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LOCAL OSCILLATIONS IN AN ANHARMONIC CRYSTAL

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In the problem of local oscillations, anharmonicity is usually considered as the cause of the damping and small shift of the local frequencies. Its influence can lead, however, also to other effects, particularly to the appearance of new local frequencies [1, 2].

It is natural to expect the influence of anharmonicity on the properties of local oscillations to become most strongly pronounced in crystals with large zero-point oscillation amplitudes (quantum crystals), when the usual method of expanding the potential energy in terms of the displacements of the nuclei is not valid. In such systems, the behavior of even an isotropic defect can be significantly different than in a harmonic lattice, for the anharmonicity of the oscillations causes the change of mass to give rise to a change in the effective force constants. We shall show below that under certain assumptions the properties of an isotropic defect in an anharmonic crystal are radically altered.

We consider a one-dimensional crystal containing 2N + 1 atoms, of which 2N have a mass m and one, located at the zeroth site, has a mass m' = Qm. We shall take into account only the nearest-neighbor approximation, which is described by a Morse potential

$$\phi(r) = D[e^{-(r-r_0)/\rho} - 1]. \tag{1}$$

Here D and ρ are constants, r_0 is the distance between sites, and r the instantaneous distance between atoms. We assume also that no external forces act on the system.

To describe the dynamics of this system, we shall use the method of [3 - 6], in which it is not assumed that the anharmonicity is small, and which makes it possible to take into account all the orders of perturbation theory. Although this method was used in the cited papers only for ideal crystals, it is easy to formulate it in a manner that does not presuppose that the lattice is ideal. Disregarding damping processes (pseudoharmonic approximation), this method applied to the potential (1) leads to the following self-consistent system of equations[1)]

$$\omega^2 G_{nn'}(\omega) = \delta_{nn'} + \sum_{n''} D_{nn''} G_{n''n'}(\omega), \quad D_{nn'} = \frac{K_{nn'}}{\sqrt{m_n m_{n'}}}; \tag{2a}$$

[1)] We follow here [4, 5], where the Morse potential is specially considered.

$$K_{n,n-1} = -f\exp\left[-\langle (u_n - u_{n-1})^2\rangle/\rho^2\right], \sum_{n'=n-1}^{n+1} K_{nn'} = 0; \tag{2b}$$

$$\langle u_n u_{n'}\rangle = \frac{\hbar}{\pi}\int_0^\infty d\omega \operatorname{cth}\frac{\hbar\omega}{2kT}\operatorname{Im} G_{nn'}(\omega - i0+). \tag{2c}$$

Here $G_{nn'}(\omega)$ is the Fourier transform of the equal-time Green's function defined for the atom displacements u_n from the statistical equilibrium premises, and $f = D/\rho^2$ is the harmonic force constant.

The solution of the system (2) can be obtained by an iteration method. We assume the harmonic approximation as the first step. The problem then reduces to the solution of Eq. (2a), which describes the dynamics of the isotropic defect in the harmonic approximation. The Green's functions have in this case simple analytic representations (cf., e.g., [7]). To proceed to the next iteration it is necessary to determine the correlators (2c), which determine the effective force constants $K_{nn'}$. At T = 0°K, the expression for the correlator $\langle(u_n - u_{n-1})^2\rangle$ takes the form ($n \geq 1$):

$$\frac{2\hbar}{\pi m\omega_M}\left\{2 + \frac{Q-1}{2-Q}\sum_{k=0}^{\infty}\left(\frac{Q}{Q-2}\right)^k\prod_{j=1}^{3}\left(k - 2n + \frac{2j-1}{2}\right)^{-1} + \right.$$

$$\left. + 2\pi\frac{1-Q}{(2-Q)^3}\left(\frac{Q}{2-Q}\right)^{2n-5/2}\right\}, \quad Q < 1, \tag{3}$$

$$\frac{2\hbar}{\pi m\omega_M}\left\{2 + \frac{1-Q}{Q}\sum_{k=0}^{\infty}\left(\frac{Q-2}{Q}\right)^k\prod_{j=1}^{3}\left(k + 2n + \frac{2j-5}{2}\right)^{-1}\right\}, \quad Q \geq 1,$$

where $\omega_M = \sqrt{4f/m}$ is the maximum frequency of the harmonic lattice. Comparing (3) with (2b) we see that as a result of the anharmonicity the isotopic defects changes the effective force constants for any pair of atoms of the chain. The force constants decrease if Q < 1 and increase if Q > 1. Their change is a monotonic function of the parameter (Q - 1). At large distances from the impurity, the correction to $K_{nn'}$ behaves like n^{-3}, i.e., the perturbation potential is short-range and the number of bound states is therefore finite [8].

After calculating the effective force constants with the aid of (3) and (2b) we return to Eq. (2a), which now includes also the changes of the force constants. In view of the short-range character of the perturbation potential, we can use the Lifshitz method [9] for the solution of (2a). For this purpose, it is necessary to rewrite (2a) in the form of a Dyson equation and take into account the changes of the force constants in a finite albeit sufficiently large region. As a result we arrive at a determinantal equation of order (2p + 1) (p is the number of nearest neighbors of the impurity, for which the change of $K_{nn'}$ is taken into account). The solutions of this determinantal equation determine, at $\omega > \omega_M$, the local frequencies in the pseudoharmonic approximation. The equation obtained in this manner was investigated numerically with a computer. It was assumed that p = 10 (further expansion of the defect region does not alter the results), $r_0 = 4 \times 10^{-8}$ cm, m = 4 a.m.u., and D = 10.2°K (all these parameters pertain to He^4 [10]); $\rho = r_0/6$ (see [5]).

The results of the calculation were quite unexpected. At $Q < 1$, the decrease of the force constants fully offsets the change of the mass, and no local oscillations arise. To the contrary, for a heavy impurity, owing to the increase of the force constants, local oscillations do occur, but only with low frequencies. There can exist altogether two local oscillations, the first of which (odd) occurs at $Q \gtrsim 1.3$, and the second (even) at $Q > 9$. As $Q \to \infty$, the local frequencies approach from below a common limit equal to $\sim 1.0059\omega_M$ (at finite Q, the even oscillations has the lower frequency). Thus, only minute local oscillations can exist in the model under consideration, and the condition for their occurrence is the opposite of the case of a harmonic crystal.

The results are determined, naturally, by the chosen value of the parameter ρ characterizing the degree of anharmonicity. The assumed value of ρ corresponds to strong anharmonicity. With increasing ρ, at a fixed value of ω_M, the degree of anharmonicity decreases, and the local oscillations acquire the same properties as in a harmonic lattice.

Thus, in spite of the simplified character of the investigated model, it can be stated that the dynamic properties of the defects can undergo considerable changes in strongly anharmonic crystals, and an experimental study of these properties would be of definite interest.

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COULOMB EXCITATION OF NUCLEI BY HEAVY POLARIZED PARTICLES

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The existing methods for determining the magnetic moments (m.m.) of short-lived nuclear states are based on the study of the interaction of the m.m. with the magnetic field [1]. The spin precession under the influence of the m.m. interaction with the magnetic field leads either to a perturbation of the $\gamma\gamma$ correlation[1)] or to a Zeeman splitting of the levels of the excited nucleus. The latter is observed in a number of cases with the aid of the Mossbauer effect.

[1)] Resonant scattering of a γ quantum is also possible in this case.