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Classical ϕ^6-field theory in (1+1) dimensions. A model for structural phase transitions

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Abstract. The classical ϕ^6-field theory in (1+1) dimensions, is considered as a model for the first order structural phase transitions. The equation of motion is solved exactly; and the presence of domain wall (kink) solutions at and below the transition point, in addition to the usual phonon-like oscillatory solutions, is demonstrated. The domain wall solutions are shown to be stable, and their mass and energies are calculated. Above the transition point there exists exotic unstable kink-like solutions which takes the particle from one hill top to the other of the potential. The partition function of the system is calculated exactly using the functional integral method together with the transfer matrix techniques which necessitates the determination of the eigenvalues of a Schrödinger-like equation. Thus the exact free energy is evaluated which in the low temperature limit has a phonon part and a contribution coming from the domain wall excitations. It was shown that this domain wall free energy differs from that calculated by the use of the domain wall phenomenology proposed by Krumhansl and Schrieffer. The exact solutions of the Schrödinger-like equation are also used to evaluate the displacement-displacement, intensity-intensity correlation functions and the probability distribution function. These results are compared with those obtained from the phenomenology as well as the ϕ^4-field theory. A qualitative picture of the central peak observed in structural phase transitions is proposed.

Keywords. ϕ^6-field theory; structural phase transitions; central peak; soft mode

1. Introduction

The structural phase transition (SPT) observed in ferroelectric crystals is usually associated with a soft phonon mode whose frequency decreases as the temperature is lowered towards its critical value (T_c) (Lines and Glass 1977). Besides the soft phonon mode a central peak near zero frequency is also observed in these transitions. The central peak is characterised by a negligible width and its strength grows as one approaches T_c from above (Riste *et al* 1971; Shapiro *et al* 1972). Even though, some understanding of the soft mode has emerged the central peak phenomenon still remains a puzzle (Bruce 1978). Conventionally, in describing the SPT one takes recourse to two different types of models namely the order-disorder and the displacive transitions. Whereas in the former case the on-site energy of the atoms is much larger than the intersite coupling, in the latter case the reverse is true. However, lately it has been realized that both these transitions can occur within the same model (Bruce *et al* 1979). The major advancement in the understanding of SPT, and in particular the central peak phenomenon has emerged from one-dimensional model