Self-consistent potential of intrinsic localized modes: Application to diatomic chain

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A mean-field theory of intrinsic localized modes (ILMs) in anharmonic lattices is proposed, which allows one to perform calculations for macroscopically large lattices of arbitrary dimensions with realistic pair potentials. In the theory, the original nonlinear problem is reduced to a linear problem of mode localization on the self-consistent harmonic local potential. This enables us to apply the Lifshitz method of the perturbed local dynamics of phonons for the calculations of ILMs. In order to check the theory, the characteristics of the ILMs in a diatomic chain with the Born-Mayer-Coulomb pair potential are found and compared with the corresponding molecular-dynamics simulations. The results of both considerations are in a very good agreement.

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I. INTRODUCTION

It is already a well-known fact that localized vibrational excitations can exist in perfect anharmonic lattices.[1–10] Such excitations are called intrinsic localized modes (ILMs),[4] discrete breathers,[8] or discrete solitons.[10] The main approach, which has been used for the study of these excitations so far, is molecular-dynamics (MD) simulations, which are based on the numerical integration of the classical equations of motion in the lattices with a finite number of the degrees of freedom. The approach is rather efficient in the case of simple one-dimensional lattices (see, e.g., Refs. 11–19), but it requires very lengthy computations in the case of two-dimensional and three-dimensional lattices due to a rapid growth of the number of numerical operations with the increase of the number of the vibrational degrees of freedom (see Refs. 20 and 21). Therefore, it is of interest to develop other methods for studying ILMs that will allow us to reduce the amount of numerical computations.

In this paper, we have developed a mean-field-type theory of ILMs that gives a possibility to perform calculations for macroscopically large lattices of arbitrary dimensions with realistic pair potentials. The theory is based on the consideration of small variations of the ILM amplitude. The equations for these variations include the characteristics of an ILM. This allows one to reduce the nonlinear problem of an ILM to a linear problem of the perturbed phonon dynamics; the perturbation comes from the ILM and is determined self-consistently. To describe the effect of perturbation, we apply the Green's function method of locally perturbed harmonic lattices (the Lifshitz method, see also Refs. 22 and 23, where an analogous idea was applied to ILMs in the lattices with cubic and quartic anharmonicities). In contrast to Ref. 4, where the Green's-functions method was used to take into account anharmonic terms for strongly localized ILMs of a large amplitude, our method uses the Green's functions for the description of harmonic (small) vibrations and is applicable generally, including the case with rather poor localization of ILMs. To demonstrate how our method works, we apply it to ILMs in a diatomic chain with a realistic Born-Mayer-Coulomb pair potential. For verification, the molecular-dynamics simulations of these ILMs are carried out as well. The results of both calculations are in very good agreement.

II. DESCRIPTION OF INTRINSIC LOCALIZED MODES

Let us start with the classical equations of the motion of atoms in a lattice:

$$M_n \ddot{u}_n = -\partial V/\partial u_n, \tag{1}$$

where u_n is the displacement of the atom n, M_n is its mass (the subscript n includes both the site number and the number of the Cartesian component), and $V \equiv V(\{u_n\})$ is the potential energy:

$$V = \frac{1}{2}\sum_{n_1 n_2} V^{(2)}_{n_1 n_2} u_{n_1} u_{n_2} + V_{anh},$$

where the first term is its harmonic part and the second term is its anharmonic part.

We are considering a localized solution of Eq. (1), describing a stable ILM. For such a solution, the displacements of atoms are of the form $u_n(t) = A_n \cos \omega_l t + \xi_n + O(\omega_l)$, where $|A_n|$ is the amplitude of the ILM at the site n, ω_l is the frequency of the ILM, which lies outside the phonon spectrum, ξ_n is the shift of the equilibrium position of the atom n (i.e., the dc component of the ILM; this component differs from zero due to odd anharmonicities), and $O(\omega_l)$ is the sum of higher harmonics. The contributions of these harmonics are usually rather small if the amplitude of the ILM is small as compared to the lattice constant(s).[3–9] Below, they will be neglected.

Our further consideration is based on the fact that $\tilde{u}_n = A_n \cos[\omega_l(t+\tau)] + \xi_n$ is also a solution of Eq. (1). Taking τ to be infinitesimal, we get $\tilde{u}_n(t) = u_n(t) + q_n(t)$, where $q_n = -A_n \omega_l \tau \sin \omega_l t$ is an infinitesimal variation of the ILM. It also oscillates in time with the frequency ω_l but its phase is shifted by $-\pi/2$.

Taking into account the relation $V(\{u_{n'}\}, \tilde{u}_n) = V + (\partial V/\partial u_n) q_n$ (here, $n' \neq n$) and subtracting the equation of motion for u_n from that for $\tilde{u}_n$, we find the following equation for q_n:

$$M_n\ddot{q}_n = -\sum_{n'} [V^{(2)}_{nn'} + v_{t,nn'}]q_{n'}, \tag{2}$$

where

$$v_{t,nn'} = \partial^2 V_{anh}/\partial u_n \partial u_{n'}. \tag{3}$$

We are searching for the solution of Eq. (2), which has the basic frequency ω_l like that of the ILM and the phase shifted by $-\pi/2$. Let us apply the rotating wave approximation (RWA), which corresponds to the neglecting of higher-order harmonics in this equation. To do this, we need to extract the $\propto \sin \omega_l t$ term in the product $v_{t,nn'}q_{n'}$, with $q_{n'} \propto \sin \omega_l t$.

The time dependence of $v_{t,nn'}$ is given by the sum of the terms $\propto \cos^m \omega_l t$, $m=1,2,\ldots$. Only the terms with even $m=2n$ give the required contribution. The $\propto e^{i\omega_l t}$ terms of the product $v_{t,nn'} \sin \omega_l t$ come (a) from the time-independent part of $\cos^{2n} \omega_l t$ [it equals $2^{-2n}(2n)!/n!n!$] and (b) from the $\propto e^{2i\omega_l t}$ part of $\cos^{2n} \omega_l t$ [it equals $-2^{-2n}(2n)!/(n-1)!(n+1)!$]. Summing up these two contributions and taking also into account the $\propto e^{-i\omega_l t}$ terms, we get

$$\cos^{2n} \omega_l t \sin \omega_l t = \frac{2^{-2n}(2n)!}{n!(n+1)!} \sin \omega_l t + O[(2k+1)\omega_l],$$

$k \geqslant 1$. Here, $O[(2k+1)\omega_l]$ denotes higher harmonics which are neglected in RWA. Note that the above factor in front of $\sin \omega_l t$ coincides with the time-independent term of the product $2 \cos^{2n} \omega_l t \sin^2 \omega_l t$. In other words, the amplitude of the first harmonic of the term $v_{t,nn'}q_{n'}$ in Eq. (2) equals to the time-independent term of the Fourier series expansion of $2v_{t,nn'} \sin^2 \omega_l t$. This observation allows one to rewrite Eq. (2) in the form

$$M_n\ddot{q}_n = -\sum_{n'} [V^{(2)}_{nn'} + v_{nn'}]q_{n'}, \tag{4}$$

where

$$v_{nn'} = 2\langle v_{t,nn'} \sin^2 \omega_l t\rangle,$$

$$\langle \cdots \rangle = \frac{\omega_l}{2\pi}\int_0^{2\pi/\omega_l} \ldots dt \tag{5}$$

denotes the averaging over the period $2\pi/\omega_l$. The averaging procedure in Eq. (5) cancels out all oscillating in time terms. Note that the obtained dynamical matrix $v_{nn'}$ leads to the same mean value of the potential energy of the small vibration as the matrix $v_{t,nn'}$.

A. Equilibrium position shifts

The dc shifts ξ_n, entering together with the amplitudes A_n into Eq. (5), are not independent parameters of the problem; they can be expressed through A_n. To find them, we are considering the shifts x_{0j} of the equilibrium positions of the normal coordinates x_j caused by an ILM. These shifts can be found from the following condition of the vanishing of the linear terms in the mean potential energy of phonons of the lattice with the ILM:

$$\omega_j^2 x_{0j} + \sum_n (\partial u_n/\partial x_j)\langle \partial V_{anh}/\partial u_n\rangle = 0.$$

Taking into account the relation $u_n = \Sigma_j e_{nj}x_j/\sqrt{M_n}$, we get $x_{0j} = -\omega_j^{-2}\Sigma_n e_{nj}\langle \partial V_{anh}/\partial u_n\rangle/\sqrt{M_n}$, where $e_{nj} \propto e^{ik_j n}$ is the component of the polarization vector of the normal mode j of the perfect lattice, and k_j is the wave number of the mode j. This gives for $\xi_n = \Sigma_j e_{nj}x_{0j}/\sqrt{M_n}$ the relation

$$\xi_n = \sum_{n'} g_{nn'}\langle \partial V_{anh}/\partial u_{n'}\rangle, \tag{6}$$

where $g_{nn'} = G^{(0)}_{nn'}(0)/\sqrt{M_n M_{n'}}$ are the parameters of the harmonic lattice, and $G^{(0)}_{nn'}(0)$ is the static limit ($\omega=0$) of the Green's function of the perfect lattice[24,25]

$$G^{(0)}_{nn'}(\omega) = \sum_j e_{nj}e_{n'j}/(\omega^2 - \omega_j^2).$$

B. Mean field for ILM

Our approach to determining the parameters of ILMs is based on the observation that Eq. (4) corresponds to the following harmonic potential energy:

$$V_{MF} = \frac{1}{2}\sum_{nn'} [V^{(2)}_{nn'} + v_{nn'}]q_n q_{n'}. \tag{7}$$

This potential energy, when the amplitude parameters A_n of the ILM are chosen correctly, should lead to the appearance of the linear local mode that is an infinitesimal part of the ILM. The potential V_{MF} constitutes a mean field for the linear mode and therefore also for the ILM. The matrix $v_{nn'}$ gives the required change of elastic springs.

The potential V_{MF} should be determined self-consistently. This can be done by using the Lifshitz method[24] for the description of the small variation of the ILM. In this method, the ratios of the amplitudes of a local mode (in our case, these are equal to the ratios of the amplitudes of the ILM) satisfy the relations

$$A_n/A_0 = G_{n0}(\omega_l)/G_{00}(\omega_l), \tag{8}$$

where $G(\omega)$ is the matrix of the perturbed Green's function[24]

$$G(\omega) = [I - G^{(0)}(\omega)v]^{-1}G^{(0)}(\omega), \tag{9}$$

the frequency ω_l is given by the position of the pole of $G(\omega)$ outside the phonon spectrum.

$$I - G^{(0)}(\omega_l)v = 0. \tag{10}$$

Since the amplitude parameters A_n enter into the perturbation matrix v, Eq. (8) and (9) constitute self-consistency equations.

We calculate an ILM by determining the amplitudes A_n, the dc shifts ξ_n, and the frequency ω_l iteratively. One starts by choosing the main amplitude(s) of the ILM. Using these, one finds the dc shifts ξ_n by solving Eq. (6). By inserting the obtained ξ_n into Eq. (5), one calculates the matrix v. After that, one computes the frequency of the ILM by using Eq. (10) and then the new amplitudes by using Eq. (8). One repeats the procedure with newly found amplitudes until the amplitudes converge to the required accuracy. Our examples show that usually the procedure converges rather quickly.

III. DIATOMIC CHAINS WITH REALISTIC PAIR POTENTIALS

Let us calculate ILMs in a chain with a realistic pair potential. We take into account the nearest-neighbor interactions only. In this case, the potential energy of a chain has the form

$$V = \sum_n V(\bar{u}_n),$$

where $V(x)$ is the pair potential of two adjacent particles which are at the distance $d+x$, d is the distance between the equilibrium positions of the particles, and $\bar{u}_n = u_n - u_{n-1}$ is the difference of the shifts of the particles n and $n-1$. In this model, an ILM causes a weakening of springs. Therefore, ILMs can exist only if the chain has gaps in the phonon spectrum.[6,19,21] Here, we consider the simplest chain of this type—a diatomic chain.

In this model, the perturbation matrix v equals

$$v_{nn'} = \delta_{n,n'}(\gamma_{n+1} + \gamma_n) - \delta_{n-1,n'}\gamma_n - \delta_{n+1,n'}\gamma_{n+1}, \quad (11)$$

where

$$\gamma_n = 2\langle \sin^2 \omega_L t \partial^2 V_{anh}/\partial \bar{u}_n^2 \rangle \quad (12)$$

is the renormalization of the elastic spring between the particles n and $n-1$. In this equation, $\partial^2 V_{anh}/\partial \bar{u}_n^2$ should be found for $\bar{u}_n = \bar{A}_n \cos \omega_l t + \bar{\xi}_n$, where

$$\bar{A}_n = A_n - A_{n-1}, \quad \bar{\xi}_n = \xi_n - \xi_{n-1}.$$

In the case under consideration, the dc shifts $\bar{\xi}_n$ can be found from the following condition of the zero force:

$$\langle \partial V(\bar{u}_n)/\partial \bar{u}_n \rangle = 0. \quad (13)$$

The Green's functions of the diatomic chain read

$$G^{(0)}_{nn'} = \sum_k \sum_{j=0,1} \frac{e_{jl}(k)e_{jl'}(k)\cos[(n-n')k]}{\omega^2 - \omega_j^2(k)}$$

$(-\pi/2 > k \geqslant \pi/2,\ l,l' = 1,2)$, where $\omega_j^2(k)$ and $e_{jl}(k)$ are the eigenvalues and the eigenvectors of the dynamical matrix in the k representation, and $j=0$ corresponds to the acoustic branch of phonons, while $j=1$ stands for the optical branch, the odd n (light atoms) correspond to $l=1$, the even n (heavy atoms) correspond to $l=2$; ω^2 is considered as the limit $\omega^2 - i\varepsilon$, $\varepsilon \to +0$.

Below, we are using the maximal frequency of phonons for the unit ($\omega_m = 1$). Then, the phonon spectrum is described by the equation

$$\omega_j^2(k) = \frac{1}{2}[1 + (2j-1)\sqrt{1 + 4\alpha^2(\cos^2 k - 1)}],$$

where $\alpha = \sqrt{M_1 M_2}/(M_1 + M_2)$.

A. Toda potential

To calculate ILMs, we need to find the renormalizations of the elastic springs γ_n. Let us first consider the values of these parameters for the Toda pair potential

$$V(x) = P(e^{-x/\rho} + x/\rho - 1), \quad (14)$$

where P is the characteristic energy and ρ is the characteristic distance of the repulsion between atoms. To find the amplitude-dependent perturbation of springs, one needs first to calculate the dc shifts from Eq. (13) and then γ_n from Eq. (12). To do that, we need to perform the averaging of the derivatives of V_{anh} over the vibrational period. This can be done by applying the equation

$$\langle e^{\bar{A}\cos \omega_l t/\rho} \rangle = I_0(\bar{A}/\rho). \quad (15)$$

Here and below, $I_n(x)$ is the modified Bessel function of the nth order. Further calculations for this potential are straightforward. As a result, one gets the following simple dependences of $\bar{\xi}$ and γ on the dimensionless amplitude $a = \bar{A}/\rho$:

$$\bar{\xi}/\rho = \ln[I_0(a)], \quad \gamma = -(P/\rho^2)I_2(a)/I_0(a). \quad (16)$$

B. Morse potential

The Morse potential

$$V(x) = (P/2)(e^{-x/\rho} - 1)^2 \quad (17)$$

is analogous to the Toda potential. Using the dimensionless amplitude $a = 2\bar{A}/\rho$, we get

$$\bar{\xi}/\rho = \ln[I_0(a)/I_0(a/2)] \quad (18)$$

and

$$\gamma = (P/\rho^2)\left\{ \frac{4I_0(a/2)}{aI_0(a)}\left[\frac{I_0(a/2)I_1(a)}{I_0(a)} - I_1(a/2) \right] - 1 \right\}. \quad (19)$$

C. Born-Mayer-Coulomb potential

One often uses the Born-Mayer-Coulomb potential

$$V(x) = P\left(e^{-x/\rho} - \frac{d^2/\rho}{d+x} + d/\rho - 1 \right). \quad (20)$$

Here, $P = \alpha_M q^2 \rho/d^2$, α_M is the Madelung constant, q is the effective charge, and ρ describes the repulsion between the

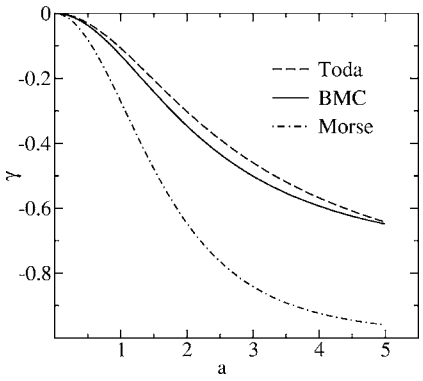

FIG. 1. The dependence of γ on the dimensionless amplitude a for the Toda, Morse, and Born-Mayer-Coulomb potentials (in the P/ρ^2 units). For the Morse potential, $a=2\bar{A}/\rho$, while for the Toda and for the Born-Mayer-Coulomb potentials, $a=\bar{A}/\rho$; for the latter potential, $\rho/d=0.1117$ (the value of this parameter in NaBr).

atoms. Note that in our units, the repulsion part of this potential coincides with that of the Toda potential. Moreover, for usual values of the ratio $d/\rho \sim 10$ and for a reasonably small x, this potential differs but little from the Toda potential.

To find the $\bar{A}$ dependence of the renormalization of springs, we need to perform also the averaging of the derivatives of the Coulomb term over the vibrational period. This can be done by applying the equation

$$\langle 1/(d+\bar{\xi}+\bar{A}\cos\omega_l t)\rangle = 1/\sqrt{(d+\bar{\xi})^2-\bar{A}^2}. \qquad (21)$$

Using Eq. (13) and the above relations (15) and (21), we get the following equation for $\bar{\xi}_n$:

$$e^{-\bar{\xi}/\rho}I_0(\bar{A}/\rho) - d^2(d+\bar{\xi})/[(d+\bar{\xi})^2-\bar{A}^2]^{3/2} = 0. \qquad (22)$$

Analogously, we get the equation for γ_n:

$$\gamma = (P/\rho^2)\Big((2\rho/\bar{A})e^{-\bar{\xi}/\rho}I_1(\bar{A}/\rho) - 1 - (2\rho/d)\{d^3/[(d+\bar{\xi})^2-\bar{A}^2]^{3/2}-1\}\Big). \qquad (23)$$

Equation (22) allows one to find the dependence of $\bar{\xi}$ on $\bar{A}$. By inserting the obtained $\bar{\xi}$ to Eq. (23), one can also find γ.

Note that for all potentials, in the small $|\bar{A}|$ limit, $\bar{\xi}$ and $\gamma \propto \bar{A}^2$. This means that the dc changes of the distances of the nearest atoms and the renormalization of bonds converge on the tails of an ILM rather fast—faster than the amplitudes itself.

In Fig. 1, the dependence of γ on the dimensionless amplitude a for all three above-considered potentials is presented (in $P/\rho^2=1$ u). As expected, the values of γ are negative for all amplitudes. Note that for the reasonable values of $a \lesssim 5$, the Morse potential has the strongest anharmonic effect, while for the Toda and Born-Mayer-Coulomb potentials, it is smaller and, as expected, differs but little.

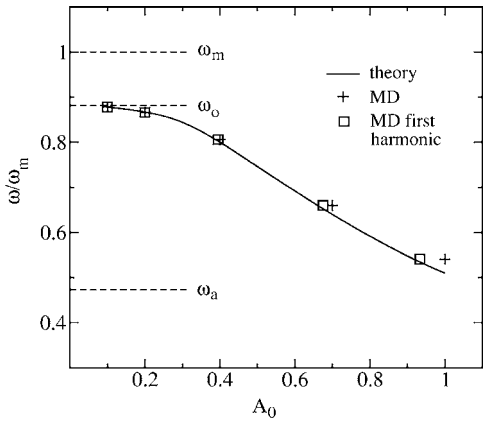

FIG. 2. The dependence of the dimensionless frequency ω/ω_m of an odd ILM on the amplitude A_0 (in Å) of the central atom (Na) in a NaBr-type diatomic chain; ω_m is the top phonon frequency, ω_o is the bottom of the optical band, and ω_a is the top of the acoustic band.

D. Numerical examples

For numerical considerations, we choose the NaBr-type diatomic chain with a Na-Br coupling, given by the Born-Mayer-Coulomb potential, and calculate the odd ILMs centered on a Na atom. The parameters of this potential are known: $d=2.981$ Å $\rho=0.333$ Å, $q=e$, $\alpha_M=1.7475$, $M_1=22.99$ amu, and $M_2=79.90$ amu. In this case, the top of the acoustic band is at $\omega_a=0.473\omega_m$; the bottom of the optical band is at $\omega_a=0.881\omega_m$.

To find the characteristics of an ILM, we use an iteration procedure: we choose the trial values of the amplitudes of a few central atoms (usually, we include into consideration the amplitudes of 13 central atoms) and then calculate the shifts ξ_n and the changes of the elastic springs γ_n by using Eqs. (22) and (23). Inserting obtained γ_n into Eqs. (8)–(11), we calculate the frequency and new amplitudes. Then, we repeat the calculations with these new amplitudes. We do that many times for every different value of the initial amplitudes. Commonly, the iteration procedure converges fast (in less than ten steps), but because of an extremely short time of a single iteration, we do approximately 40 iteration steps for every case.

The results of our calculations are given in Fig. 2 and in Table I (upper lines). As it should be, the ILMs with small amplitudes have rather a large size; their frequency is close to the bottom of the optical band. The enlargement of the amplitudes results in the increasing of localization and in the decreasing of the frequency.

E. Comparison with MD simulations

We also carried out MD simulations of the ILMs in the same model. A special care was taken to achieve high precision; for details, see Ref. 26. A comparison of the obtained

TABLE I. Frequencies ω, amplitudes A_n, and changes of atomic distance $\bar{\xi}_n$ (in Å) for odd ILMs in a NaBr-type chain with the Born-Mayer-Coulomb pair potential. For every amplitude A_0 of the central atom (Na) two values, the theoretical (up) and the result of the MD simulations (down) are given.

ω/ω_m	A_0	$-A_1$	$-A_2$	A_3	A_4	$-A_6$
0.878	0.100	0.001	0.094	0.003	0.080	0.063
0.878	0.100	0.001	0.095	0.002	0.083	0.068
0.867	0.200	0.009	0.149	0.011	0.092	0.054
0.867	0.200	0.008	0.151	0.011	0.094	0.056
0.799	0.400	0.049	0.101	0.017	0.033	0.014
0.805	0.400	0.048	0.102	0.017	0.035	0.012
0.640	0.700	0.107	0.082	0.033	0.024	0.007
0.660	0.700	0.106	0.081	0.030	0.024	0.007
0.507	1.000	0.193	0.075	0.099	0.032	0.018
0.541	1.000	0.177	0.066	0.066	0.029	0.012
ω/ω_m	$\bar{\xi}_1$	$\bar{\xi}_2$	$\bar{\xi}_3$	$\bar{\xi}_4$	$\bar{\xi}_5$	$\bar{\xi}_6$
0.878	0.009	0.008	0.008	0.005	0.006	0.003
0.878	0.009	0.008	0.008	0.006	0.006	0.003
0.867	0.038	0.018	0.023	0.006	0.009	0.002
0.867	0.038	0.018	0.023	0.006	0.009	0.002
0.799	0.162	0.003	0.013	0.000	0.001	0.000
0.805	0.159	0.003	0.013	0.000	0.002	0.000
0.640	0.440	0.000	0.012	0.000	0.001	0.000
0.660	0.428	0.002	0.010	0.000	0.001	0.000
0.507	0.793	0.013	0.027	0.004	0.007	0.001
0.541	0.756	0.016	0.018	0.002	0.003	0.000

results with our theoretical calculations (see Table I and Fig. 2, the line and the crosses) demonstrates a good agreement of both calculations. In fact, for the case of ILMs with a small amplitude and rather a substantial size, the agreement is just excellent. This clearly demonstrates an advantage of the proposed method as compared to the method of Ref. 4, which allows one to calculate only strongly localized ILMs.

One can see that the difference between the theoretical results and the MD simulations increases with the increasing of the amplitude of the ILM. For example, the frequency difference of the ILM with $A_0=1$ Å reaches 7%. This discrepancy is connected with the RWA used above: the increasing of amplitudes results in the increasing of the contribution of higher-order harmonics, which are neglected in this approximation. This conclusion is fully supported by our MD calculations of the first harmonics of ILMs (see Fig. 2, squares): the MD frequencies of ILMs with the same amplitude of the first harmonics, as it is in the theory, are situated very close to the theoretical line.

IV. CONCLUSION

To conclude, we have developed a theory of intrinsic localized modes, which allows one to make use of harmonic approximation results and to perform calculations for a macroscopically large lattice of an arbitrary dimension. We have derived the equations describing small variations of ILM amplitudes, which allowed us to reduce the original nonlinear problem to the linear problem of phonon localization on the local effective potential. The latter is created by the ILM itself and it is determined self-consistently. This enabled us to apply the Lifshitz method of the perturbed local dynamics of phonons for the calculations of the ILMs. To test the method, we calculated the ILMs in diatomic chains. We have also carried out the MD calculations of the ILMs in diatomic chains. A comparison of the results obtained by both methods (see Table I and Fig. 2) shows a good agreement.

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