_{n-1})^2. \tag{23}$$

Once again, the partition function of the model can be written in terms of an integral transfer operator, which in this case is given by [compare with Eq. (21)]

$$\mathbf{T}\phi(y) = \int_{-\infty}^{A} dx \exp[-\beta(W(y, x) + \tfrac{1}{2}[V(y) + V(x)])]\, \phi(x) \tag{24}$$

where the upper limit in the integral, A, is a cutoff introduced for technical reasons, but the limit $A \to \infty$ is well defined.

The problem with the Dauxois–Peyrard model is that it is not possible to solve exactly for the eigenvalues of the transfer operator. However, in ref. 27 the combined use of analytical approximations and numerical computation of the eigenvalues allowed the authors to provide compelling evidence for a phase transition in the anharmonic case [$\alpha \neq 0$ in the Hamiltonian (23)]. Indeed, their numerical results show, much as in the Chui–Weeks's model, a single eigenvalue in the discrete spectrum that merges the band of the continuous spectrum at a finite temperature. The result agrees very well with numerical simulations of the model, showing that above the critical temperature the double strand denaturates (i.e., the two strands separate to a macroscopically large distance or, equivalently, the mean value of y_n diverges), whereas below the critical temperature the two strands remain bound. Most interestingly, the predictions of the model compare very well with experiments on short chains.[30] The authors claim[28] that van Hove's theorem does not apply here, among other reasons, because of the presence of the external field term given by the Morse potential. Actually, we want to go beyond their claim and stress that van Hove's theorem has nothing to do with this model, because it does not fulfill other hypotheses as well (although, admittedly, the most noticeable violation is the external potential, which breaks the required translation invariance). Therefore, this phase transition should not be discussed in the framework of van Hove's theorem: As we will see in the next section, the transfer operator is likely to be excluded of the more general theorem we will present, thus making it possible the existence of this phase transition.

4. A GENERAL THEOREM ON THE NON-EXISTENCE OF PHASE TRANSITIONS

Once established the existence of phase transitions in one-dimensional systems with finite-range interaction, we will consider the formulation of an impossibility theorem sufficiently general as to include all known particular cases of proven nonexistence of phase transitions (namely, the theorems of van Hove,[8] Ruelle,[9, 14] and Perron–Frobenius,[11, 12] at least).

Our guideline to look for such a generalization will be the Perron–Frobenius theorem for nonnegative matrices. This theorem applies to homogenous lattice models in which the state variables defined on each node take on values from a finite set (like, e.g., Ising or Potts variables) and interact only with a finite set of neighbors. The partition function of those models can be defined in terms of the eigenvalues of a finite nonnegative (its elements are Boltzmann's factors) transfer matrix, the kind of object to which Perron–Frobenius theorem applies. But general one-dimensional models may differ from those lattice models in at least one of two ways:

they can be continuum models, and state variables can take values on an infinite (either discrete or continuum) set. In these cases the partition function can be expressed in terms of a transfer operator on a certain infinite-dimensional linear space. Integral operators or infinite matrices are two particular instances of such operators, but they are not the only ones.

The problem to generalize Perron–Frobenius theorem to operators more general than finite matrices is to extend the notions of nonnegativeness and irreducibility. This amounts to equip functional spaces with an order which allows comparing functions (at least in certain cases). The theory resulting from introducing order in Banach spaces and its consequences for the spectral theory of linear operators defined on them has been a topic of active research for mathematicians for quite some time,[31, 32] and it is at the heart of this realm where the desired extension is found.

4.1. Mathematical Background

Much as the proof of non-existence of phase transitions in 1D lattice models with finite-state variables interacting through a short-range potential is based upon Perron–Frobenius theorem, that of general 1D models is based on a generalization of that theorem to a class of transfer operators. Such a generalization, known as Jentzsch–Perron theorem (a special case of which was employed by van Hove to obtain his result[8]) reads as follows (the present statement is a slightly simplified version of Corollary 4.2.14 on p. 273 of ref. 31):

Theorem 3 (Jentzsch–Perron). Let E be a Banach lattice and $\mathbf{T} \neq 0$ a linear, positive, irreducible operator in E. Assume $\mathbf{T}^k$ is compact for some $k \in \mathbb{N}$. Then its spectral radius $\rho(\mathbf{T}) > 0$ is an eigenvalue of $\mathbf{T}$ with multiplicity one.

The proof of this theorem roots deeply into the theory of Banach lattices. The interested reader is urged to study the specialized literature[31, 32] to discover the rich structure that order induces in ordinary Banach spaces. Instead of that, we are simply giving here the necessary clues to make this theorem a practical tool to investigate phase transitions in models whose partition function can be written in terms of a transfer operator.

4.1.1. Banach Lattices in a Nutshell

A vector space, E, is said to be an *ordered vector space* if a partial order ($\leqslant$) is defined between its elements such that if f, g are elements of E, (i) $f \leqslant g$ implies $f + h \leqslant g + h$ for any $h \in E$ and (ii) $f \geqslant 0$ implies $\alpha f \geqslant 0$

for every $\alpha \geqslant 0$ in $\mathbb{R}$ (we then say that the order is *compatible* with the vector space structure). If $(E, \leqslant)$ is also a *lattice* (a mathematical notion not to be confused with physical lattices), i.e., if for any $f, g \in E$, $\sup\{f, g\}$ and $\inf\{f, g\}$ are in E, then we call E a *Riesz space*.

In a real Riesz space it makes sense to define the *absolute value* of a vector as $|f| = \sup\{f, -f\}$, because a Riesz space is a lattice. The extension of this notion to complex Riesz spaces is $|f| = \sup\{\mathrm{Re}(fe^{-i\theta}), 0 \leqslant \theta < 2\pi\}$ (notice that the latter definition reduces to the former one for real elements of the Riesz space). This element, though, is not guaranteed to belong to the Riesz space or even to exist at all.

When a Riesz space E has a norm, $\|\cdot\|$, such that for $f, g \in E$, $|f| \leqslant |g|$ implies $\|f\| \leqslant \|g\|$ (i.e., *compatible* with the order), then E is a *normed Riesz space*. If the normed Riesz space E is complete in the norm (i.e., every Cauchy sequence converges in E or, in other words, if E is a Banach space), then E is called a *Banach lattice*. In a complex Banach lattice, completeness ensures that $|f|$ (see above) is always a well-defined element of it.

Physically Relevant Examples of Banach Lattices. The most common Banach spaces are also Banach lattices with the natural order. For instance, l^p $(1 \leqslant p < \infty)$, the sequences $x = (x_n)_{n \in \mathbb{N}}$ of complex numbers with $\sum_{n \in \mathbb{N}} |x_n|^p < \infty$, ordered componentwise (i.e., for $x, y \in l^p$, $x = (x_n)_{n \in \mathbb{N}}$, $y = (y_n)_{n \in \mathbb{N}}$, we say that $x \leqslant y$ if $\mathrm{Re}\, x_n \leqslant \mathrm{Re}\, y_n$ and $\mathrm{Im}\, x_n \leqslant \mathrm{Im}\, y_n$). We have the same property for spaces $L^p(X, \mu)$, the complex functions on the point set X (to be precise, the classes of functions which are equal "almost everywhere") having $\int_X |f|^p \, d\mu < \infty$. The order is then pointwise almost everywhere, i.e., for $f, g \in L^p(X, \mu)$, $f \leqslant g$ if $\mathrm{Re}\, f(x) \leqslant \mathrm{Re}\, g(x)$ and $\mathrm{Im}\, f(x) \leqslant \mathrm{Im}\, g(x)$ for all $x \in X$, except for a set of vanishing μ-measure.

4.1.2. Linear Operators on Banach Lattices

An important subset of a Riesz space is its *positive cone*, $E_+ = \{f \in E : f \geqslant 0\}$. A linear operator, $\mathbf{T}: E \mapsto E$ is said to be a *positive operator* if $\mathbf{T}E_+ \subset E_+$. Every positive operator in a Banach lattice is automatically (norm) bounded. We say that one such linear operator is *irreducible* if the only invariant ideals are $\{0\}$ and E. In short, a vector subspace $A \subset E$ is an *ideal* of the Riesz space E if for any $x \in A$ it contains all $y \in E$ such that $|y| \leqslant |x|$. As we will show below, for some very common types of operators there is a simpler characterization of irreducibility.

We say that $\mathbf{T}$ is a *compact operator* if it maps the unit ball ($\{x \in E : \|x\| \leqslant 1\}$) in a relatively compact set (one whose closure is a compact set)

of E. Compact operators are the closest to finite matrices because of the very simple structure of their spectra.[31] The continuous and residual spectra of compact operators are empty. Also, every $\lambda \neq 0$ in the spectrum is an eigenvalue of finite multiplicity. There is a finite or countable number of eigenvalues, and if not finite, they can be arranged in a sequence $(\lambda_n)_{n \in \mathbb{N}}$ such that $\lambda_n \to 0$ as $n \to \infty$ ($\lambda = 0$ may or may not be itself an eigenvalue). Thus each $\lambda_n \neq 0$ is an isolated point in the spectrum. In general, one of the easiest ways to prove that an operator is *not* compact is showing that part of its spectrum is continuous.

Physically Relevant Examples of Linear Operators. In the Banach lattice $\mathbb{C}^n$ every linear operator (an $n \times n$ complex matrix) is, of course, compact. In ℓ^2 a linear operator $\mathbf{T}$ can be represented by an "infinite by infinite" matrix $(t_{ij})_{i,j \in \mathbb{N}}$. A sufficient (not necessary) condition for $\mathbf{T}$ to be compact is $\sum_{i,j \in \mathbb{N}} |t_{ij}|^2 < \infty$; or if $\mathbf{T}$ is of the special type that $t_{ij} = 0$ for $|i-j| > r$, for some fixed r (a $2r+1$-diagonal operator), then a necessary and sufficient condition for $\mathbf{T}$ to be compact is $\lim_{ij \to \infty} t_{ij} = 0$ (i.e., every diagonal is a null sequence).[33] In $L^2(X, \mu)$, an integral operator $(\mathbf{T}f)(x) = \int_X t(x, y)\, f(y)\, d\mu_y$ with a kernel $t(x, y)$ of the Hilbert–Schmidt type (i.e., with $\int_{X^2} |t(x, y)|^2\, d\mu_x\, d\mu_y < \infty$) is compact.

For these particular classes of operators there are also simpler tests of irreducibility. In the case of $\mathbb{C}^n$ or ℓ^2, $\mathbf{T} = (t_{ij})$ is reducible if and only if there exists a finite nonempty subset $A \subset \mathbb{N}$ such that $\sum_{i \in A} \sum_{j \in A^c} t_{ij} = 0$ (A^c stands for the complementary set of A). Likewise, in the case of a Hilbert–Schmidt integral operator in $L^2(X, \mu)$, $\mathbf{T}$ is reducible if and only if there exists $A \subset X$ with $0 < \mu(A) < \mu(X)$ such that $\int_{A^c} \int_A |t(x, y)|^2\, d\mu_x\, d\mu_y = 0$.

4.1.3. Analyticity of the Spectrum

As in the case of finite matrices, there only remains to complete this theorem with another one which guarantees the analyticity of the maximum eigenvalue. Such a theorem is (from ref. 23, Section VII.1.3):

Theorem 4. For every β in a simply connected set $D \subset \mathbb{C}$, let $\mathbf{T}(\beta)$ be a linear operator in a closed domain of a Banach space X (hence $\mathbf{T}(\beta)$ is a bounded operator). Assume that $\mathbf{T}(\beta)$ is analytic in D either in the strong or in the weak convergence sense. Let Σ be any finite set of isolated eigenvalues of $\mathbf{T}(\beta)$ whose number of elements is constant in D. Then each eigenvalue has constant multiplicity and can be expressed as an analytic function in D, $\lambda_j(\beta)$ ($j = 1, \ldots, |\Sigma|$).

4.2. The Theorem

We are now in a position to formulate our result in precise terms. Let us consider any statistical mechanical model whose partition function can be expressed as

$$\mathscr{Z}_N = \varphi(\mathbf{T}(\beta)^N), \tag{25}$$

where $\mathbf{T}(\beta)$ is a transfer operator of any kind for every $\beta > 0$, and $\varphi(\cdot)$ is a real, linear functional. Typical instances of φ are $\varphi(\mathbf{T}) = \mathrm{tr}(\mathbf{T})$, or $\varphi(\mathbf{T}) = \langle f, \mathbf{T}g \rangle$ with $\langle \cdot, \cdot \rangle$ a scalar product, as in Kittel's model [cf. Eq. (8)], etc. Notice in passing that the partition function of every 1D model with short-range interaction fits in Eq. (25), but not only. Models in $D > 1$ can also have a partition function given by Eq. (25); the only constraint is that $\mathbf{T}$ does not depend on N.

For such models we can now state the following theorem, consequence of Theorems 3 and 4, which defines a class of models for which there is *no* phase transition:

Theorem 5 (Nonexistence of Phase Transitions). Let $\mathbf{T}(\beta)$ be a compact, positive, irreducible, linear operator on the Banach lattice E for every β in a complex neighborhood containing $\beta > 0$. Let $\lambda_{\max}(\beta)$ and $\mathbf{P}_{\max}(\beta)$ be, respectively, the maximum eigenvalue of $\mathbf{T}(\beta)$ and the projector on its corresponding eigenspace. Let $\varphi(\cdot)$ be a real, linear functional on the space of bounded, linear operators on E such that $\varphi(\mathbf{P}_{\max}(\beta)) \neq 0$. Then

$$\lim_{N \to \infty} \frac{1}{N} \ln \mathscr{Z}_N = -\ln \lambda_{\max}(\beta) \tag{26}$$

is an analytic function on $\beta > 0$, where $\mathscr{Z}_N$ is given by Eq. (25).

Proof. Since $\mathbf{T}(\beta)$ is compact we know that its spectrum is purely discrete and of the form $\sigma(\mathbf{T}(\beta)) = \{\lambda_n(\beta)\}_{n \in I}$, where I is a finite or countable set of indices. Zero may or not be included, and, if I is countable, the remaining eigenvalues can be sorted in such a way that $\lambda_n \to 0$ as $n \to \infty$. Then

$$\mathscr{Z}_N = \sum_{n \in I} \lambda_n(\beta)^N \varphi(\mathbf{P}_n(\beta)). \tag{27}$$

Notice that if I is countable, the above series will be convergent for sufficiently large N. By factoring $\lambda_{\max}(\beta)$ out of the series

$$\mathscr{Z}_N = \lambda_{\max}(\beta)^N [\varphi(\mathbf{P}_{\max}(\beta)) + \epsilon_N], \quad \epsilon_N = \sum_{n \in I'} \left(\frac{\lambda_n(\beta)}{\lambda_{\max}(\beta)} \right)^N \varphi(\mathbf{P}_n(\beta)), \tag{28}$$

where I' is I with the index corresponding to $\lambda_{\max}(\beta)$ removed. Equation (26) simply follows from the fact that

$$\lim_{N \to \infty} [\varphi(\mathbf{P}_{\max}(\beta)) + \epsilon_N]^{1/N} = 1 \tag{29}$$

because $\varphi(\mathbf{P}_{\max}(\beta)) \neq 0$.

Now, $\mathbf{T}(\beta)$ fulfills the hypothesis of Theorem 3, thus $\lambda_{\max}(\beta) > 0$ has multiplicity one. Then taking $\Sigma = \{\lambda_{\max}(\beta)\}$ in Theorem 4 it follows that this eigenvalue is an analytic function in $\beta > 0$ and the proof is complete. ▌

4.3. Discussion

4.3.1. Boundary Conditions

Among the hypotheses of the theorem, the only one whose significance may not be evident is $\varphi(\mathbf{P}_{\max}(\beta)) \neq 0$. As stated in the proof, this is actually needed to show that the partition function can be written in terms of the maximum eigenvalue. Actually, the condition is related to the choice of boundary conditions for the system. In the examples mentioned above, $\varphi(\mathbf{T}) = \mathrm{tr}(\mathbf{T})$ arises from periodic boundary conditions, whereas $\varphi(\mathbf{T}) = \langle f, \mathbf{T}g \rangle$ arises from fixed boundary conditions given by the two vectors f and g. The condition is then excluding boundary conditions that would suppress the eigenstates of the maximum eigenvalue as allowed states for the model. Otherwise nothing can be said about the existence or not of phase transitions and, in fact, they are possible: As an illustrative example, consider a transfer matrix for a three-state system of the form

$$\mathbf{T} \equiv \begin{pmatrix} 3 & 1 & 1 \\ 1 & b & 1 \\ 1 & 1 & b \end{pmatrix}. \tag{30}$$

This is a positive, irreducible matrix which, according to Perron–Frobenius theorem, can not have a phase transition. However, the spectrum of this matrix is

$$\sigma(\mathbf{T}) = \{b-1, \tfrac{1}{2}(4+b \pm \sqrt{12-4b+b^2})\}. \tag{31}$$

Choosing now the boundary conditions to be given by an eigenvector orthogonal to that of the maximum eigenvalue, $(4+b+\sqrt{12-4b+b^2})/2$, the hypothesis on the projector of the theorem will not be fulfilled. One can easily check that in that particular case, as there is a crossing of the second and third eigenvalues at $b=3$, the model has a thermodynamic phase transition even if it is described by a positive, irreducible matrix. Of course, this occurs only for those specific boundary conditions, and in general the model will behave in the usual way. Admittedly, this is an academic example because if matrix (30) were to represent the transfer matrix of a physical system, both the energy of the first state and the boundary conditions (through the corresponding eigenvectors) would be temperature dependent. It is conceivable, though, that operators with such features could arise in more realistic systems. In any event, it is clear that the hypothesis on the projector is needed to prevent pathological situations like this one.

4.3.2. Previous Examples of Phase Transitions in the Context of the Theorem

Once we have the general result on the absence of phase transitions above, it is the time to address the issue as to the two examples of phase transitions discussed in Sections 3.2 and 3.3, namely the Chui–Weeks's and the Dauxois–Peyrard's models. The fact that they do not conform to the type of operator in the theorem is clear in view that both operators possess continuous spectrum, which as mentioned in Section 4.1.2, makes it impossible for them to be compact. However, in using this mathematical condition to show that some model is outside the range of applicability of the theorem one must consider several subtleties:

Analytical Calculations. For the Chui–Weeks's model, the spectrum of the infinite transfer matrix is obtained analytically, and therefore noncompactness is rigorously established. Nevertheless, this needs not be the case in general. A good example is provided by the 1D sine-Gordon model, thoroughly discussed in ref. 34 and defined by the following Hamiltonian:

$$\mathscr{H}=\sum_{i=1}^{N}\left\{\frac{J}{2}(h_{i-1}-h_i)^2+V_0[1-\cos(h_i)]\right\}. \tag{32}$$

From the fact that the potential term is periodic in h, it follows by Floquet–Bloch theorem that the spectrum of the corresponding transfer integral operator is continuous,[35] which would in turn imply that the model does not fulfill the hypothesis of the theorem and subsequently, it could exhibit phase transitions. Note that this does not imply that it must exhibit a phase transition: indeed, in ref. 34 it was shown that a suitable change of

variables casts the operator in a form compatible with the theorem, thus establishing the impossibility of phase transitions in this model (and in fact in a much wider class). Interestingly, the same problem arises in van Hove's theorem;[8] van Hove writes first his general transfer operator in a non-compact form, but he is able to rewrite it as a compact operator and to prove his theorem. The difference with respect to the Chui–Weeks's model is that in this case it is possible to calculate the spectrum and prove that there is actually an eigenvalue crossing. These considerations indicate that non-compactness of the transfer operator merely excludes it from the theorem, but is not enough to say anything definite about the possibility of phase transitions.

Numerical Calculations. The situation is more complicated with the Dauxois–Peyrard model, where the spectrum cannot be computed analytically, and only numerical results are available. Resorting to numerical algorithms to study the spectrum of such an integral operator implies several difficult issues. To begin with, there are two sources of numerical error involved: the discretization of the integral and the truncation of the integration range. In some cases, such as the sine-Gordon model, the latter problem can be avoided by a change of variable, see ref. 36; however, the former one cannot be cured. Further, when discretizing an integral operator such as the ones we are discussing here, the result is *always* a finite matrix that is necessarily positive and hence irreducible: i.e., it is subject to the Perron–Frobenius theorem and cannot have singularities in the largest eigenvalue. Hence, all that one can see in a numerical calculation of the spectrum of an integral operator is a possibly rapid, but anyway smooth, change of the behavior of the largest eigenvalue. In fact, if discontinuities are observed, they must come from the lack of precision of the computation, which leads to the vanishing of very small matrix elements that effectively yield the matrix reducible. It is very important then to complete the study of the eigenvalues with other quantities, preferably the eigenstates themselves. A good example of such an analysis is given in refs. 27 and 28, where the existence of a phase transition in the Dauxois–Peyrard's model is firmly established even if it cannot be rigorously proven.

5. CONCLUSIONS

In this paper, we have attempted to convey two main conclusions: First, there are true thermodynamic phase transitions in one dimensional systems with short range interactions, in spite of the widespread belief on the opposite; and second, we have provided a very general theorem about non-existence of those transitions. In this closing section we discuss both conclusions and their implications.

To be sure, the existence of phase transitions in 1D systems with short range interactions is not a new result. In this respect, what we have done here is to collect and present within a unified framework a few, selected instances of such phase transitions, the earliest of which were proposed already in the sixties. In our opinion there are two main reasons which can explain why part of the scientific community do not believe in its existence. The first one is the fact that, indeed, *most* 1D systems with short range interaction do not undergo a phase transition (except maybe a zero or infinite temperature). Van Hove's rigorous result, Ruelle's extension to lattice models and the most common exactly solvable examples of statistical physics (Ising model, Potts model, etc.) seem to suggest this conclusion. Landau's argument (not a theorem, as pointed out in the introduction, and therefore applicable to a not well defined class of models) reinforces this point of view. So far so good because we are just describing the genesis of a reasonable conjecture. The second reason, however, is not scientific. It has recently been pointed out that a big deal of papers contain cites which the authors have not read.[37] This is very obvious in the case of van Hove's work, which you often see it cited as "the proof" of impossibility of phase transitions in 1D models with short range interactions, referring to models having little or nothing in common with the model van Hove deals with. This has spread the belief that such a proof exists. We hope that the present work helps to remedy this situation by tracing a neat boundary between the 1D systems about which it can be actually proved that there is no phase transition and those about which nothing can be said.

A second point that we want to stress is that, even if we have discussed just three basic examples, there are many more (and there will surely be more to come). It is important to realize that whereas Kittel's model is largely academic, Chui–Weeks's and Dauxois–Peyrard's models are relevant in physical situations of the importance of surface growth/wetting and DNA denaturation, respectively. This means that they cannot be disregarded as "academic, non realistic systems" and that phase transitions in 1D problems must be considered in their own right. Furthermore, the examples we have discussed represent three different stages in complexity of the model description in terms of transfer operators: finite matrices, infinite matrices, and integral operators. However, there are transfer operators that do not belong in any of these classes, such as the ones defined through the evolution of dynamical systems.[38] These are in principle much more difficult to tackle, but on the other hand they open new fields to the study of 1D phase transitions.

Moving now to the other result of the paper, the theorem presented here is a very general result about non-existence of phase transitions in 1D, short-ranged systems, and hence it constitutes the chief original contribution

of this work. Improving on the starting point of van Hove's theorem, we have proven a rigorous result valid for any system whose partition function can be written in terms of a transfer operator independent on the system size. We want to emphasize this formulation because it goes beyond the dimensionality of the models, although we could as well define 1D models as those whose transfer operator does not depend on the size. In any event, the theorem presented here applies to a much wider class of problems than the original van Hove's theorem, as we have removed two of its main three limitations discussed in Section 2: our result is valid for point-like particles and in the presence of external fields.

Notwithstanding the considerations above on the virtues of the theorem we have proven, it is most important to realize that it is not the final answer to this issue yet. One direction in which much work is needed is to turn this result into an "if-and-only-if" theorem. Clearly, this is a very ambitious goal and, in addition, it might not even be reachable. In fact, the present result gives already some hints that this is the case. Indeed, compactness is needed to show that there cannot be phase transitions in 1D systems, but its absence does not imply anything, as there are models with non-compact transfer operators with (Dauxois–Peyrard) and without (sine-Gordon) phase transition. It can be argued at this point that the latter case can finally be rewritten as a compact operator, but then the question arises as to what is the class of "apparent non-compact" operators, i.e., non-compact operators that can be recast as compact. This is obviously not an easy question. In this respect, it is interesting to note that in the theory of dynamical systems a more general class of transfer operators arises (quasi-compact operators), whose spectral properties also allow to show the impossibility of phase transitions (whatever this means for a dynamical system). However, showing that an operator is quasi-compact without resorting to determine its spectrum is far more difficult than the already difficult task of proving compactness, and we know of no instance of an equilibrium statistical-mechanical 1D system described by one such operator. The reader interested in this generalization can consult refs. 39 and 40. As for positiveness, we face the same kind of problems: Kittel's model with non-degenerate open states is described by a non-positive, reducible 2×2 matrix which does not have a phase transition (rather, the transition temperature is infinite). It appears then that if an "if-and-only-if" version of the theorem exists, it will need much refinement of the present hypotheses.

Another comment that stems from the discussion in the previous paragraph is that the theorem, being general and with clear-cut hypotheses, is not very easy to apply. The case of systems with a finite number of states per site is well dealt with, and the consequence of Perron–Frobenius theorem is that forbidden energy configurations are necessary in order to

have a 1D phase transition in that case; otherwise, the corresponding finite matrix is always within the theorem applicability irrespective of any other ingredient of the model. However, as the complication of transfer operators increases, it becomes more and more difficult to show whether or not they verify the hypotheses of the theorem. Among the three basic conditions, namely positiveness, irreducibility, and compactness, the case for the first two is again simpler, as in general irreducibility needs non-positivity and this is usually linked to the existence of configurations with infinite energy. The problem arises with compactness, as, aside from the simplest operators, it is not a trivial task either to prove or to disprove it. As we have discussed in Sections 4.1.2 and 4.3.2, the spectrum of the operator may be of help, but it does not provide a general tool. This is then the key point in characterizing operators to check for the possibility of phase transitions.

Finally, it must be borne in mind that all the results and discussion in this paper relate to *homogeneous systems*. Of the three conditions for van Hove's theorem to apply mentioned above, this is the only one we have not been able to remove, as the study of non-homogeneous systems involves stupendous mathematical difficulties. At the level of systems with a finite number of states per site, the theory of random matrices might shed some light on the problem, although we have not been able to find guidance to this end among the available results. For more complex systems, with infinite matrices or integrals as transfer operators, this is a largely unknown territory. We referred in Section 2 to examples of true phase transitions in specific disordered systems[13] which grant that the problem is an interesting, physically relevant one, albeit one that needs much more effort.

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REFERENCES

1. E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic Press, London, 1966).
2. J. Bernasconi and T. Schneider, *Physics in One Dimension* (Springer, Berlin, 1981).

3. D. H. Dunlap, H. L. Wu, and P. Phillips, *Phys. Rev. Lett.* **65**:88 (1990).
4. F. A. B. F. de Moura and M. L. Lyra, *Phys. Rev. Lett.* **81**:3735 (1998).
5. P. Carpena, P. Bernaola-Galván, P. C. Ivanov, and H. E. Stanley, *Nature* **418**:955 (2002).
6. P. Carpena, P. Bernaola-Galván, P. C. Ivanov, and H. E. Stanley, *Nature* **421**:764 (2003).
7. M. R. Evans, *Brazilian J. Phys.* **30**:42 (2000).
8. L. van Hove, *Physica* **16**:137 (1950) (reprinted in ref. 1, p. 28).
9. D. Ruelle, *Statistical Mechanics: Rigorous Results* (Addison–Wesley, Reading, 1989).
10. L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Part 1 (Pergamon, New York, 1980).
11. C. D. Meyer, *Matrix Analysis and Applied Linear Algebra* (SIAM, Philadelphia, 2000).
12. R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge University Press, Cambridge, 1985).
13. G. Forgacs, J. M. Luck, T. M. Nieuwenhuizen, and H. Orland, *Phys. Rev. Lett.* **57**:2184 (1986); B. Derrida, V. Hakim, and J. Vannimenus, *J. Stat. Phys.* **66**:1189 (1992); G. Giguliarelli and A. L. Stella, *Phys. Rev. E* **53**:5035 (1996); P. S. Swain and A. O. Parry, *J. Phys. A* **30**:4597 (1997); T. W. Burkhardt, *J. Phys. A* **31**:L549 (1998).
14. D. Ruelle, *Comm. Math. Phys.* **9**:267 (1968).
15. G. Rushbrooke and H. Ursell, *Proc. Cambridge Phil. Soc.* **44**:263 (1948).
16. F. J. Dyson, *Comm. Math. Phys.* **12**:91 (1969).
17. J. Fröhlich and T. Spencer, *Comm. Math. Phys.* **81**:87 (1982).
18. C. Kittel, *Am. J. Phys.* **37**:917 (1969).
19. J. F. Nagle, *Am. J. Phys.* **36**:1114 (1968).
20. H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford University Press, Oxford, 1971).
21. K. Huang, *Statistical Mechanics* (Wiley, Singapore, 1987).
22. M. Plischke and B. Bergersen, *Equilibrium Statistical Physics* (World Scientific, Singapore, 1994).
23. T. Kato, *Perturbation Theory for Linear Operators* (Springer, Berlin, 1995).
24. S. T. Chui and J. D. Weeks, *Phys. Rev. B* **23**:2438 (1981).
25. J. M. Yeomans, *Statistical Mechanics of Phase Transitions* (Oxford University Press, Oxford, 1992).
26. T. W. Burkhardt, *J. Phys. A* **14**:L63 (1981).
27. T. Dauxois, M. Peyrard, and A. R. Bishop, *Phys. Rev. E* **47**:R44 (1993); T. Dauxois and M. Peyrard, *Phys. Rev. E* **51**:4027 (1995).
28. N. Theodorakopoulos, T. Dauxois, and M. Peyrard, *Phys. Rev. Lett.* **85**:6 (2000); T. Dauxois, N. Theodorakopoulos, and M. Peyrard, *J. Stat. Phys.* **107**:869 (2002).
29. N. Theodorakopoulos, http://arxiv.org/abs/cond-mat/0210188 (2002).
30. A. Campa and A. Giansanti, *Phys. Rev. E* **68**:3585 (1998).
31. P. Meyer-Nieberg, *Banach Lattices* (Springer, Berlin, 1991).
32. A. C. Zaanen, *Introduction to Operator Theory in Riesz Spaces* (Springer, Berlin, 1997).
33. N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space* (Dover, New York, 1993).
34. J. A. Cuesta and A. Sánchez, *J. Phys. A* **35**:2373 (2002).
35. T. Tsuzuki and K. Sasaki, *Progr. Theoret. Phys. Supp.* **94**:73 (1988).
36. S. Ares, J. A. Cuesta, A. Sánchez, and R. Toral, *Phys. Rev. E* **67**:046108 (2003).
37. M. V. Simkin and V. P. Roychowdhury, *Complex Sys.* **14**:269 (2003).
38. C. Beck and F. Schlögl, *Thermodynamics of Chaotic Systems: An Introduction* (Cambridge University, Cambridge, 1993), Chapter 21.
39. D. Ruelle, *Thermodynamic Formalism* (Addison–Wesley, Reading, 1978).
40. V. Baladi, *Positive Transfer Operators and Decay of Correlations* (World Scientific, Singapore, 2000).