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NON-LINEAR DYNAMICAL EXCITATIONS IN SOLIDS

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Abstract.— Vibrational excitations can exist in non-linear systems which have no counterpart in the corresponding linear systems. In this paper we investigate such excitations in systems where the non-linearity is of an on-site character. In particular, we analyze the existence conditions for localized (and delocalized) excitations, and their interaction with external fields.

In this paper we discuss the properties of non-linear periodic lattice waves in models of perfect and imperfect crystals. Our model Hamiltonians contain a fourth-order on-site electron-ion potential reminiscent of $\phi^4$-models. This approach is motivated by the success of the self-consistent phonon approximation (SPA) for the investigations of ferroelectric-type phase transitions in terms of such models (refer to Bussmann et al., this Conference).

2. General Solution to the Dynamical Monomer Problem

The monomer (Fig. 1) consists of one anion and one cation. If the center of mass motion is factored out, the system is described by two coupled variables, which may be chosen as the displacement, $u$, of the cation relative to the anion core and the displacement, $w$, of the anion shell relative to its core. The oscillation frequency of the monomer is displayed in Fig. 2 as a function of $w^2$, where $w_o$ is the maximum displacement from the origin. The range $w^2 > w^2_{\text{crit}}$ belongs to anharmonic oscillations which traverse the origin $w=0$ (the solution at $w^2=0.4$ is the only harmonic one). The range $w^2 < w^2_{\text{crit}}$ describes oscillations which are localized in one or another of two equivalent potential wells. The minimum squared displacement from the origin increases from zero to the left of $w^2_{\text{crit}}$ until it coincides with $w^2_o$ at $-g^2/g_4$ (notice that the frequency does not go to zero at this point).

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We now turn to the consideration of a problem in which a nonlinearly polarizable atom is present as a substitutional impurity in a monatomic linear chain (Fig. 3). We seek a solution for the displacement field in the chain that decays exponentially with increasing distance from the impurity site, i.e., a localized mode.

We can obtain an exact solution to the equations of motion of the chain with the Ansatz

\[ \omega = A \cos \omega t \]  
\[ u_0 = B(1) \cos \omega t + B(3) \cos 3\omega t \]  
\[ u_n = (-1)^n [C(1)e^{-n\lambda \cos \omega t} + C(3)e^{-n\mu \cos 3\omega t}] \]  
\[ n \geq 1, \]  

where \( \omega_0 \) is the relative shell-core displacement of the impurity atom, and \( u_n \) is the displacement of the \( n \)th core, when we assume in addition that \( u_{-n} = u_n \). In Eq. (3.2c) the quantities \( \lambda \) and \( \mu \) are the real quantities given by \( \lambda = 2 \cosh^{-1}(\omega/\omega_0) \), \( \mu = 2 \cosh^{-1}(3\omega/\omega_L) \), where \( \omega_L = (4\gamma/M)^{1/2} \) is the maximum normal mode frequency of the unperturbed chain. The frequency of the localized mode must therefore be larger than \( \omega_L \) for the solution (3.2) to exist. The equation determining \( \omega \) is

\[ \frac{9M\omega^2 - 9Mw^2 - f - \gamma(1 + e^{-\mu})}{2f - 9Mw^2 - \gamma(1 + e^{-\mu})} = 1. \]  

(3.3)

With \( \omega \) determined from this equation the amplitude \( A \) is found from the relation

\[ A^2 = \frac{4g_2}{3g_4} \left[ 1 + \frac{2f/g_2}{(2f/M\omega^2) - \delta} \right] > 0, \]  

(3.4)
where \( X = \left[ M \omega^2 - \gamma (1 + e^{-\lambda}) \right] / \left[ \omega^2 - \gamma (1 + e^{-\lambda}) \right] \).

It should be pointed out that for \( g_2 < 0 \), Eqs. (3.3) - (3.4) have a solution even if \( M' = M \) and \( f = \gamma \) provided that \( |g_2|/\gamma > 2.8 \). In this case the localized mode has no counterpart in the harmonic approximation.

4. Response to External Electric Fields

If the periodon solutions to the nonlinear equation of motion of a crystal containing atoms or ions possessing nonlinear polarizabilities are to be observed experimentally, it is likely to be through features they contribute to the functions characterizing the response of such crystals to external probes. We have therefore begun a study of the periodon-type solutions of the equations of motion of a monatomic linear crystal of this type (Fig. 4), in the presence of an external spatially and temporally varying electric field.

We consider an electric field given by \( E_n(t) = E_0 \cos(n\phi - \omega t) \). In this case the equations of motion of the crystal have the exact solution

\[
\begin{align*}
\omega_n(t) &= A \cos(n\phi - \omega t) \\
u_n(t) &= B(1) \cos(n\phi - \omega t) + B(3) \cos(3n\phi - \omega t)
\end{align*}
\]

provided that the frequency and wave vector are related through \( \omega^2 = 4(f + f')/9M \sin^2 \frac{3\phi}{2} \).

We then have that the amplitude \( A \) is obtained in terms of the electric field amplitude \( E_0 \) from the equation

\[
\frac{4fA \sin^2 \frac{1}{2} \phi}{Z E_0 g_2 A - \frac{3}{4} g_4 A^3} = \frac{M \omega^2 - 4(f + f') \sin^2 \frac{1}{2} \phi}{M \omega^2 - 4f' \sin^2 \frac{1}{2} \phi} ,
\]

while

\[
\begin{align*}
B(1) &= \frac{Z E_0 g_2 A - \frac{3}{4} g_4 A^3}{M \omega^2 - 4f' \sin^2 \frac{1}{2} \phi} \\
B(3) &= \frac{g_4 A^3}{16f \sin^2 \frac{3}{2} \phi}
\end{align*}
\]

where \( Z \) is the charge on each core and \(-Z\) is the charge on each shell. Generalizations of this solution can be obtained by adding higher odd harmonics to the right hand sides of Eqs. (4.1). However, in that case a solution in finite terms, like that given by Eqs. (4.1) - (4.3), is no longer possible.

+ refer to Büttner and Bilz, (this Conference)