NONLINEAR EXCITATIONS IN ANISOTROPIC X-Y MODELS*

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Abstract

We consider a 1-D ferrodisorptive X-Y model and illustrate the importance of phase-amplitude coupling in the dominant low T elementary excitations.

Recent studies^[1,2,3,4] have indicated the role of nonlinear equations in phenomenological characterizations of the statistical mechanics of several 1-D problems. These include complex order parameter Ginzburg-Landau free energy expansions with discrete phase symmetry, in the limits of constant phase^[1,2,4] and constant amplitude^[3,4]. The essential idea is that the basic features of the formal statistical mechanics^[1,3] can be well described by isolating dominant solutions of the nonlinear partial differential equations of motion governing the order parameter. Spatially localized 'kink-like' solutions characteristic of many nonlinear equations^[5], have been emphasized. In 1-D, it has been shown^[1-4] that these, taken together with linearized perturbations, yield an excellent phenomenological description of the classical free energy, correlation functions, etc., at low temperatures. The kink solutions may be considered as elementary excitations and are physically distinctive in many contexts^[3,4], so that it is important to understand their properties, for example as cluster walls in ferroelectric models^[1]. While many more problems are posed in higher dimensions, molecular dynamics simulations^[6] have demonstrated the importance of nonlinear cluster patterns above and below critical temperatures.

We are currently considering a general class of problems in 1-D with discrete phase symmetry that may be described with a complex order parameter. These include Fröhlich charge density-wave phenomena^[3] and a variety of anisotropic X-Y models. We are solving the exact statistical mechanics^[1], but here we will be concerned with the complementary aspect of studying the coupled nonlinear equations in the amplitude and phase order parameter components, to isolate the important elementary excitations.

To be explicit we will consider a 1-D ferrodistorptive X-Y model with harmonic intersite coupling: $H = \int d(z/L) K(x,y;z)$, where

$$K = \frac{1}{2\pi} (\pi_x^2 + \pi_y^2) - A(x^2 + y^2) + B(x^4 + y^4) + C(x'^2 + y'^2) \quad (1)$$

m is the mass of the particle, l is the lattice spacing, π_x is the canonical momentum $m\dot{x}$ and A , B , and C are nonnegative constant coefficients; $\dot{x}$ and x' signify dx/dt and $dx/d(z/l)$ respectively. We have introduced a continuum representation, limiting ourselves to strong intersite coupling ($C \gg A$) and extended displacement patterns^[1]. This is one limit of a model recently treated^[7] in a 2-D molecular dynamics simulation, which showed the formation of clusters in the angular displacement field separated by 90° walls. Our purpose here is to describe these walls in the analogous 1-D problem in some detail. In particular we will see explicitly the coupling between the radial and angular displacements, which is of very general importance in such two-component order-parameter problems^[3]. This is an improvement to the approximate domain wall description given in^[7], which assumed a 'Sine-Gordon' equation^[5] for the angular displacement field and a constant radial component.

For clarity we introduce polar coordinates r and θ so that the on-site potential $V(r, \theta)$ has a 'wine-bottle-bottom' form with discrete (rather than continuous) rotational symmetry. The potential trough is defined by $r_{\min}(\theta) = r_0(2 - \sin^2 2\theta)^{-1/2}$, where $r_0 = (A/B)^{1/2}$. Thus $V(r_{\min}(\theta)) < V(r=0)$, all θ , and there are four degenerate minima at $r = r_0$, $\theta = \pi/4, 3\pi/4, 5\pi/4, 7\pi/4$. If a displacement gradient is to be formed, particle positions must move from one potential well to an adjacent one. Classically, the energetically preferred trajectory is the one crossing the potential barrier at its lowest point. At low temperatures this is expected to be the dominant nonlinear excitation of the anharmonic hamiltonian(1). At any finite temperature a subtle phonon-dressing of the kinks is crucial [2,3] and other nonlinear excitations also contribute.

Hamilton's equations for the simplest travelling wave solutions $r, \theta = r, \theta(z - vt)$ are

$$0 = -u_{ss} + u\psi_s^2 - u + u^3 (2 - \cos^2 2\psi) \quad (2a)$$

$$0 = -2u u_s \psi_s - u^2 \psi_{ss} + \frac{1}{2} u^4 \sin 4\psi, \quad (2b)$$

where $u = r/r_0$, $\psi = \theta - \pi/4$, $u_s = du/ds$, $s = \gamma(z-vt) \ell^{-1} \alpha^{-1/2}$, $\gamma = (1 - v^2/c_0^2)^{-1/2}$, $c_0^2 = 2C/\mu$, $\alpha = A/c$. We see immediately that there is a cut-off velocity of propagation c_0 , relativistic scaling of length (and energy), and a wall thickness $\propto \alpha^{-1/2}$. Inspection of (2) shows that u and ψ are strongly coupled. The simple Sine-Gordon equation corresponding to constant u in (2b) has been used elsewhere [7] to describe domain wall formation. The only such solution consistent with (2a) is the trivial one of constant ψ in which the particles stay at the bottom of one of the on-site potential wells.

The initial value problem for the coupled system of ordinary differential equations (2) is easily solved numerically using Hamming's Predictor-Corrector Method [8]. It should be emphasized that this procedure is not intended to predict the energetically preferred excitation patterns - these are chosen on the basis of physical intuition. Indeed the physically favored trajectory we have investigated is particularly sensitive to initial conditions in our numerical procedure. [Considerable insight and motivation can be gained from a mechanical analogue interpretation of (2) in which a particle moves in the negative of the physical on-site potential.]

The results of our calculation are illustrated in Fig. 1, which reveals not only the well-defined 90° domain wall but also the strong coupling between ψ and u . Defining the width L of a 90° wall as the change in s between $\psi = 0 + \Delta$ and $\psi = \pi/2 - \Delta$ where Δ is 0.1% of $\pi/2$, we find in the reduced units of (2), $L = 8.017 \pm 0.002$, whereas the approximate Sine-Gordon solution ($\psi = \tan^{-1} \exp \pm (s\langle u \rangle/2)$) gives $9.130/\langle u \rangle$: not only does this approximation give an inaccurate classical picture of the low T elementary excitations but it also describes an artificially widened wall. Both of these shortcomings make

the simple Sine-Gordon theory inappropriate for a detailed phenomenological description of the 1-D X-Y ferrodistorive hamiltonian, in the spirit of Refs. [1-4].

In conclusion we have indicated the importance of phase-amplitude coupling in describing the details of dominant low temperature elementary excitations for a lattice dynamic X-Y model. Such considerations will be important in many similar complex order parameter problems and the methods described here are equally applicable.

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Figure Captions

Figure 1 The radial (solid line) and angular (dashed line) displacement fields as functions of position along the chain, for a 90° wall (see text).