# Statistical Mechanics of Lamé Solitons

Ioana Bena\*

Department of Theoretical Physics, University of Geneva, CH-1211 Geneva 4, Switzerland

Avinash Khare<sup>†</sup>

Institute of Physics, Bhubaneswar, Orissa 751005, India

Avadh Saxena<sup>‡</sup>

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

(Dated: February 2, 2008)

## Abstract

We study the exact statistical mechanics of Lamé solitons using a transfer matrix method. This requires a knowledge of the first forbidden band of the corresponding Schrödinger equation with the periodic Lamé potential. Since the latter is a quasi-exactly solvable system, an analytical evaluation of the partition function can be done only for a few temperatures. We also study approximately the finite temperature thermodynamics using the ideal kink gas phenomenology. The zero-temperature "thermodynamics" of the soliton lattice solutions is also addressed. Moreover, in appropriate limits our results reduce to that of the sine-Gordon problem.

PACS numbers: 05.20.-y, 03.50.-z, 05.45.Yv, 11.10.Lm

<sup>\*</sup> Ioana.Bena@physics.unige.ch

<sup>&</sup>lt;sup>†</sup> khare@iopb.res.in

<sup>&</sup>lt;sup>‡</sup> abs@viking.lanl.gov

### 1. Introduction

Systems described by one-dimensional nonlinear scalar fields and governed by nonlinear energy functionals are ubiquitous in physics. Frequently the governing dynamical equations of these fields admit large-amplitude, localized, robust, particle-like solutions – the solitary waves [1]. In anharmonic models of various condensed-matter systems [2, 3] the presence of these nonlinear excitations is thermally controlled. It is therefore important to proceed to a statistical mechanics investigation of the system, considering the different excitations that are potentially present, as well as their interactions, since they contribute nontrivially to the thermodynamical properties.

Over the years, extensive research has been carried out seeking the soliton solutions of the integrable sine-Gordon (sG) equation [1] and its (non-integrable) counterpart, the double sine-Gordon equation (DsG) [4, 5, 6]. The statistical and thermodynamical properties for both the sG and DsG potentials were studied [7, 8].

There have also been advances in the study of the *hyperbolic* analogues of these problems, the sine-hyperbolic Gordon (shG) equation [9], respectively the double sine-hyperbolic Gordon (DshG) equation [10] (which is non-integrable). The statistical mechanics of double sinh-Gordon solitons was also addressed in [10].

However, the study of the *elliptic* analogues of the sG and DsG problems is less advanced. The elliptic generalization of the sG is the *Lamé equation* [11] and its single soliton and soliton lattice solutions have been worked out only recently [12]. One would surmise that the elliptic generalization of the DsG equation is the Associated Lamé equation [13, 14, 15]. Nevertheless, we found [12] that this is not the case, and this generalization is still an open problem.

There are many physical contexts in which the Lamé equation arises, such as, e.g., bondorder and charge density wave systems [16], nonlinear elasticity [17], phase slips in superconductors and vortex oscillations in a Josephson junction [18], magnetoelastic interaction on curved surfaces and symmetric monopoles [19]. The Lamé equation appears in systems with a single periodicity, for instance a one-dimensional elastic solid comprising identical atoms with a certain strength of the potential [20], or Hartree equation for spinless fermions, or Hartree-Fock equation for spin-1/2 fermions [21]. It also arises in field theory contexts such as sphaleron solutions of the Abelian Higgs model [22], in connection with elliptic CalogeroMoser systems [23], and in group theoretical aspects of algebraic potentials [24].

Our goal here is to address the problem of the statistical mechanics of thermally controlled excitations in a nonlinear system with a Lamé potential. The presented results find applications in the various classes of physical systems enumerated above. Note, however, that the Lamé equation is a *quasi-exactly solvable* problem, which means that one cannot obtain analytically the complete band spectrum of the corresponding Schrödinger equation, but only a part of the spectrum, and that only for certain values of the parameters of the potential, as it will be discussed below. Therefore, it is not possible to obtain analytically the corresponding partition function for arbitrary temperatures, but only for a set of temperatures.

The plan of the paper is as follows. In Sec. 2 we describe the soliton-like solutions of the Lamé potential. For the sake of completeness, we review some previously obtained results [12] and then present a new family of kink lattice solutions. We also address the zero-temperature (T = 0K) "thermodynamics" of the kink crystals and discuss their stability. The single topological kink solution is also described, as well as the asymptotic interaction energy between kinks. The sine-Gordon results are recovered in an appropriate limit. Section 3 describes an approximate method of treating the low-temperature statistical mechanics of this kink-bearing system, namely the ideal kink gas phenomenology. In Sec. 4 we present the transfer operator formalism for an exact calculation of the grand-canonical partition function of the system, with some computational details relegated to the Appendix. Finally, conclusions and perspectives are presented in Sec. 5.

### 2. Soliton Solutions of the Lamé Potential

The Lamé potential [13, 14, 15] with a dimensionless parameter  $\nu$  is defined as

$$V_L(\phi) = \nu(\nu+1) k^2 \operatorname{sn}^2(\phi, k), \qquad (1)$$

where  $\nu(\nu + 1) > 0$  for the situations of physical relevance. Here  $\operatorname{sn}(\phi, k)$  is the sineamplitude Jacobi elliptic function of real modulus k ( $0 \leq k \leq 1$ ) and period 4K(k); K(k)denotes the complete elliptic integral of the first kind, see Refs. [25, 26]. Lamé potential is periodic with a period 2K(k),

$$V_L(\phi + 2K(k)) = V_L(\phi), \qquad (2)$$

and has one minimum  $V_{min} = 0$  at  $\phi = 0$  and one maximum  $V_{max} = \nu(\nu+1)k^2$  at  $\phi = K(k)$ , see Fig. 1.

Consider a classical dimensionless scalar field  $\phi(x, t)$  with  $V_L(\phi)$  as the interaction energy density. Its dynamics is described by the Euler-Lagrange equation

$$\frac{\partial^2 \phi}{\partial t^2} - c^2 \frac{\partial^2 \phi}{\partial x^2} = -\omega_0^2 \frac{\partial V_L}{\partial \phi} \tag{3}$$

corresponding to a Hamiltonian density

$$\mathcal{H}(x, t) = A\left[\frac{1}{2}\left(c^2\phi_x^2 + \mathcal{P}^2\right) + \omega_0^2 V_L(\phi)\right].$$
(4)

Here  $\mathcal{P}(x,t) = \partial \phi/\partial t \equiv \phi_t$  is the conjugate field momentum density, and  $\phi_x \equiv \partial \phi/\partial x$ . In view of the periodicity of the Lamé potential, the field  $\phi$  is defined modulo 2K(k). The velocity c, the frequency  $\omega_0$ , and the constant A (that has the dimensions [energy]·[time]<sup>2</sup>/[length]) are the parameters of the system defining the characteristic time  $(1/\omega_0)$ , length  $(c/\omega_0)$ , and energy  $(Ac\omega_0)$  scales. In the following we shall use dimensionless quantities based on this scaling.

The total energy

$$E_{\Lambda}[\phi, \mathcal{P}] = \int_{-\Lambda}^{\Lambda} \mathcal{H}(x, t) \, dx \tag{5}$$

and the topological charge (or the winding number) of the system

$$W_{\Lambda} = \frac{1}{2K(k)} \int_{-\Lambda}^{\Lambda} \frac{\partial \phi}{\partial x} dx = \frac{1}{2K(k)} \left[ \phi |_{x=\Lambda} - \phi |_{x=-\Lambda} \right]$$
(6)

are constants of the motion for fixed boundary conditions (2 $\Lambda$  is the length of the system,  $-\Lambda \leq x \leq \Lambda$ ). In the "thermodynamic limit"  $\Lambda \to \infty$ , as seen below, the topological charge is simply the difference between the numbers of kinks and antikinks in the system.

In the stationary case the equation for the field  $\phi(x)$  reduces simply to

$$\frac{d^2\phi}{dx^2} = \frac{\partial V_L}{\partial\phi},\tag{7}$$

that can be integrated by quadratures, see below. In view of the covariant form of Eq. (3), the time-dependent solutions  $\phi(x,t)$  are immediately obtained from  $\phi(x)$  by a "Lorentz boosting" to velocity v, i.e.,  $x \to (1 - v^2)^{-1/2}(x - vt)$ .

There are two families of kink lattice solutions of (7). From the perspective of the dynamical systems theory, the first family of non-topological kinks corresponds to closed periodic orbits in the  $(\phi, \phi_x)$  phase plane, while the second family of topological kinks corresponds to open periodic orbits in the phase plane. These different kink lattices reduce to the same single solution solution in the appropriate limit.

#### 2.1. First family of kink lattice solutions

A first type of stationary solutions is given by

$$\pm\sqrt{2}(x - x_0) = \int_{\phi(x_0)}^{\phi(x)} \frac{d\phi'}{\sqrt{V_L(\phi', k) - \nu(\nu + 1)k^2 a^2}},$$
(8)

where  $x_0$  and  $a^2$  are the two integration constants. We fix  $x_0$  through the convention  $\phi(0) = K(k)$ . The control parameter  $a^2$ , with  $0 \leq a^2 < 1$ , determines the appropriate integration domain in Eq. (8), the profile and the properties of the field  $\phi(x)$ .

When extended to the whole real axis  $\Lambda \to \infty$ , Eq. (8) leads to a *soliton lattice* solution:

$$\operatorname{sn}^{2}(\phi, k) = \frac{(1 - k^{2}a^{2}) - (1 - a^{2})\operatorname{sn}^{2}(y, t)}{(1 - k^{2}a^{2}) - k^{2}(1 - a^{2})\operatorname{sn}^{2}(y, t)},$$
(9)

where  $t \equiv \sqrt{(1-a^2)/(1-k^2a^2)}$  and  $y \equiv \sqrt{2\nu(\nu+1)k^2(1-k^2a^2)}x$ . This represents an array of *nontopological* solitons, i.e., a periodic sequence of "small" (nontopological) kink– antikink pairs. In Fig. 2 we show a typical profile of this type of soliton lattice solution (i.e., the field  $\phi$  as a function of x) for a fixed value of  $a^2$ . The spatial size of one kink/antikink (which represents half of the spatial period of the lattice) is a function of the control parameter  $a^2$ 

$$2L(a^2) = \frac{2K(t)}{\sqrt{2\nu(\nu+1)k^2(1-k^2a^2)}},$$
(10)

and the topological charge of such a "small" kink/antikink is, respectively,  $\pm [1 - \sin^{-1}(a, k)/K(k)].$ 

The energy per kink/antikink of the lattice, as a function of  $a^2$ , can be computed as

$$E_{KL}(a^2) = 2\sqrt{\frac{2\nu(\nu+1)k^2}{1-k^2a^2}} \left[ \left(\frac{1}{k^2} - \frac{a^2}{2}\right) K(t) - \frac{k'^2}{k^2} \Pi(k^2t^2, t) \right],$$
(11)

where  $\Pi(k^2t^2, t)$  denotes the complete elliptic integral of the third kind [25, 26].

## 2.1.1. Kink lattice "thermodynamics" at T = 0K

One can immediately compute the thermodynamic characteristics of the ground state of this classical kink-antikink crystal. The ground-state energy per kink is expressed by Eq. (11), while the specific volume per kink is given by Eq. (10). Correspondingly, the thermodynamic pressure is obtained as

$$P_{KL} = -\left(\frac{\partial E_{KL}}{\partial (2L)}\right)_{T=0K} = -\frac{dE_{KL}/d(a^2)}{d(2L)/d(a^2)} = -\nu(\nu+1)k^2a^2.$$
(12)

(in deriving the last equality we have used the properties of the derivatives of the elliptic functions [25, 26]). Thus, the internal energy of the crystal increases with increasing volume under these isothermal conditions. The equation of state can be obtained formally by eliminating the parameter  $a^2$  between Eqs. (10) and (12).

The chemical potential at zero temperature  $\mu_{KL}$  is just the enthalpy per kink,

$$\mu_{KL} = E_{KL} + 2LP_{KL} = 2\sqrt{\frac{2\nu(\nu+1)k^2}{1-k^2a^2}} \left[\frac{1-k^2a^2}{k^2}K(t) - \frac{{k'}^2}{k^2}\Pi(k^2t^2,t)\right],$$
(13)

where the complementary modulus  $k'^2 = 1 - k^2$ . Finally, the isothermal compressibility at T = 0K is

$$\chi_{KL} = -\frac{1}{2L} \frac{\partial(2L)}{\partial P_{KL}} = -\frac{1}{2L} \frac{d(2L)/d(a^2)}{dP_{KL}/d(a^2)} = \frac{K(t) - (1/a^2) E(t)}{2\nu(\nu+1)k^2(1-a^2)K(t)}.$$
 (14)

Here K(t) and E(t) are, respectively, the first- and second-kind complete elliptic integrals of modulus t, see [25, 26]. One notices that  $\chi_{KL}$  can change sign upon variation of the parameters  $k^2$  and  $a^2$ , the states with  $\chi_{KL} < 0$  being "mechanically" unstable. The corresponding stability diagram of this kink lattice solution at T = 0K in the plane of the parameters  $(k^2, a^2)$  is presented in Fig. 3.

#### 2.1.2. The sine-Gordon limit

As discussed in [12], the Lamé potential (1) reduces to the sine-Gordon (sG) potential in the limit

$$k \to 0, \quad \nu(\nu+1) \to \infty, \quad \text{with} \quad \nu(\nu+1)k^2 \to Q = \text{finite}.$$
 (15)

In this limit the above nontopological kink lattice solution reduces to  $\phi_{sG}(x)$ :

$$\sin^2(\phi_{sG}) = 1 - (1 - a^2) \operatorname{sn}^2(\sqrt{2Q}x, \sqrt{1 - a^2}) = \operatorname{dn}^2(\sqrt{2Q}x, \sqrt{1 - a^2}), \quad (16)$$

where  $dn(\sqrt{2Qx}, \sqrt{1-a^2})$  is the delta-amplitude Jacobi elliptic function [25, 26]. The kink/antikink width is  $2L_{sG}(a^2) = 2K(\sqrt{1-a^2})/\sqrt{2Q}$ , and the energy per kink/antikink

$$E_{sGKL} = 2\sqrt{2Q} \left[ E(\sqrt{1-a^2}) - (a^2/2)K(\sqrt{1-a^2}) \right].$$
(17)

The pressure of the sine-Gordon kink lattice at T = 0K is  $P_{sGKL} = -Qa^2$ , and the chemical potential  $\mu_{sGKL} = 2\sqrt{2Q}[E(\sqrt{1-a^2}) - (a^2/2)K(\sqrt{1-a^2})]$ . The isothermal compressibility

$$\chi_{sGKL} = \frac{K(\sqrt{1-a^2}) - 1/a^2 E(\sqrt{1-a^2})}{2Q(1-a^2)K(\sqrt{1-a^2})},$$
(18)

is always negative, which means that this class of sG kink lattice solution is *unstable* (see the  $k \rightarrow 0$  limit in Fig. 3 and [27]).

## 2.2. Second family of kink lattice solutions

The second type of stationary solutions is given by

$$\pm \sqrt{2} \left( x - x_0 \right) = \int_{\tilde{\phi}(x_0)}^{\tilde{\phi}(x)} \frac{d\phi'}{\sqrt{V_L(\phi', k) + \nu(\nu+1) k^2 a^2}},$$
(19)

where  $x_0$  and  $a^2 \ge 0$  are the two integration constants. Here again we fix  $x_0$  through the convention  $\tilde{\phi}(0) = K(k)$ . One notices that this family of solutions can be obtained *formally* from the previous one, Eq. (9), by replacing  $a^2$  by  $-a^2$ , and thus:

$$\operatorname{sn}^{2}(\tilde{\phi}, k) = \frac{1 - \operatorname{sn}^{2}(\tilde{y}, \tilde{t})}{1 - k^{2} \operatorname{sn}^{2}(\tilde{y}, \tilde{t})}, \qquad (20)$$

where  $\tilde{t} = \sqrt{(1+k^2a^2)/(1+a^2)}$  and  $\tilde{y} = \sqrt{2\nu(\nu+1)k^2(1+a^2)}x$  with  $a^2 \ge 0$ . This is a *topological* kink lattice solution, see Fig. 4, i.e., a succession of topological kinks (or antikinks), of kink/antikink width (half lattice period)

$$2\tilde{L}(a^2) = \frac{2K(\tilde{t})}{\sqrt{2\nu(\nu+1)k^2(1+a^2)}}.$$
(21)

The energy per kink/antikink of the lattice is found to be:

$$\tilde{E}_{KL} = 2\sqrt{\frac{2\nu(\nu+1)k^2}{1+a^2}} \left[ \left(\frac{1}{k^2} + \frac{a^2}{2}\right) K(\tilde{t}) - \frac{k'^2}{k^2} \Pi(k^2, \tilde{t}) \right].$$
(22)

## 2.2.1. T = 0K "thermodynamics"

Proceeding as in the previous case of the first family of kink lattice solutions, one obtains for the pressure of the ground state of the second type lattice solutions

$$\tilde{P}_{KL} = \nu(\nu + 1)k^2 a^2 \,, \tag{23}$$

and for the corresponding chemical potential

$$\tilde{\mu}_{KL} = 2\sqrt{\frac{2\nu(\nu+1)k^2}{1+a^2}} \left[ \left(\frac{1}{k^2} + a^2\right) K(\tilde{t}) - \frac{k'^2}{k^2} \Pi(k^2, \tilde{t}) \right].$$
(24)

Finally, the isothermal compressibility

$$\tilde{\chi}_{KL} = \frac{k^2 K(\tilde{t}) + (1/a^2) E(\tilde{t})}{2\nu(\nu+1)k^2(1+k^2a^2)K(\tilde{t})},$$
(25)

which is always positive, and thus the kink lattice solution of the second type is stable at T = 0K.

## 2.2.2. The sine-Gordon limit

In the sine-Gordon limit (15), the above kink lattice solution reduces to

$$\sin^2(\tilde{\phi}_{sG}) = 1 - \operatorname{sn}^2(\sqrt{2Q(1+a^2)}x, 1/\sqrt{1+a^2}) = \operatorname{cn}^2(\sqrt{2Q(1+a^2)}x, 1/\sqrt{1+a^2}), \quad (26)$$

of spatial period  $2\tilde{L}_{sG}(a^2) = 2K(1/\sqrt{1+a^2})/\sqrt{2Q(1+a^2)}$ , where  $\operatorname{cn}(\sqrt{2Q(1+a^2)}x, 1/\sqrt{1+a^2})$  is the cosine-amplitude Jacobi elliptic function [25, 26]. The corresponding energy per kink is

$$\tilde{E}_{sGKL} = 2\sqrt{\frac{2Q}{1+a^2}} \left[ (1+a^2)E(1/\sqrt{1+a^2}) - (a^2/2)K(1/\sqrt{1+a^2}) \right], \qquad (27)$$

the chemical potential is  $\tilde{\mu}_{sGKL} = 2\sqrt{2Q(1+a^2)}E(1/\sqrt{1+a^2})$ , and the pressure is  $\tilde{P}_{sGKL} = Qa^2$ . The positiveness of the isothermal compressibility  $\chi_{sGKL} = E(1/\sqrt{1+a^2})/[2Qa^2K(1/\sqrt{1+a^2})]$  confirms the *thermodynamic stability* of the sG kink lattice of the second type. These results are in agreement with those found previously in [7] for the sG potential.

#### 2.3. The single soliton solution

For the sake of completeness we consider the single soliton solution as well. The corresponding single soliton solution can be obtained from *either* of the above soliton lattices in the limit of "infinite kink dilution", i.e., when the period of the lattice becomes infinite,  $L, \tilde{L} \to \infty$ , which corresponds to the control parameter  $a^2 \to 0$ . It is a *topological*, "large" kink/antikink of charge

$$\frac{1}{2K(k)} \int_{-\infty}^{\infty} \phi_x \, dx = \pm 1 \,, \tag{28}$$

given by

$$\operatorname{sn}(\phi, k) = \pm \frac{1}{\sqrt{1 + k^{2} \sinh^{2}(y^{*})}}, \qquad (29)$$

where  $y^* = \sqrt{2\nu(\nu+1)k^2} x$  and  $k'^2 = 1 - k^2$ . The characteristic "spatial extent" of such a soliton is  $\xi_{kink} = 2/\sqrt{2\nu(\nu+1)k^2}$ . In Fig. 5 we present the typical profile of a single kink.

The energy (rest mass) of the static single kink/antikink is shown [12] to be

$$E_K = \sqrt{2\nu(\nu+1)} \ln\left(\frac{1+k}{1-k}\right)$$
 (30)

In view of the covariant form of equation (3), a kink moving with a velocity v has an energy

$$E_K(v) = (1 - v^2)^{-1/2} E_K = (E_K^2 + \mathcal{P}^2)^{1/2}, \qquad (31)$$

where  $\mathcal{P} = E_K v (1 - v^2)^{-1/2}$  is the "relativistic" momentum.

One can also compute the energy of the interaction of one kink/antikink in the lattice with the rest of the lattice as  $U(a^2) = E_{KL}(a^2) - E_K$  (for the first type kink lattice) or as  $\tilde{U}(a^2) = \tilde{E}_{KL}(a^2) - E_K$  (for the second type kink lattice). From these expressions one can deduce (through a Taylor expansion in the parameter  $a^2$ ) the *long-distance* interaction energy between two kinks.

Note that there is another, more general way to obtain the asymptotic interaction energy between two solitons – Manton's method [12, 28]. Given the asymptotic shape of the single kink (29), that in our case reads (e.g., for  $x \to \infty$ )

$$\phi_{as} \approx \frac{2}{\sqrt{1-k^2}} \exp\left(-\sqrt{2\nu(\nu+1)k^2}x\right) \,, \tag{32}$$

one obtains for the asymptotic interaction energy between two solitons separated by a distance  $D \gg 1/\sqrt{2\nu(\nu+1)k^2}$ :

$$U_{as}(D) \approx \pm \frac{8\sqrt{2\nu(\nu+1)k^2}}{1-k^2} \exp\left(-\sqrt{2\nu(\nu+1)k^2}D\right).$$
 (33)

The positive sign corresponds to a repulsive interaction between solitons of the same topological charge, while between a kink and an antikink the interaction is attractive. For the particular case of the first type of soliton lattice, in the limit of "high kink dilution" ( $a^2 \ll 1$ ), one has

$$D = 2L(a^2) \approx 1/\sqrt{2\nu(\nu+1)k^2} \ln\left[\frac{16}{a^2(1-k^2)}\right] \gg 1/\sqrt{2\nu(\nu+1)k^2}, \quad (34)$$

and thus the asymptotic attractive interaction energy between a kink and an antikink in the lattice is

$$U_{as}(a^2) \approx -a^2 \sqrt{\nu(\nu+1)k^2/2}$$
. (35)

The same expression is obtained in the limit of "high kink dilution" for the second type of soliton lattice. Finally, there is no difficulty or surprise in obtaining the properties of the sG single soliton in the appropriate limit (15), see also [7].

Next, let us briefly consider the question of the behavior of the single kink solution of the Lamé potential with respect to small perturbations of its shape. For small oscillations  $\psi(x) \exp(i\omega t)$  around the stationary kink solution (29), the linearized dynamics equation reads

$$\left\{-\frac{d^2}{dx^2} + 2\nu(\nu+1)k^2\left[1 - 2(1+k^2)\operatorname{sn}^2(\phi,k) + 3k^2\operatorname{sn}^4(\phi,k)\right] - \omega^2\right\}\psi(x) = 0.$$
(36)

Consider the following change of variables:

$$z = \frac{2}{(1-k^2)\cosh(2y^*) + (1+k^2)},$$
(37)

and

$$\psi = \left[ (1 - k^2) z/2 \right]^s \chi(z), \qquad s \equiv \sqrt{\frac{1}{4} - \frac{\omega^2}{8\nu(\nu+1)k^2}}. \tag{38}$$

With these new variables, the stability equation (36) becomes Heun's equation [29]:

$$\frac{d^2\chi}{dz^2} + \left(\frac{2s+1}{z} + \frac{1/2}{z-1} + \frac{1/2}{z-1/k^2}\right)\frac{d\chi}{dz} + \frac{(s-1/2)(s+3/2)z - (s+1)(2s-1)(1+k^2)/(2k^2)}{z(z-1)(z-1/k^2)}\chi = 0,$$
(39)

that is a subject of current intensive research in mathematical physics [30]. Further on, following [29], one can make a new change of variables

$$z = \operatorname{sn}^{2}(u, k), \qquad f(u) = \left[\operatorname{sn}(u, k)\right]^{(4s+1)/2} \chi(z(u)), \qquad (40)$$

and the Heun equation above reduces to the Schrödinger equation

\_

$$-\frac{d^2 f(u)}{du^2} + \tilde{V}(u)f(u) = hf(u)$$
(41)

with the "potential"  $\tilde{V}(u) = (15/4)k^2 \operatorname{sn}^2(u, k) + (16s^2 - 1)/[4 \operatorname{sn}^2(u, k)]$  and a fixed "energy"  $h = 9(1 + k^2)/4$ .

As explained in detail in, e.g., [3], and also checked directly, these stability equations always admit the Goldstone  $\omega = 0$  (s = 1/2) mode as a solution, thus restoring the translational invariance of the original Hamiltonian (4) broken by the introduction of the kink into the system. In addition to the translation mode at  $\omega = 0$ , although difficult to find exactly, there may exist additional *bound states* with nonzero frequency of the stability equations. These solutions represent *internal oscillations of the kink* (or shape modes), corresponding to harmonically varying kink shape around the kink center. They are strongly localized around the static kink. Besides these discrete bound state solutions, there exist continuum states (extended modes) corresponding to phonons (see below Sec. 3.2) that are scattered by the kink (asymptotically, i.e., far from kink's center, this scattering results simply in a phase shift as compared to the kink-free system). Note that the degrees of freedom of the bound states (internal modes of the kink) are obtained at the expense of the phonon field (whose local density is altered by the presence of the kink), i.e., the excitation of these internal modes can be seen as a 'capture' of phonons by the kink, see [3] for a detailed discussion of this point.

One could legitimately address the question of the linear stability in the case of the kink lattice solutions, too. However, the corresponding linearized evolution equation of the perturbation (although reminiscent of a Heun's equation) is more complicated and will not be discussed further.

## 3. Finite-temperature thermodynamics: The ideal kink gas approximation

### 3.1. The contribution of the kinks

A first approach to the study of the finite-temperature T > 0 K thermodynamics of the field  $\phi$  can be discussed within the framework of the *ideal kink gas approximation*, see [3, 8, 31] for a more detailed description of the method. This approximation consists of assuming that, at sufficiently low temperatures, very few kink-like excitations are present, and thus the mean distance between them is very large as compared to their typical size  $\xi_{kink}$ . Therefore, these kinks and antikinks behave like *independent*, *non-interacting particles*, with an energy (when moving with velocity v) given by Eq. (31). Moreover, the interaction between individual kinks and the phonons (see below) is also neglected, i.e., kinks and phonons contribute independently to the thermodynamic properties of the system.

Let us concentrate first on the contribution of the kink gas. Suppose there are  $N_K$  kinks and  $N_{\overline{K}}$  antikinks in the system; then  $W_{\Lambda} = N_K - N_{\overline{K}}$  is the constant topological charge (winding number), Eq. (6). There is no restriction on the ordering of these kinks and antikinks along the system. Let  $N_{\Lambda} = N_K + N_{\overline{K}} = 2N_K - W_{\Lambda}$  be the total number of kink-like excitations in the system. Then the grand-canonical partition function is simply:

$$\Xi_{\Lambda}(\beta,\mu) = \sum_{N_{\Lambda}=0}^{\infty} \exp(\mu\beta N_{\Lambda}) Z_{\Lambda}(\beta) , \qquad (42)$$

where  $\mu$  is the chemical potential associated with the creation of a kink-like excitation in the system, T is the temperature,  $\beta = 1/(k_B T)$ , and  $Z_{\Lambda}(\beta)$  is the canonical partition function,

$$Z_{\Lambda}(\beta) = \frac{(2\Lambda)^N}{N!h^N} \left\{ \int_{-\infty}^{+\infty} d\mathcal{P} \exp\left[-\beta (E_K^2 + \mathcal{P}^2)^{1/2}\right] \right\}^N$$
(43)

(with h Planck's constant). Thus, finally

$$\Xi_{\Lambda}(\beta,\mu) = \exp\left[(4E_K\Lambda/h)K_1(\beta E_K)\exp(\beta\mu)\right]$$
$$\approx \exp\left\{(2\Lambda/h)(2\pi E_K/\beta)^{1/2}\exp[\beta(\mu - E_K)]\right\}$$
(44)

with the approximation holding for low temperatures  $\beta \gg 1$  ( $K_1$  is the modified Bessel function [25]). This leads to a pressure

$$P_K = (2\pi E_K / \beta^3 h^2)^{1/2} \exp[\beta(\mu - E_K)], \qquad (45)$$

and to an average kink-density (i.e., number of kinks per unit length)

$$n_{K} = (\partial P_{K} / \partial \mu)_{T} = (2\pi E_{K} / \beta h^{2})^{1/2} \exp[\beta(\mu - E_{K})].$$
(46)

The situation of physical relevance is that when there is no external constraint on the number of kink-like excitations in the system, i.e., the kink density is solely determined by the temperature; this amounts to setting  $\mu = 0$  in the above equation, thus obtaining

$$n_K = (2\pi E_K / \beta h^2)^{1/2} \exp(-\beta E_K), \qquad (47)$$

which shows that the kink density is *exponentially small* at low temperatures  $\beta \gg 1$ .

The free energy density (i.e., the free energy per unit length of the system) of this ideal kink gas is then simply

$$F_K = -(1/\beta) n_K, \qquad (48)$$

and the internal energy density

$$U_K = \partial(\beta F_K) / \partial\beta = [E_K - 1/(2\beta)] n_K.$$
(49)

Finally, the specific heat per unit length is

$$C_K = k_B \left[ (\beta E_K - 1/2)^2 - 1/2 \right] n_K.$$
(50)

In analogy with the correlation functions for periodic potentials [8, 32], e.g.  $\langle \sin \phi(0), \sin \phi(x) \rangle$  for the sine-Gordon case, an appropriate measure of the static field-field spatial correlation function is given by the following expression:

$$\mathcal{C}(x) = \left\langle \operatorname{sn}(\phi(0), k) \operatorname{sn}(\phi(x), k) \right\rangle, \tag{51}$$

where  $\langle ... \rangle$  designates the usual thermal average (in agreement with the convention in Sec. II,  $\phi(0) = K(k)$ ). The choice of the function  $\operatorname{sn}(\phi, k)$  for the study of the spatial correlations of the field  $\phi$  is related to its "sensitivity" to the presence of a kink (antikink); indeed, if a kink (i.e., a "jump" of 2K(k) in the field  $\phi$ ) is present on the segment of length x, this leads to a change in the sign of  $\operatorname{sn}(\phi, k)$ . The value of  $\mathcal{C}(x)$  can be easily estimated using the following qualitative argument [8]: at low kink density the probability  $\operatorname{Prob}(n, x)$  of finding n kinks in a segment of length x is simply a Poisson distribution of mean  $\langle n \rangle = n_K x$ , i.e.,

$$\operatorname{Prob}(n,x) = \frac{(n_K x)^n}{n!} \exp(-n_K x).$$
(52)

Correspondingly,  $\operatorname{sn}(\phi(0), k) \operatorname{sn}(\phi(x), k) = (-1)^n \operatorname{sn}(\phi(0), k) = (-1)^n$ . Thus the correlation function is simply

$$C(x) = \sum_{n=0}^{\infty} (-1)^n \operatorname{Prob}(n, x) = \exp(-2n_K x), \qquad (53)$$

which corresponds to a correlation length  $\xi_K = 1/(2n_K)$  of the field  $\phi$ .

## 3.2. Linear modes (phonons)

Let us briefly turn to the description of the phonons, i.e., the small-amplitude harmonic vibrations in the Lamé potential well. The equation of motion (7) for the field  $\phi$  can be linearized around the minimum  $\phi = 0$  of the potential  $V_L(\phi)$ , thus leading to the following dispersion relation for the phonons:

$$\omega_q^2 = q^2 + 2\nu(\nu+1)k^2 \,. \tag{54}$$

All the frequencies are real for all  $q \ge 0$ . In the semiclassical approximation, the contribution of the phonons to the free energy *per unit length* of the system at a temperature T is thus given by

$$F_{ph} = \frac{1}{\beta \Delta x} \ln\left(\frac{h\beta}{2e \Delta x}\right) + \frac{1}{2\beta} \sqrt{2\nu(\nu+1)k^2}, \qquad (55)$$

where  $\Delta x$  is the size of a spatial cell corresponding to the smallest-wavelength linear mode of the system, i.e., to the Debye cut-off in terms of frequency (usually,  $\Delta x$  corresponds to the unit-cell length of the corresponding discrete lattice of the system under study). Taking the continuum limit  $\Delta x \to 0$  leads to the well-known "ultraviolet catastrophe". The contribution of the phonons to the internal energy density is then

$$U_{ph} = \partial(\beta F_{ph})/\partial\beta = 1/(\beta \Delta x), \qquad (56)$$

while the specific heat per unit length is a constant,  $C_{ph} = 1/\Delta x$ . No interaction of the phonons with the kinks is taken into account in the above thermodynamic expressions.

The total pressure, free energy density, internal energy density, and specific heat per unit length of the classical field  $\phi$  is the sum of the independent contributions of the phonons and the ideal kink gas, respectively. In a more refined approach [3], one can take into account the interaction between phonons and individual kinks as a 'trapping' of phonons by the kinks, i.e., the excitation of the internal bound modes of the kinks at the expense of the degrees of freedom of the phonon field. However, this results only in a transfer of energy between the linear modes (phonons) and nonlinear ones (kinks), i.e., it does not affect the global thermodynamic properties of the system inside the limits of the approximate ideal kink gas scheme.

Of course, all the thermodynamic properties of the field in the low-temperature limit are dominated by the contribution of the phonons, since the kink density, Eq. (47), is exponentially small at low temperatures. However, as discussed, for example in [3], the density of kinks may be important for some transport properties that are insensitive to phonons, e.g. dc conductivity in charge-density-wave systems and transport coefficients in general [33], which are related to the correlation functions of the field.

#### 4. Finite-temperature thermodynamics: The transfer operator formalism

The above approximate theory becomes inappropriate at high temperatures  $\beta \leq 1$ , when one can no longer neglect the interaction between the various nonlinear and linear excitations present in the system. There exists an *exact* general formal method for computing the grand-canonical partition function, by mapping the problem onto the spectral problem of a Schrödinger operator. Let us briefly apply this so-called *transfer operator formalism* [7, 31, 32] to the case of the Lamé potential.

The canonical partition function for the field  $\phi(x)$  can be written as a functional integral over the conjugated fields  $\phi(x, t)$  and  $\mathcal{P}(x, t) = \partial \phi / \partial t$ :

$$Z_{\Lambda}(\beta) = \int \mathcal{D}\mathcal{P} \int \mathcal{D}\phi \, \exp\left\{-\beta E_{\Lambda}[\phi, \mathcal{P}]\right\} \,.$$
(57)

One can define the path integral by dividing the system into M cells of length  $\Delta x = 2\Lambda/M$ and replacing the continuous fields  $\phi(x, t)$  and  $\mathcal{P}(x, t)$  by two discrete sets of (M + 1) field variables  $\{\phi_i(t) = \phi(x_i, t)\}$  and  $\{\mathcal{P}_i(t) = \mathcal{P}(x_i, t)\}, x_i = -L + 2iL/M, i = 0, ..., M$ . At the end, one would consider the continuum limit  $M \to \infty$ . We shall consider fixed boundary conditions

$$\phi_0(t) = 0, \ \phi_M(t) = 2K(k)W_\Lambda; \ \mathcal{P}_0(t) = \mathcal{P}_M(t) = 0,$$
(58)

that assure the constancy of both the total energy  $E_{\Lambda}$  and the topological charge  $W_{\Lambda}$ . Moreover, we impose that  $W_{\Lambda}$  is an integer, i.e., in the "thermodynamic limit"  $\Lambda \to \infty$ the system supports topological kinks/antikinks, and  $W_{\Lambda}$  represents simply the difference between the numbers of kinks and antikinks.

The partition function factorizes into a kinetic energy part  $Z^{\mathcal{P}}_{\Lambda}(\beta)$  (determined by the momentum variables  $\{\mathcal{P}_i\}$ ):

$$Z^{\mathcal{P}}_{\Lambda}(\beta) = \left(\frac{2\pi\,\Delta x}{\beta h^2}\right)^{(M-1)/2},\tag{59}$$

and a configurational (potential energy) part  $Z^{\phi}_{\Lambda}(\beta)$ . The evaluation of the latter can be carried out using the formalism of the *transfer operator* [7, 31, 32], that allows an exact mapping of this problem onto the problem of finding the eigenvalues of an integral operator. In the continuum limit  $M \gg 1$  ( $\Delta x \ll \Lambda$ ), this problem can be further simplified to finding the energy eigenvalues of the following Schrödinger equation for the Lamé potential, with a temperature-dependent "mass":

$$\left[-\frac{1}{2\beta^2}\frac{d^2}{d\phi^2} + V_L(\phi) - \varepsilon_n\right]\Phi_n(\phi) = 0, \qquad (60)$$

where  $\Phi_n(\phi)$  are the Lamé functions [11, 16, 34]. More precisely,

$$Z^{\phi}_{\Lambda}(\beta) = \left(\frac{2\pi\Delta x}{\beta}\right)^{M/2} \sum_{n} \exp(-2\Lambda\beta\varepsilon_n)\Phi_n(0)\Phi^*_n(2K(k)W_{\Lambda}), \qquad (61)$$

where  $(...)^*$  denotes the complex conjugate, and n labels the "quantum states".

In view of the periodicity of the Lamé potential, Eq. (2), the eigenvalues of the Schrödinger equation (60) lie in allowed bands, separated by forbidden bands. In each such allowed band the energy varies continuously with the wavenumber

$$\tilde{k} \equiv \frac{q\pi}{K(k)}, \quad \text{where} \quad -1/2 \leqslant q \leqslant 1/2$$
(62)

 $(\tilde{k} \text{ is restricted to the first Brillouin zone})$ . In the "thermodynamic limit"  $\Lambda \to \infty$ , and using Bloch's theorem for the eigenfunctions, one can simplify further the expression (61) to:

$$Z^{\phi}_{\Lambda}(\beta) = \left(\frac{2\pi\Delta x}{\beta}\right)^{M/2} \int_{-1/2}^{1/2} dq \exp\left[-2\Lambda\beta\varepsilon_1(q) - 2\pi i q W_{\Lambda}\right] |\Phi_q(0)|^2, \tag{63}$$

where  $\Phi_q(\phi)$  is the eigenfunction in Eq. (60) corresponding to the eigenvalue  $\varepsilon_1(q)$  that lies within the *first allowed band*.

The *total* canonical partition function in the continuum limit  $M \gg 1$  is thus given by:

$$Z_{\Lambda}(\beta) = \left(\frac{2\pi}{\beta}\right)^M \int_{-1/2}^{1/2} dq \exp\left[-2\Lambda\beta\varepsilon_1(q) - 2\pi i q W_{\Lambda}\right] |\Phi_q(0)|^2.$$
(64)

One cannot pick out directly the most significant contribution to the integral above as the term of largest magnitude, because the phase  $2\pi q W_{\Lambda}$  also plays a role. The way to avoid this problem is to go to the grand canonical ensemble, whose partition function is:

$$\Xi_{\Lambda}(\beta,\mu) = \exp(2\Lambda\beta P) = \sum_{W_{\Lambda}=-\infty}^{\infty} Z_{\Lambda}(\beta) \exp(\mu\beta W_{\Lambda}) = \\ = \left(\frac{2\pi}{\beta}\right)^{M} \int_{-1/2}^{1/2} dq \exp[-2\Lambda\beta\varepsilon_{1}(q)] |\Phi_{q}(0)|^{2} \sum_{W_{\Lambda}=-\infty}^{\infty} \exp[-(2\pi i q - \mu\beta)W_{\Lambda}].$$
(65)

Here  $\mu$  is the chemical potential associated with the creation of one topological charge in the system, and P is the thermodynamic pressure. Recall that  $W_{\Lambda}$  represents the difference between the number of topological kinks and antikinks in the system, and that is why it runs between  $-\infty$  and  $+\infty$ . Allowing the chemical potential  $\mu$  to take imaginary values

$$\mu\beta = 2\pi i\lambda\,,\tag{66}$$

one can immediately perform the summation over  $W_{\Lambda}$ , given that

$$\sum_{W_{\Lambda}=-\infty}^{\infty} \exp[-2\pi i (q-\lambda) W_{\Lambda}] = \delta(q-\lambda) \,. \tag{67}$$

Thus

$$\Xi_{\Lambda}(\beta,\mu) = \left(\frac{2\pi}{\beta}\right)^{M} \exp[-2\Lambda\beta\varepsilon_{1}(\lambda)]|\Phi_{\lambda}(0)|^{2}, \qquad (68)$$

from which one obtains the pressure

$$P(\mu,\beta) = \frac{M}{2\Lambda\beta} \ln\left(\frac{2\pi\Delta x}{\beta h}\right) - \varepsilon_1(\lambda) = \frac{1}{\beta\Delta x} \ln\left(\frac{2\pi\Delta x}{\beta h}\right) - \varepsilon_1\left(-i\frac{\mu\beta}{2\pi}\right).$$
(69)

Note that the first term in the r.h.s.,  $\frac{1}{\beta\Delta x} \ln\left(\frac{2\pi\Delta x}{\beta h}\right)$  (corresponding to  $V_L = 0$ ), is nothing else but the contribution of the classical phonon field, see also [3, 31].

We must now analytically continue the chemical potential back onto the real axis, which is the situation of physical relevance. This problem has been analyzed in detail in [35] for general periodic symmetric potentials, and it was shown that under rather general circumstances the first allowed energy band of complex wavenumber maps onto the first forbidden energy band of real wavenumber. One is thus led finally to the important conclusion that in order to obtain the thermodynamics of the system, Eq. (69), one has to compute the lowest allowed and forbidden energy bands corresponding to the associated Schrödinger equation (60) with the Lamé potential.

This is a nontrivial spectral problem, and some details are presented in the Appendix. No general results are known for arbitrary values of  $\beta$  and  $\nu$ . However, for the case when  $2\beta^2\nu(\nu+1)$  is of the form  $\ell(\ell+1)$ , with  $\ell$  an integer that is either strictly positive, or  $\ell \leq -2$ , the energy bands are known under an implicit form that allows for combined analytical and numerical calculations. This means that, for a fixed value of  $\nu$ , the thermodynamic properties of the field  $\phi$  can be computed for a discrete set of values of the temperature given by:

$$\beta = \sqrt{\frac{\ell(\ell+1)}{2\nu(\nu+1)}}, \quad \ell \in \mathcal{Z} \setminus \{0, -1\}.$$
(70)

As an example, we give below the analytical expression for the set of parameters with  $2\beta^2\nu(\nu+1) = 2$  (i.e.,  $\ell = 1$ ). In this case, the expression (69) for the pressure of the system becomes:

$$P\left(\mu,\beta=1/\sqrt{\nu(\nu+1)}\right) = \frac{M\sqrt{\nu(\nu+1)}}{2\Lambda} \ln\left(\frac{2\pi\Delta x\sqrt{\nu(\nu+1)}}{h}\right) - \frac{\nu(\nu+1)}{2} \left[1 - \frac{k^{\prime 2}}{\operatorname{cn}^{2}(\overline{\delta},k)}\right].$$
(71)

Here  $k' = \sqrt{1 - k^2}$  is the complementary modulus of the elliptic functions, and the value of the parameter  $\overline{\delta}$  follows from the implicit equation:

$$\frac{\mu}{2\pi\sqrt{\nu(\nu+1)}} = -\frac{\overline{\delta}}{2K(k')} - \frac{K(k)}{\pi} \left[ F(\gamma, k) - E(\gamma, k) + \tan\gamma \sqrt{1 - k^2 \sin^2\gamma} \right], \quad (72)$$

where  $F(\gamma, k)$  and  $E(\gamma, k)$  are incomplete elliptic integrals of the first and second kind [25, 26], respectively, and

$$\sin\gamma = \operatorname{sn}(\overline{\delta}, k) \,. \tag{73}$$

From it one can compute, in principle, the thermodynamic properties of the system at this fixed temperature, e.g., the density of kinks,

$$n_{K} = \left(\frac{\partial P}{\partial \mu}\right)_{T} = -\frac{k^{\prime 2}\sqrt{\nu(\nu+1)}}{2\pi} \frac{\operatorname{sn}(\overline{\delta}, k)\operatorname{dn}(\overline{\delta}, k)}{\operatorname{cn}^{3}(\overline{\delta}, k)} \left[\frac{1}{2K(k^{\prime})} + \frac{K(k)}{\pi} \frac{\operatorname{dn}^{2}(\overline{\delta}, k)}{\operatorname{cn}^{2}(\overline{\delta}, k)}\right]^{-1}.$$
 (74)

One has now to consider the  $\mu \to 0$  limit in the above expressions, that corresponds to the physically relevant situation of thermally activated excitations of the field, i.e., no external constraint on the topological charge of the system.

To complete the discussion of statistical mechanics, we need to compute the field-field correlation function (51) whose Fourier transform is related to the static structure factor [3, 7, 10]. The corresponding correlation length is a measure of average distance between kink excitations. As discussed in [3, 8] for general periodic potentials, C(x) is obtained from the knowledge of the lowest Lamé band wavefunctions [16, 24], and in the asymptotic limit  $|x| \gg 1$  it is  $C(x) \sim \exp(-2n_K|x|)$ , in agreement with the expression found in the low kink density limit, Sec. III. Its general expression, however, cannot be obtained in a closed analytical form. Similarly, the correlation function involving field fluctuations [3, 32] for the Lamé case remains an open question. Finally, as a general remark [3], the results of the transfer matrix formalism reduce in the low-temperature limit, through a WKB-type of approximation, to the ideal kink gas results in Sec. III.

### 5. Conclusions

We have obtained two types of kink lattice solutions of the Lamé equation and their common limit of the single-kink solution. We studied the T = 0K "thermodynamics" of these kink crystals. Using the ideal kink gas formalism, we studied first the approximate low-temperature thermodynamics, which takes into account separately the contribution of independent kinks and phonons, while the interactions between them are not properly accounted for. Then we invoked the transfer integral approach to calculate exactly the partition function. This maps the statistical mechanics problem onto the spectral problem of the Schrödinger equation for the Lamé potential, see also [7]. Unlike the sine-Gordon equation, Lamé equation is not exactly solvable but quasi-exactly solvable: the band structure of the corresponding Schrödinger equation is not known analytically for all the values of the parameter  $\ell$  of the potential. The band structure of the Lamé equation is known in explicit form [11, 16, 24] for  $\ell = 1$ , and in implicit form for higher integer values of  $\ell$ , see the Appendix. Due to this limitation, we have been able to obtain closed form expressions for thermodynamic quantities only for a set of temperatures. Similar constraints hold in the case of another periodic system, namely the double sine-Gordon equation [8]. Although we have not been able to present analytic results for all temperatures, our approach provides insight into this system and other related periodic quasi-exact solvable systems.

#### Acknowledgments

I.B. acknowledges partial support from the Swiss National Science Foundation. This work was supported in part by the U.S. Department of Energy.

# APPENDIX A: SPECTRAL PROPERTIES OF THE LAMÉ POTENTIAL

Let us consider the dimensionless Schrödinger equation

$$\left[-\frac{d^2}{d\phi^2} + V_L(\phi)\right]\psi(\phi) = \varepsilon\psi(\phi).$$
(A1)

The Lamé potential with  $\nu = \ell$  a strictly positive integer is well-known to be exactly solvable, see, e.g., [11, 34]. The energy  $\varepsilon$  and the wavenumber  $\tilde{k}$  are expressed parametrically as

$$\varepsilon = \sum_{n=1}^{\ell} \frac{1}{\operatorname{sn}^2 \alpha_n} - \left[ \sum_{n=1}^{\ell} \frac{\operatorname{cn} \alpha_n \operatorname{dn} \alpha_n}{\operatorname{sn} \alpha_n} \right]^2, \qquad (A2)$$

and

$$\tilde{k} = i \sum_{n=1}^{\ell} Z(\alpha_n, k) - \frac{\ell \pi}{2K(k)}, \qquad (A3)$$

respectively, where Z(u, k) is the Jacobi's zeta function [25, 26],

$$Z(u,k) = E\left(\sin^{-1}(\sin(u,k)),k\right) - (E(k)/K(k))u.$$
 (A4)

The parameters  $\alpha_1, \ldots, \alpha_\ell$  are subject to  $(\ell - 1)$  independent constraints

$$\sum_{p=1}^{\ell} \frac{\operatorname{sn}\alpha_p \operatorname{cn}\alpha_p \operatorname{dn}\alpha_p + \operatorname{sn}\alpha_n \operatorname{cn}\alpha_n \operatorname{dn}\alpha_n}{\operatorname{sn}^2\alpha_p - \operatorname{sn}^2\alpha_n} = 0, \quad p \neq n, \quad n = 1, \dots, (\ell - 1).$$
(A5)

The allowed energy bands correspond to a real value of the wavenumber  $\tilde{k}$ , i.e., to the condition

$$\operatorname{Re}\left[\sum_{n=1}^{\ell} Z(\alpha_n, k)\right] = 0, \qquad (A6)$$

and there are  $(\ell+1)$  allowed bands ( $\ell$  finite bands followed by a continuum band), separated by  $\ell$  forbidden bands.

Closed analytical results can be obtained in the  $\ell = 1$  case. In particular, for the lowest allowed band one obtains the parametric equations [24, 34] for the energy

$$\varepsilon_1 = 1 - k^2 \operatorname{cn}^2(\eta + K(k'), k'), \quad k^2 \leqslant \varepsilon_1 \leqslant 1, \quad 0 \leqslant \eta \leqslant K(k'),$$
(A7)

and the corresponding wavenumber (for half of the first Brillouin zone, the other half being obtained by symmetry)

$$\tilde{k} = Z(\eta, k') - \frac{\pi}{2K(k)} \left( 1 - \frac{\eta}{K(k')} \right) - \sqrt{\frac{(\varepsilon_1 - k^2)(1 - \varepsilon_1)}{1 + k^2 - \varepsilon_1}}.$$
(A8)

Here  $k' = \sqrt{1 - k^2}$  is the complementary modulus of the elliptic functions. With a change of parametrization and using the properties of the elliptic functions [25, 26], these formulae can be reduced to the following (more familiar to physicists) expressions [16, 21]:

$$\varepsilon_1 = 1 - k'^2 \operatorname{cn}^2(p, k'), \quad k^2 \leqslant \varepsilon_1 \leqslant 1, \quad -K(k') \leqslant p \leqslant K(k'),$$
 (A9)

and for the wavenumber in the first Brillouin zone

$$\tilde{k} = Z(p, k') + \frac{\pi p}{2K(k)K(k')}.$$
(A10)

Note that (as demonstrated in a more general context in [35]) the results for the first forbidden band can be obtained *formally* from those concerning the first allowed band simply by replacing p in (A9) and (A10) by  $i\overline{p}$ . One obtains thus for the energy levels of the first forbidden band:

$$\overline{\varepsilon}_1 = 1 - \frac{k^2}{\operatorname{cn}^2(\overline{p}, k)},\tag{A11}$$

where the parameter  $\overline{p}$   $(-K(k') \leq \overline{p} \leq K(k'))$  corresponds to a *complex* wavenumber given by:

$$\tilde{k} = i \left[ F(\gamma, k) - E(\gamma, k) + \tan\gamma \sqrt{1 - k^2 \sin^2 \gamma} \right] + i \frac{\overline{p}\pi}{2K(k)K(k')}, \qquad (A12)$$

with

$$\sin\gamma = \operatorname{sn}(\overline{p}, k) \,. \tag{A13}$$

One realizes, however, that with increasing  $\ell$  the complexity of the implicit equations (A2), (A3),(A5), and (A6) (that one has to solve in order to obtain the dispersion relations for the allowed bands) increases, up to becoming prohibitive even for present-day powerful computers.

Fortunately, a recent paper by Maier [36] offers an alternative to the above-described Hermite-Halperin method of band computation. It is shown, using the so-called Hermite– Krishever Ansatz, that the dispersion relations for any integer  $\ell$  can be expressed in terms of the  $\ell = 1$  relations. Moreover, the effective construction of these dispersion relations, whose technical details will not be given here, makes use of relatively simple polynomials and rational functions. This represents an enormous gain in the efficacy of symbolic calculation of the dispersion relations.

To our knowledge, there is no information yet on the spectrum of the Lamé potential when  $\nu$  is not a positive integer. In these cases one has to obtain the results strictly from numerical evaluations.

See, e.g., Drazin, P. G., and Johnson, R. S., "Solitons: An Introduction" (Cambridge University Press, Cambridge, 1989); Rajaraman, R., "Solitons and Instantons" (North-Holland,

Amsterdam, 1989); Remoissenet, M., "Waves Called Solitons: Concepts and Experiments" (Springer-Verlag, Berlin, 1999); ed. Scott, A., "Nonlinear Science" (Oxford University Press, New York, 1999).

- [2] For a review see, e.g., Bishop, A. R., in "Lattice Dynamics and Structural Phase Transitions", Proceedings, Paris 1977, ed. Balkanski, M.; "Solitons and Condensed Matter Physics", Proceedings of the Symposium on Nonlinear Structure and Dynamics in Condensed Matter, eds. Bishop, A. R., and Schneider, T. (Springer-Verlag, New York, 1978).
- [3] Currie, J. F., Krumhansl, J. A., Bishop, A. R., and Trullinger, S. E., Phys. Rev. B 22, 477 (1980).
- [4] Leung, K. M., Phys. Rev. B 26, 226 (1982); Phys. Rev. B 27, 2877 (1983).
- [5] Campbell, D. K., Peyrard, M., and Sodano, P., Physica **19 D**, 165 (1986).
- [6] Saxena, A., and Dandoloff, R., Phys. Rev. B 58, R563 (1998).
- [7] Gupta N., and Sutherland, B., Phys. Rev. A 14, 1790 (1976).
- [8] DeLeonardis, R. M., and Trullinger, S. E., Phys. Rev. B 27, 1867 (1983).
- [9] Ablowitz, M. J., Kaup, D. J., Newell, A. C., and Segur, H., Stud. Appl. Math. 53, 249 (1974);
   McKean, H. P., Comm. Pure Appl. Math. 34, 197 (1981).
- Behera, S.N. , and Khare, A., J. Phys. (Paris) C6, 314 (1981); Khare, A., Habib, S., and Saxena, A., Phys. Rev. Lett. 79, 3797 (1997); Habib, S., Khare, A., and Saxena, A., Physica D 123, 368 (1998).
- [11] Arscott, F. M., "Periodic Differential Equations" (Pergamon, Oxford, 1981).
- [12] Bena, I., Khare, A., and Saxena, A., J. Math. Phys. 45, 2323 (2004).
- [13] Magnus, W., and Winkler, S., "Hill's Equation" (Wiley, New York, 1966).
- [14] Khare, A., and Sukhatme, U., J. Math. Phys. 40, 5473 (1999); J. Math. Phys. 42, 5652 (2001).
- [15] Ganguly, A., Mod. Phys. Lett. A 15, 1923 (2000); J. Math. Phys. 43, 1980 (2002).
- [16] Horovitz, B., Phys. Rev. Lett. 46, 742 (1981); Phys. Rev. B 35, 734 (1987).
- [17] Zhuravchak, L. M., Mater. Sci. **36**, 33 (2000).
- [18] Fetter, A. L., and Stephen, M. J., Phys. Rev. 168, 475 (1968).
- [19] Sutcliffe, P. M., J. Phys. A **29**, 5187 (1996).
- [20] Sutherland, B., Phys. Rev. A 8, 2514 (1973).
- [21] Shastry, B. S., Phys. Rev. Lett. **50**, 633 (1983).
- [22] Brihaye, Y., Giller, S., Kosinski, P., and Kunz, J., Phys. Lett. B 293, 383 (1992).

- [23] Enolskii, V. I., and Eilbeck, J. C., J. Phys. A 28, 1069 (1995).
- [24] Li, H., Kusnezov, D., and Iachello, F., J. Phys. A 33, 6413 (2000).
- [25] For the properties of the Jacobi elliptic functions and integrals see Gradshteyn, I. S., and Ryzhik, I. M., "Tables of Integrals, Series, and Products" (Academic Press, New York, 1980).
- [26] Byrd, P. F., and Friedman, M. D., "Handbook of Elliptic Integrals for Engineers and Scientists" (Springer, Berlin, 1971).
- [27] Balakrishnan, R., and Saxena, A., Phys. Rev. B 58, 14383 (1998).
- [28] Manton, N. S., Nucl. Phys. B **150**, 397 (1979).
- [29] Brihaye, Y., Giller, S., and Kosinski, P., J. Phys. A: Math. Gen. 28, 421 (1995).
- [30] Maier, R. S., "The 192 Solutions of the Heun Equation", preprint, arXiv: math-ph/0408317;
   J. Diff. Eqs. 213, 171 (2005).
- [31] Krumhansl, J.A., and Schrieffer, J. R., Phys. Rev. B 11, 3535 (1975).
- [32] Scalapino, D. J., Sears, M., and Ferrell, R. A., Phys. Rev. B 6, 3409 (1972).
- [33] Rice, M. J., Bishop, A. R., Krumhansl, J. A., and Trullinger, S. E., Phys. Rev. Lett. 36, 432 (1976).
- [34] Whittaker E. T., and Watson, G. N. "A Course of Modern Analysis" (Cambridge University Press, Cambridge, 1980), Ch. XXIII.
- [35] Kohn, W., Phys. Rev. **115**, 809 (1959).
- [36] Maier, R. S., "Lamé polynomials, hyperelliptic reductions and Lamé band structure", preprint, arXiv: math-ph/0309005; J. Diff. Eqs. 198, 16 (2004).

## FIGURE CAPTIONS

FIGURE 1: Typical profile of the Lamé potential  $V_L(\phi)$  over a period [0, 2K(k)].

FIGURE 2: Typical profile of a kink lattice solution of the first type (an array of nontopological kink-antikink pairs) over a spatial period 4L of the lattice (for a fixed value of the control parameter  $a^2$ ,  $0 < a^2 < 1$ .)

FIGURE 3: The stability diagram of the kink lattice solution of the first type, at T = 0K, in the plane of the parameters  $k^2$  (of the Lamé potential) and  $a^2$  (the control parameter).

FIGURE 4: Typical profile of a kink lattice solution of the second type (an array of topological kinks/antikinks) over a spatial period 4L of the lattice (for a fixed value of the control parameter  $a^2 > 0$ ). Note that we have plotted  $|\tilde{\phi}(x)|$  modulo 2K(k); there are no "cusps" in the field  $\tilde{\phi}(x)$ .

FIGURE 5: The profile of the topological single kink solution.

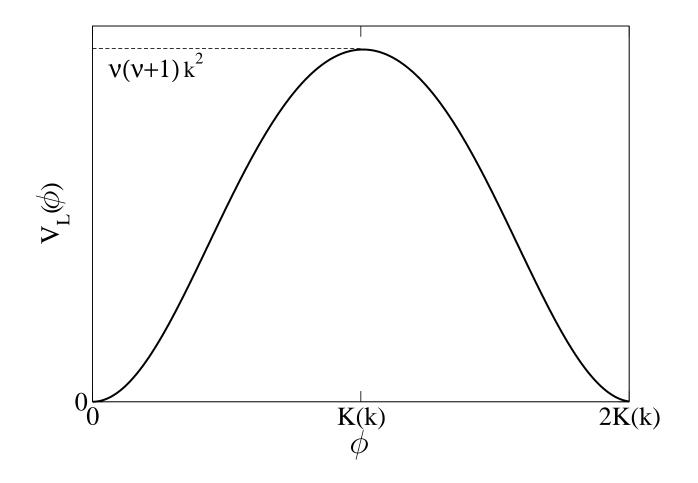


FIG. 1:

FIGURE 1

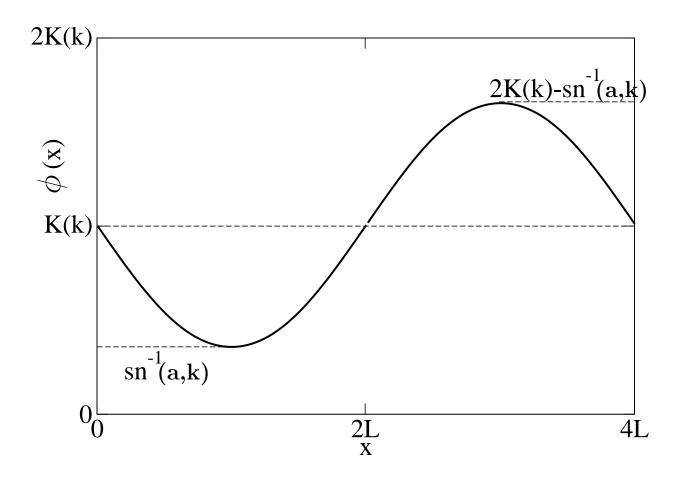


FIG. 2:

FIGURE 2

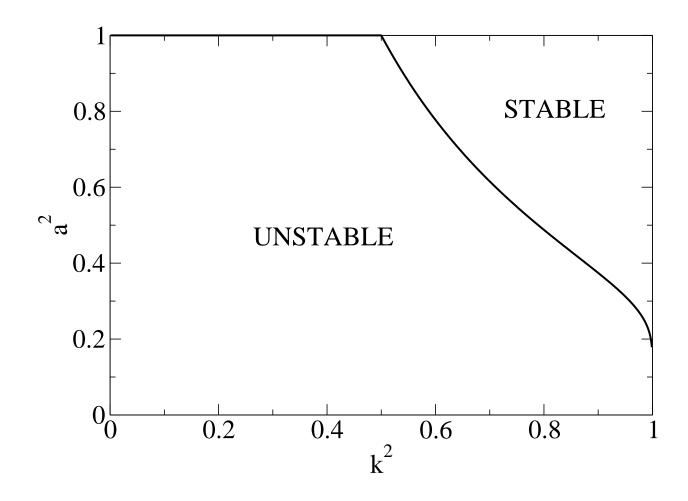


FIG. 3:

FIGURE 3

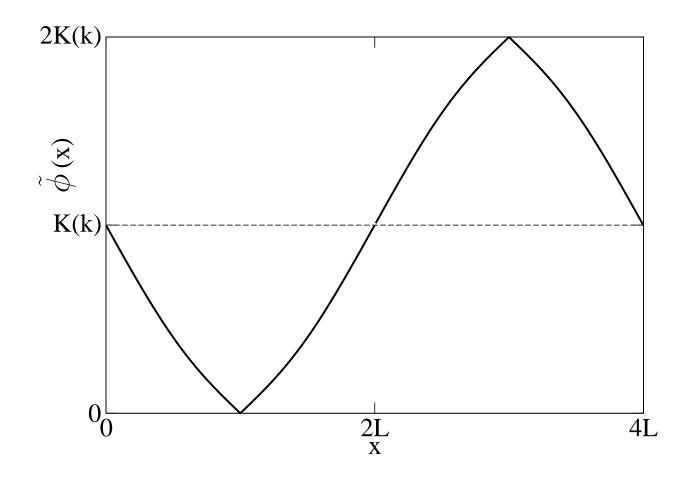


FIG. 4:

FIGURE 4

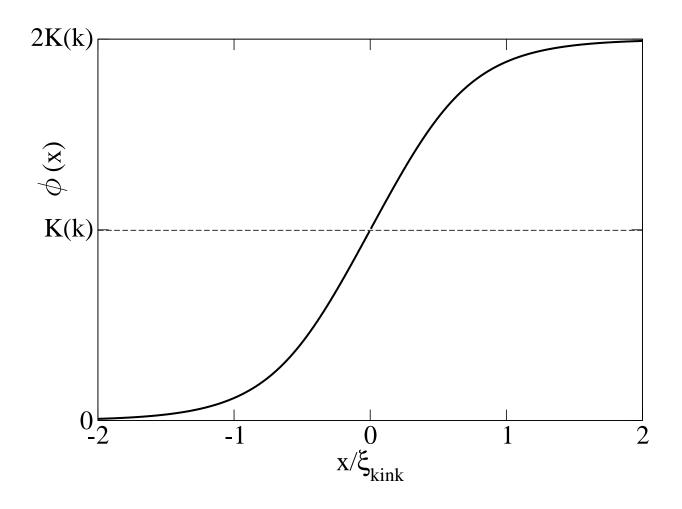


FIG. 5:

FIGURE 5