Thermally Activated Generation, Motion and Annihilation of Localized Modes in the Anharmonic Chains

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During the studies of the first-order phase transitions in crystals (e.g. melting), a precursor of the transition has been detected by the fluorescence method [T. Shigenari, E. Kojima, Y. Ino and K. Abe, Phys. Rev. Lett. **66** (1991) 2112]. The critical speeding-up of the fluorescence lifetime was ascribed to the increase of the displacement fluctuations. Among the possible mechanisms of the critical increase of fluctuations, the intrinsic localized modes (ILM) [A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61** (1988) 970] or other localized modes can be discussed. Thus, the study of localized modes in a discrete system will be useful to interpret the observations.

The aim of the present study is to discuss the existence of the ILM near the first-order phase transition and the possibility of their experimental indication by the fluorescence lifetime measurements. To our knowledge, up to now, no experimental methods are known for indirect observation of the ILM in crystals. The main difficulty here is to separate the contribution of ILM from the contributions of other localized modes. Our approach is the numerical study of energy localization in the thermalized nonlinear chains and the comparison of the results obtained at different temperatures and different degrees of discreteness.

We investigate numerically the thermalized Frenkel-Kontorova (FK) chain and the one-dimensional chain of particles having two degrees of freedom. In the continuum limit, the FK model reduces to the sine-Gordon equation, which supports the topological solitons (kinks) and the oscillatory two-soliton solutions, called here continuous breathers (CB). CB perturbed by discreteness shows a very long lifetime [J. A. D. Wattis, Nonlinearity **9** (1996) 1583]. Thus, one can expect the existence of at least two kinds of localized modes, ILM and CB, in the system. However, the ILM cannot exist in a weakly discrete system and hence the comparison of behavior of the system at different degrees of discreteness can show us the influence of ILM.

For setting the initial conditions we used the equipartition theorem, according to which, in the statistical equilibrium state, the energy of the chain is shared equally among harmonic modes and there is no phase correlation between them. Then we studied the time evolution of the nonlinear system. We observed the energy localization in different forms and the kink-pair nucleation process. Finally, the system reached the equilibrium state in which a part of energy was carried by the localized modes. The relaxation time is smaller in the system with a greater discreteness.

Unexpected effects found in this study are the abrupt change of kink's drift velocity in a highly discrete system and the propagation of kinks with well-defined velocities in a weakly discrete system. The continuum theory predicts the acceleration of the kinks by phonon wave packet as long as there is an energy flux through the kink [W. Hasenfratz, R. Klein, Physica **89A** (1977) 191]. Thus, the theory explains the Brownian-like motion of the kinks but the abrupt change of the drift velocity is not predicted. The change of kink's velocity is probably due to the collision with ILM. However, it has been shown that the energy exchange between CB and kink may take place even at a weak discreteness [S. V. Dmitriev, T. Miyauchi, K. Abe and T. Shigenari, Phys. Rev. **E61** (2000) 5880]. Thus, the highly discrete and the weakly discrete systems were found to show different behavior. However, at the present stage we cannot separate the contributions of different kinds of localized modes in energy fluctuations. Further investigations are necessary to see what kind of localized modes can be responsible for the critical increase of energy fluctuations near the first-order phase transition in a crystal.