

Quantum theory of anharmonic gap modes

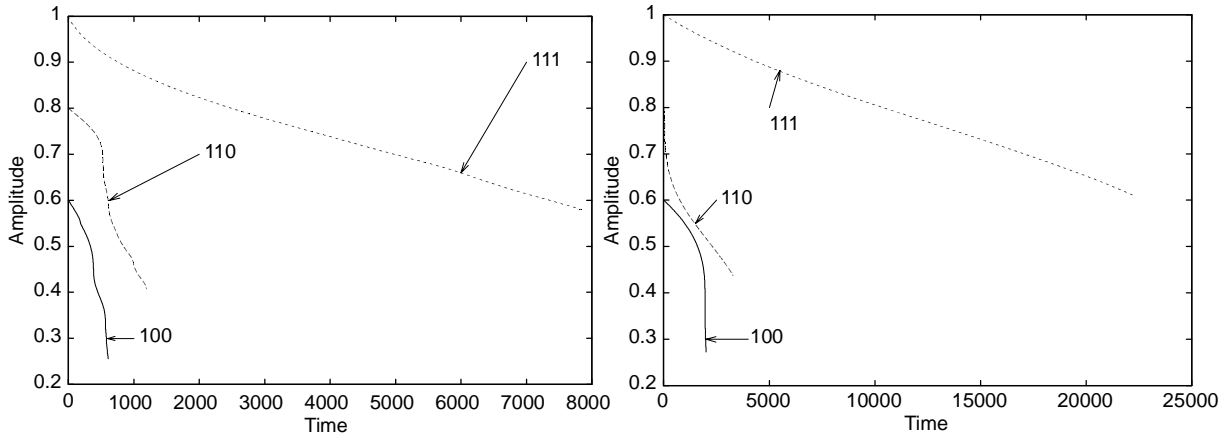
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It has been shown that stable localized vibrations of large amplitude (called intrinsic local modes (ILMs) or discrete breathers) can exist in anharmonic lattices within the gaps in the phonon spectrum [1]. The observation of gap ILMs in three-dimensional lattices brings certain computational difficulties. Here we apply an analytical method, which allows us to reduce the ILM problem to a simpler inverse problem of phonons scattering on a local potential. Using this method we have calculated the dependence of the frequency of odd gap ILMs (localized on the light ion) on their amplitude in alkali halide crystals. The method also allows one to describe quantum effects of the ILMs. The ILMs quantization is based on the calculation of the effective potential energy operator $U(Q)$. We introduce the reduced amplitude of the ILM $A = \sum_{mn} a_{mn}$, where a_{mn} is the reduced amplitude of the n 'th harmonic of the atom m . Two classical turning points of the ILM equal $Q_{1,2} = A + A_0$, where $A_0 = \sum_m a_{m0}$ is the DC-component of the ILM. For the given amplitude and frequency ω one finds the maximal value of the kinetic energy $E_{kin} = (\omega^2/2) \sum_m [\sum_n n a_{mn}]^2$. From the energy conservation law one gets $E_{kin} = U(Q_{1,2})$. The procedure allows us to find $U(Q)$ numerically. Then, approximating $U(Q)$ by an analytic expression, one can do the quantization. In this approach the effective mass of the ILM equals unity.

The ILMs are stable only in the classical limit; taking into account the zero-point fluctuations of the lattice leads to the multiphonon decay of these modes. The peculiarity of the problem is that, due to the large amplitude of the mode, standard perturbation theory is not applicable for the calculation of the decay rate. To solve the problem, we apply the nonperturbative theory of two-phonon decay [2].



Results showing the gap mode amplitude (in Å) in NaI (left) and KI crystals versus time (in ω_I/π units) for 3 directions are presented in the Fig. above ($\omega_I = 2 \cdot 10^{13} \text{ sec}^{-1}$ is the lowest frequency of the optic band). The gap modes in the (111) direction (lifetime $\sim 10^{-8}$ sec) are most stable. Such a long lifetime should not restrict the experimental observation of intrinsic localized gap modes.

1. S.A. Kiselev, and A.J. Sievers, Phys. Rev. B **55**, 5755 (1997).
2. V. Hizhnyakov, Phys. Rev. B **53**, 13981 (1996); V. Hizhnyakov and D. Nevedrov, Phys. Rev. B **56**, R2908 (1997).