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1995 J. Phys.: Condens. Matter 7 6187

(http://iopscience.iop.org/0953-8984/7/31/003)

J. Phys.: Condens. Matter 7 (1995) 6187–6196. Printed in the UK

A structural viewpoint on the sine–Gordon equation in incommensurate phases

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Received 6 March 1995, in final form 1 May 1995

Abstract. The spatially inhomogeneous order parameter considered in the Landau description of incommensurate phases is analysed from a structural viewpoint using the superspace approach. All modulation functions, including that of the order parameter, are defined along the internal space. Taking a displacive case for concreteness and within the constant-amplitude approximation, a general differential equation for the order parameter phase, θ, which generalizes the well known sine–Gordon equation, is derived. No reference is made to any particular expression for the free-energy expansion; only consistency arguments between the Landau description and the structural properties of an incommensurate phase are used. It is shown that, under certain quite common conditions, this general equation can be approximately reduced to the sine–Gordon equation. The sine–Gordon equation can, therefore, be considered of rather general validity when modelling the structure of incommensurate phases irrespective of their particular thermodynamic potential. The introduction of the θ modulation along the internal space further simplifies the equation; its parameters become system independent, being a function of only the *soliton density*.

1. Introduction

One of the most successful approaches to the analysis of incommensurate (IC) modulated phases is based on a generalization of the usual Landau theory [1]. In particular, its description of two sequential phase transitions limiting the stability range of an IC phase has been successfully applied to a great variety of systems [2–14]. Below and not far from the phase transition into the IC phase, the system is described by a sinusoidal distortion, so that the position of every atom μ varies in each cell l according to the displacement modulation

$$u(\mu, l) = Q e^{\mu} \exp(\mathrm{i}2\pi \boldsymbol{q}_I \cdot \boldsymbol{l}) + \mathrm{cc} \tag{1}$$

where Q is the order parameter amplitude, e^{μ} is the polarization vector of the unstable mode and $\boldsymbol{q}_I$ its incommensurate modulation wavevector, which in general is temperature dependent. For simplicity, we limit the discussion to one-dimensional modulations, i.e. modulations with a single rationally independent wave vector. Typically, a further decrease in temperature drives the system towards a new phase transition (the lock-in phase transition), after which the modulation wavevector is locked into a simple rational value $\boldsymbol{q}_L$ and, therefore, a strict crystalline state is recovered. As the lock-in transition is approached, the importance of higher-order harmonics, frozen together with the first harmonic (the

0953-8984/95/316187+10$19.50

order parameter), should increase [15, 16] and, consequently, the atomic modulations are expected to show increasingly anharmonic character. Instead of including higher harmonics in expressions such as (1), the usual approach to describe these anharmonic distortions is to use the lock-in phase as a reference [17], i.e. the order parameter is defined locally, its homogeneous configuration corresponding to the lock-in commensurate phase. Thus, the state of the system in the IC phase is described by a modulation of the order parameter. Thus, the atomic displacements $u(\mu, l)$ are expressed as

$$u(\mu, l) = Q(l)e^{\mu} \exp(\mathrm{i}2\pi \boldsymbol{q}_L \cdot \boldsymbol{l}) + \mathrm{cc}. \tag{2}$$

Obviously, comparing (1) and (2), when the distortion is sinusoidal, the order parameter $Q(l)$, so defined, is modulated in the form $Q(l) = Q\exp(\mathrm{i}2\pi\delta \cdot l)$, where $\delta = q_I - q_L$. If only long-wavelength variations in $Q(l)$ are considered, a continuous approximation can be introduced for the order parameter along the modulation direction in real space: $Q(x) = \rho(x)\exp(\mathrm{i}2\pi\theta(x))$, so that in the sinusoidal regime $\rho(x) = \rho$(x independent) and $\theta(x) = \delta x$, for $\delta = \delta a^*$. A Landau potential is then constructed where invariant terms with x derivatives of the field $Q(x)$ are included [18]. Under certain conditions, this Landau potential predicts the existence, previous to the lock-in phase, of a so-called soliton regime [15, 16, 19]. The soliton regime is characterized by the coexistence of almost commensurate (lock-in) and IC regions. Phenomenologically this state is a consequence of the competition of two antagonistic terms present in the Landau free-energy expansion: the Lifshitz invariant [1] and a relatively low-order umklapp term that contributes to the lock-in energy. This scheme typically appears in the free energy of those compounds whose IC wavevector is far from the Brillouin zone centre. Typical examples are A_2BX_4 compounds [20, 21] which, together with many others, are usually classified as type-I compounds [19]. The order parameter phase $\theta(x)$ progressively shows r identical steps, r being the number of possible distinct domains in the lock-in phase, e.g. $r = 4$ for $(NH_4)_2BeF_4$ and $r = 6$ in K_2SeO_4. Thus, the structure in the soliton regime is composed of periodic zones where the modulation wavevector is almost constant and equal to q_L, limited by discommensurations where the modulation phase varies rapidly. Although, out of the sinusoidal regime, the order parameter amplitude ρ also becomes inhomogeneous, this inhomogeneity is typically very weak [4, 22] and can be neglected, reducing the Landau analysis to what is called the 'constant-amplitude approximation'. Under this approximation, the temperature dependence of the inhomogeneous $\theta(x)$ is controlled by the sine–Gordon equation that is derived from the minimal Landau free-energy conditions [5, 6, 16, 20, 23]. In this paper the term 'sine–Gordon equation' will refer to its first integral:

$$\left(\frac{\mathrm{d}\theta}{\mathrm{d}x}\right)^2 = a_0 + a_1 \cos(2\pi r\theta(x)). \tag{3}$$

The parameters a_0 (> 0) and a_1 ($|a_1| \leqslant a_0$) are functions of some coefficients of the free energy expansion and the amplitude of the order parameter. Implicitly they depend on δ and, certainly, on temperature [20, 24]. Solutions of (3) range from $\theta = \delta x$ (the sinusoidal regime) to step functions whose constant steps tend in the limiting case to have an infinite length, so that they represent macroscopic domains of the commensurate lock-in phase. The degree of anharmonicity in this continuous path from a sinusoidal to an ideal step function with infinite period is quantitatively described by the so-called 'soliton density' [19, 25] which measures the ratio of the width of the discommensurations and that of the commensurate steps. Introducing the parameter $k = (2|a_1|/(a_0+|a_1|))^{1/2}$ the soliton density is then given by [25, 20] $n_s = \pi/2K(k)$, where $K(k)$ is the complete elliptic integral of the first kind. In the sinusoidal regime, $n_s = 1$ ($k = 0$) and in the ideal limit of the soliton regime $n_s = 0$ ($k = 1$).

Traditionally, IC compounds without a Lifshitz invariant in its free-energy expansion seemed to have a completely different phenomenological description [7–14, 19] and, apparently, a similar soliton regime was not possible for them. That is the case for proper ferroelectrics such as $NaNO_2$ and thiourea, which belong to the group of type II materials. However, some conclusive x-ray diffraction results [26] and a recent revision of previous theoretical approaches [27] have shown, at least in the case of thiourea, that the soliton regime is also present in type II compounds and can be modelled using the Landau theory. Moreover, the observed soliton regime was shown to be well described by the sine–Gordon differential equation (3) although the equation is not directly derived from the minimization of the Landau free energy. Hence, the difference between the behaviour of both types of IC structure was reduced more to quantitative than to qualitative features. The sine–Gordon equation seemed to have a rather general validity independently of the particular form of the Landau potential.

In this paper, we pretend to ascertain the validity limits of the sine–Gordon equation in the description of IC phases from a general viewpoint, as obtained when the usual order parameter definition is made consistent with an atomistic description of the structure. No Landau-type energy argument will be used. We shall derive the restrictions on the order parameter configuration that result from its necessary consistency with the structural properties of an IC structure and, therefore, are independent of any phenomenological theory. In particular, we demonstrate that, in general, the order parameter phase satisfies a differential equation that generalizes the sine–Gordon equation and can be reduced to this latter in certain cases, which may often be realized, independently of the expansion for the free-energy density relevant in each case.

The superspace formalism [28, 29] is used in the analysis. A simple relation exists between the inhomogeneous configuration of the order parameter in physical space with the variation in the order parameter along the internal space introduced in the superspace description of IC structures [28, 29]. The description of the distortion by means of a modulation of the order parameter along the internal coordinate v instead of a continuous physical space variable x is shown to be much better suited to a consistent practical analysis. The form of the modulation and the modulation wavevector become uncoupled in this description, i.e. the differential equation governing the transformation of the modulation with temperature becomes formally independent of the value of the modulation wavevector, its solutions having a fixed period in internal space.

2. Atomic modulation functions in the soliton regime

In general, in an IC structure the atomic displacements with respect to a reference normal structure can be described by general modulations of the form

$$u(\mu, l) = \sum_{n \geqslant 0} u_n^\mu \exp(\mathrm{i}2\pi n q_l \cdot l) + \mathrm{cc}. \tag{4}$$

Comparing (4) and (2), it is clear that equation (2) is restricting the distortion (4) to those Fourier components n, such that nq_L is equivalent to q_L and equation (4) can then be reduced to

$$u(\mu, l) = \left(\sum_n{}' u_n^\mu \exp(\mathrm{i}2\pi n \delta \cdot l) \right) \exp(\mathrm{i}2\pi q_L \cdot l) + \mathrm{cc} \tag{5}$$

where the prime in the sum indicates that it is restricted to n such that $nq_L \equiv q_L$. Comparing again equation (5) and (2), it is still necessary to assume the uniqueness of the polarization

vector for all harmonics

$$u_n^\mu = b_n e^\mu \tag{6}$$

These restrictions on the form of the atomic modulation correspond to the fact that the Landau model reduces the structural modulation to one having the symmetry of the order parameter, neglecting the presence of secondary modes with different symmetries. Using (5) and (6), the order parameter modulation can be expressed as

$$Q(l) \equiv \rho(l)\exp(\mathrm{i}2\pi\theta(l)) = \sum_n{}' b_n \exp(\mathrm{i}2\pi n\delta \cdot l) \tag{7}$$

where $\rho(l)$ and $\theta(l)$ are real.

In the superspace description, the discrete atomic displacement fields are substituted by periodic 'atomic modulation functions' $u^\mu(v)$ along the internal coordinate v [30]:

$$u^\mu(v) = \sum_n{}' u_n^\mu \exp(\mathrm{i}2\pi nv) + \mathrm{cc} \tag{8}$$

so that $u(\mu, l) = u^\mu(v = q_l \cdot l)$. It should be noted that the introduction of the internal coordinate v is not a continuous approximation; it is just a way of taking advantage of the incommensurateness of the vector q_l, so that each value of v within a period represents a certain cell in direct space. According to (6) and (8), we can write

$$u^\mu(v) = Q(v)e^\mu + \mathrm{cc} \tag{9}$$

where $Q(v)$ is defined as

$$Q(v) = \rho(v)\exp(\mathrm{i}2\pi\theta(v)) = \sum_n{}' b_n \exp(\mathrm{i}2\pi nv). \tag{10}$$

Comparing with (7), $Q(l) = Q(v = \delta \cdot l)$, which is fully consistent with (8), by the property

$$Q(v + q_L \cdot l) = Q(v)\exp(\mathrm{i}2\pi q_L \cdot l) \tag{11}$$

which is ensured by the restriction on the sum in (10) [31]. Equation (9) can also be written in a more explicit form:

$$u_\alpha^\mu(v) = 2\rho(v)\left|e_\alpha^\mu\right|\cos(2\pi\theta(v) + \Psi_\alpha^\mu) \tag{12}$$

where Ψ_α^μ is the phase of the component α of the polarization vector e^μ.

Equation (6) describes an important approximation for the structural features of IC phases which is hidden in their usual Landau description. Obviously, this approximation makes sense only when δ is small in comparison with the typical scale of variation within the Brillouin zone of the mode polarization vectors and, in addition, very high harmonics in the modulation are negligible, which is the situation usually assumed when a continuous approximation in real space is introduced for the order parameter modulation.

3. Sine–Gordon equation in internal space

According to (7) and (10), the amplitude and phase of the order parameter along the internal space, $\rho(v)$ and $\theta(v)$, coincide with the functions $\rho(x)$ and $\theta(x)$ considered in the usual continuous approximation for direct space [20, 22], except for a temperature-dependent scale factor δ^{-1} between both continuous variables. This simple relation, however, should not conceal the very different interpretations of the two descriptions. The space of the coordinate v is an adimensional phase space, and the functions $\rho(v)$ and $\theta(v)$ are well defined

whatever configuration the order parameter $Q(l)$ may take; no continuous approximation is required for their definition and they always have a clear microscopic meaning given by the equations above. In contrast with the real space functions, the functions $\rho(v)$ and $\theta(v)$ are periodic with period 1, their period being uncorrelated with the modulation wavevector and its possible temperature variation. If the phase configuration satisfies the sine–Gordon equation, as the period of the function along v is necessarily 1, the corresponding coefficients a_0 and a_1 in the sine–Gordon equation (see equation (3)) satisfy the additional condition $(a_0+|a_1|)^{1/2} = 2K(k)/\pi$, where k is the parameter defined in section 1. Consequently, the sine–Gordon equation can be written in the form

$$\dot{\theta}^2 = \frac{1}{n_s^2}\left[1 - k^2\cos^2\left(2\pi\frac{r\theta}{2}\right)\right] \qquad \text{if } a_1 < 0 \tag{13a}$$

or

$$\dot{\theta}^2 = \frac{1}{n_s^2}\left[1 - k^2\sin^2\left(2\pi\frac{r\theta}{2}\right)\right] \qquad \text{if } a_1 > 0 \tag{13b}$$

where the dot represents the derivative with respect to the internal coordinate. Hence, $\theta(v)$ is completely determined by k or n_s.

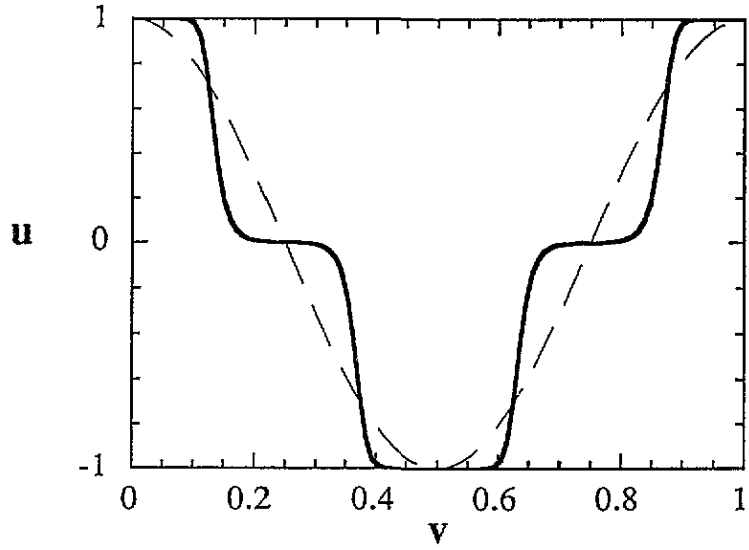

Figure 1. Example of the atomic modulation function $u(v)$ for $r = 4$ and a strong soliton density. The broken line corresponds to the sinusoidal regime.

Note that in the sinusoidal regime, when only a single first term $n = 1$ exists in the right-hand side of equation (10), $\theta(v) = v$, which is a trivial solution of equation (13) for $k = 0$ ($n_s = 1$). In figure 1 we present the effect of the function $\theta(v)$ solution of equation (13a) for $r = 4$ and $n_s = 0.2$ ($k = 0.999\,999$) on a particular atomic modulation function according to (12). It is important to note that in contrast with the function $\theta(x)$ in real space the width of the discommensurations in internal space goes to zero when the limit of the soliton regime ($k = 1, n_s = 0$) is approached. The finiteness of the discommensurations in real space in the usual Landau description is preserved by the simultaneous blow-up of the scale factor δ^{-1} as the lock-in limit is approached.

4. Generalization of the sine–Gordon equation

If tq_L (t integer) equals a reciprocal-lattice vector of the normal phase, the Fourier series (5), (7), (8) and (10) are restricted to values of n such that $n = mt + 1$ ($m \in Z$). However, condition (6) contains an implicit additional restriction on the possible Fourier terms in equation (10). The Fourier amplitudes u_n^μ for different atoms and a fixed n are symmetry related according to the superspace group of the structure. As n increases, these symmetry relations differ in general for different values of n in a cyclic way. As mentioned above, (6) implies the same symmetry relation for all terms in the sum (i.e. the symmetry of the order parameter). Therefore, the set of possible values n in the sum will in general be reduced to a subset of those mentioned above, typically $n = mr + 1$ with r being a multiple of t (it corresponds, as seen below, to the number of possible distinct commensurate domains in the lock-in phase, or steps in the order parameter phase). Hence, taking into account equation (10), this implies that:

$$\theta\left(v + \frac{1}{r}\right) = \theta(v) + \frac{1}{r} \tag{14}$$

while the period of $\rho(v)$ is $1/r$.

For simplicity, we shall restrict our considerations now to the case of IC phases with a superspace group containing at least one rotational operation that transforms q_I into $-q_I$, as it happens in all experimental cases. Under this condition, once the arbitrary phase of b_1 (the phason degree of freedom in the structure [32, 33]) is set to zero, the rest of the coefficients b_n ($n > 1$) should also be real to keep this superspace symmetry operation. If the coefficients b_n are real and we neglect the v-dependence of the order parameter amplitude, equation (10) yields

$$\dot{\theta}^2 = d_0 + \sum_{k \geqslant 1} d_k \cos(2\pi k r v). \tag{15}$$

On the other hand, from (10) and also within the constant-amplitude approximation, it can be easily derived that

$$\cos(2\pi m r \theta(v)) = \sum_t A_t^m \cos(2\pi t r v). \tag{16}$$

Comparing (16) and (15), it is then clear that, in general, we can expect that the function $\theta(v)$ satisfies the differential equation

$$\dot{\theta}^2 = a_0 + a_1 \cos(2\pi r\theta) + a_2 \cos(2\pi(2r)\theta) + a_3 \cos(2\pi(3r)\theta) + \dots . \tag{17}$$

This equation is a generalization of the sine–Gordon equation resulting from the usual Landau approach for type I materials. It has been derived from the consistent definition of the order parameter phase $\theta(v)$ in microscopic terms without any appeal to Landau energy arguments. It can therefore be considered to have general validity for any IC material, so long as the constant-amplitude approximation is satisfactory.

In the above derivation we have assumed that $q_L \neq 0$. However, the particular case $q_L = 0$ corresponding, for instance, to thiourea or sodium nitrite is not very different. Although, in this case, the actual polarization vector of the order parameter distortion is real, the complex expressions used can be maintained, if the polarization vector considered in equation (6) is the complex eigenvector corresponding to q_I. The harmonics summed up in the first term of (5) are, then, all positive integers $nr + 1$. The polarization vector is in this case a linear combination of the order parameter mode at $q_I = 0$ and the mode with which is coupled at $q_I \neq 0$ [27]. A similar situation will happen when q_L lies on the border of the Brillouin zone.

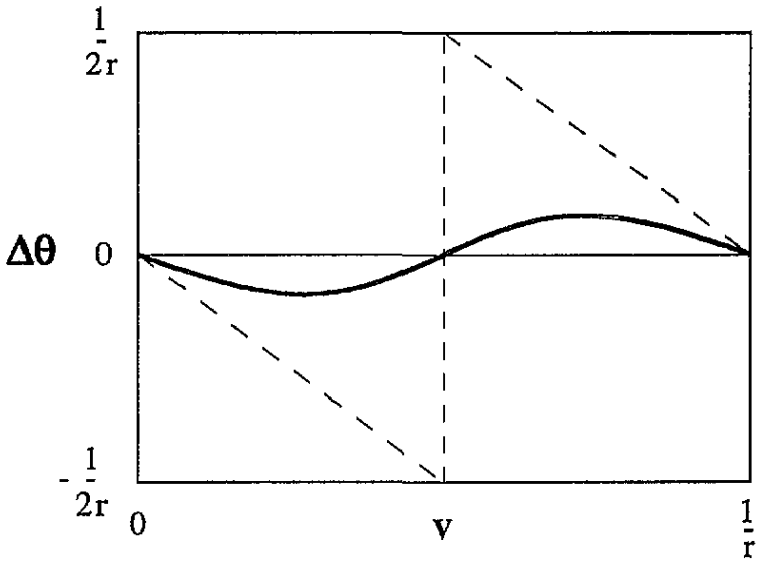

Figure 2. Function $\Delta\theta(v)$ in a generic period $[0, 1/r]$: – – –, limit case of null soliton density (equation (19*a*)); ——, solution of the sine–Gordon equation (essentially a sinusoidal function) for a soliton density $n_s = 0.6$.

From (10), it is straightforward that $\theta(v)$ should be odd and, therefore, the function $\Delta\theta(v)$ defined as $\theta(v) - v$, which according to (14) has period $1/r$, is in general given by the Fourier series

$$\Delta\theta(v) = \sum_{k=1}^{\infty} c_k \sin(2\pi k r v). \tag{18}$$

Obviously, the sinusoidal case corresponds to $\Delta\theta(v) = 0$, $c_k = 0$ for all k. On the other hand, in the extreme limit of a soliton regime, where the order parameter phase forms along the internal space r equal-spaced discontinuous steps with an increase of $1/r$ in each one, $\Delta\theta(v)$ should exhibit a sawtooth shape (figure 2) and its coefficients c_k in (18) would be

$$c_k = \frac{(-1)^k}{k\pi r} \tag{19a}$$

$$c_k = \frac{1}{k\pi r}. \tag{19b}$$

The two configurations (19) differ basically in the situation of the point $v = 0$: either in the middle of a discontinuous step ($c_1 > 0$) or in the middle of a constant-phase region ($c_1 < 0$). Equation (19*a*) corresponds to the case with the order parameter phase taking the values n/r ($n = 0, \ldots, r-1$) in the r possible domains of the commensurate phase, while the case (19*b*) represents the situation when the commensurate domains are associated with the phase values $n/r + 1/2r$ for the order parameter. Both the sinusoidal configuration and the soliton limit (19) are trivial solutions of the sine–Gordon equation ($a_n = 0, n > 1$, in equation (17)). In the latter case, $a_0 \approx |a_1|$ and is very large, with a_1 negative and positive, respectively (see equations (13)).

According to the demonstration above, in a more general situation, $\theta(v)$ satisfies an equation of the type (17). The concept of soliton density originally introduced for the

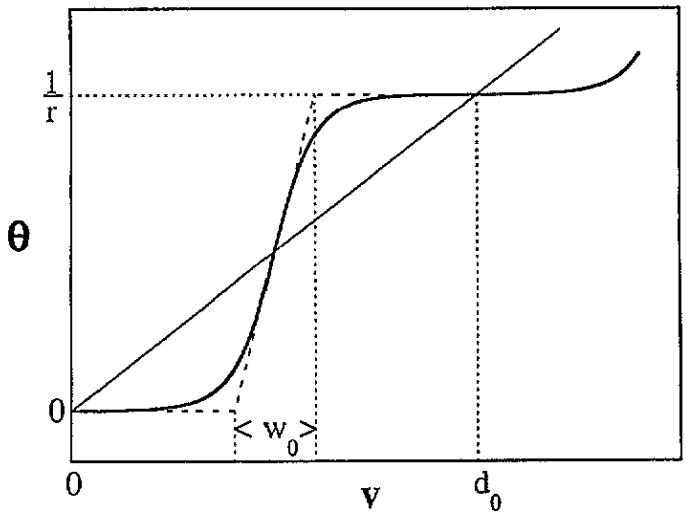

Figure 3. Schematic representation of the criterion used to define the relative width of the discommensurations in the internal space for a general regime ($n_s \neq 0$).

sine–Gordon equation can also be extended to this general equation. The soliton density measures the volume fraction of the sample occupied by discommensurations, and can be defined [20] as w_0/d_0, w_0 being the discommensuration width and d_0 the distance between two consecutive discommensurations. According to the periodicity of $\Delta\theta(v)$, $d_0 = 1/r$. On the other hand, since the stepping of θ is only exact in the limit, the width of the discommensurations is not in general unambiguous and depends on its definition. Assuming a single maximum of $\dot{\theta}$ in each discommensuration, a simple criterion [20, 34] consists in substituting the quasi-commensurate regions by strict plateaux of width $d_0 - w_0$ and the IC zones by straight lines having a slope equal to the maximum value of $\dot{\theta}$ (see figure 3). As the θ steps have a value of $1/r$, the width w_0 is then given by $1/(r\dot{\theta}_{max})$ and accordingly, $n_s = 1/\dot{\theta}_{max}$. Hence, for a general configuration satisfying (17) the soliton density could be expressed as

$$n_s = \frac{1}{\sqrt{a_0 + |a_1| - |a_2| + |a_3| + \ldots + (-1)^{n+1}|a_n| + \ldots}} \tag{20}$$

or, equivalently, in terms of the Fourier amplitudes in (18)

$$n_s = \frac{1}{1 + 2\pi r[|c_1| + 2|c_2| + 3|c_3| + \ldots + n|c_n| + \ldots]}. \tag{21}$$

These general expressions coincide with the usual definition when equation (17) is constrained to be the sine–Gordon equation.

5. Approximate validity of the sine–Gordon equation

Near the sinusoidal regime, one can expect that the first corrections to the sinusoidal configuration should come from the harmonics of next lowest order, i.e. $n = r + 1$ and $n = -r + 1$. It can be shown, comparing equations (10) and (18), that the amplitude of these harmonics is linearly related to the value of c_1 in equation (18), while their contribution to the other terms in the series is quadratic or higher. Hence, we can expect in a wide temperature range close to the sinusoidal regime (so long as the appearance of higher harmonics is not

significant) that the Fourier series (18) is limited to a single term, i.e. $c_1 \neq 0, c_n \approx 0$ for $n > 1$ (see figure 2). On the other hand, one can easily check that a single harmonic for the function $\Delta\theta(v)$ is a good approximation for the solution of the sine–Gordon equation up to soliton densities of the order of 0.6 (see figure 2). As the temperature is furthered lowered, new harmonics in (18) are bound to appear ($c_k \neq 0, k > 1$), but a weight hierarchy will be kept so long as the values of the order parameter harmonics in (10) also follow a rapidly decreasing law with their order. Deviations from the sine–Gordon equation are then expected, but these should again become negligible if the system further approaches the soliton limit mentioned above. We can assume that the ratios of the Fourier amplitudes c_k in this limiting soliton configuration are an upper bound, so that for any intermediate configuration $n|c_n| \geqslant m|c_m|$ if $m > n$, while the signs of the coefficients c_k follow the same rules as in the soliton limit (see equations (19)). Provided that the previous inequality is satisfied and using equations (15) and (17), the following approximate expressions for the first four coefficients a_i in (17) in terms of the amplitudes c_k can be obtained:

$$\begin{aligned} a_0 &= 1 + 6\pi^2 r^2 c_1^2 + \ldots \qquad a_0 > 0 \\ a_1 &= 4\pi r c_1 + 28\pi^2 r^2 c_1 c_2 - 2\pi^3 r^3 c_1^3 + \ldots \\ a_2 &= -2\pi^2 r^2 c_1^2 + 8\pi r c_2 + 52\pi^2 r^2 c_1 c_3 \ldots \\ a_3 &= 2\pi^3 r^3 c_1^3 - 12\pi^2 r^2 c_1 c_2 + \ldots . \end{aligned} \tag{22}$$

Therefore, only a very reduced number of coefficients a_i in (17) will have a non-negligible value. The sine–Gordon equation, even though it is not the most general differential equation for the phase, will constitute a good first approximation of the real differential equation for $\theta(v)$.

6. Conclusions

Independently of any actual energy calculations in the framework of the Landau theory, the sine–Gordon equation (13) is expected to be a good approximation of the general equation (17) in significant temperature ranges even for type II compounds. The sine–Gordon equation acquires a much simpler form when defined in internal space, where it is parametrized using only the soliton density.

Although the sine–Gordon equation has been systematically considered in the thermodynamic description of IC phases, it has never been used in the structural analysis of them (except for the early attempt of Yamada *et al* [35]). These results open up new perspectives in this field. Equations of the type of equation (12) can be used to model the structure of IC materials. The phase $\theta(v)$ in these equations is expected to satisfy one of the sine–Gordon equations (13), and this constraint can be introduced into the structural refinement. The eventual success of such a refinement not only will confirm the validity of the sine–Gordon equation but also will yield an experimental value of the soliton density in the structure.

Acknowledgments

This work has been supported by the DGICYT project PB91-0554 and the UPV project 063.310-EB150/92.

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