Chapter 12
Bound States of Electrons in Harmonic and Anharmonic Crystal Lattices

Larissa S. Brizhik, Alexander P. Chetverikov, Werner Ebeling, Gerd Röpke and Manuel G. Velarde

Abstract The pairing of electrons in harmonic and anharmonic one-dimensional lattices is studied with account of the electron-lattice interaction. It is shown that in harmonic lattices binding of electrons in a bound localized state called bisoliton, takes place. It is also shown that bisolitons in harmonic lattices can propagate with velocity below the velocity of the sound. Similarly, binding of electrons in singlet spin state, called bisolectron, takes place in anharmonic lattices. It is shown that the account of the lattice anharmonicity leads to the stabilization of bisolectron dynamics: bisolectrons are dynamically stable up to the sound velocity in lattices with cubic or quartic anharmonicities and can also be supersonic. They have finite values of energy and momentum in the whole interval of bisolectron velocities. The bisolectron binding energy and critical value of the Coulomb repulsion at which the bisolectron becomes unstable and decays into two independent solectrons, are calculated. The analytical results are in a good agreement with the results of numerical simulations in a broad interval of the parameter values.

L.S. Brizhik (✉)
Bogolyubov Institute for Theoretical Physics,
14b, Metrolohichna Str., Kyiv 03680, Ukraine
e-mail: brizhik@bitp.kiev.ua

A.P. Chetverikov
Department of Physics, Saratov State University,
Astrakhanskaya 83, Saratov 410012, Russia
e-mail: chetverikovap@info.sgu.ru

W. Ebeling
Institut für Physik, Humboldt-Universität Berlin, Newtonstrasse 15,
12489 Berlin, Germany
e-mail: ebeling@physik.hu-berlin.de

G. Röpke
Institut für Physik, Universität Rostock, 18051 Rostock, Germany
e-mail: gerd.roepke@uni-rostock.de

M.G. Velarde
Instituto Pluridisciplinar, Universidad Complutense,
Paseo Juan XXIII, 1, 28040 Madrid, Spain
e-mail: mgvelarde@pluri.ucm.es

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12.1 Introduction

In this chapter we will study the possibility of binding of two extra electrons or holes in a singlet localized bound state in a one-dimensional lattice with account of the electron-lattice interaction. For simplicity we will consider a chain with one 'atom' per unit cell, and, respectively, one phonon mode, which describes longitudinal displacements of atoms from their equilibrium states and is called 'acoustic mode': there is electron-lattice interaction with acoustical phonons, only. For more realistic low-dimensional molecular systems such a model corresponds to the case of very strong anisotropy when the parameters of the system in one direction are much bigger than in two other directions, so that one can identify in the system one-dimensional chains in which the acoustical mode is the most active. The interaction between the chains can be considered as weak and taken into account using perturbation method. In the general case the electron-lattice systems can be described by the Fröhlich Hamiltonian, which includes three terms, the first two of which describe, respectively, a quasiparticle (electron, hole, exciton, etc.) and undisturbed lattice, and the third term describes the interaction between the quasiparticle and lattice displacements from their equilibrium positions.

It is well established that the electron-lattice interaction plays a significant role in low-dimensional molecular systems and can result in their essentially genuine properties. Thus, electron-lattice interaction (it is called also electron-phonon interaction) leads to the lowering of the energy of quasiparticles [1, 2, 19, 31, 34, 35]. Such phenomenon is known as polaron effect. Unfortunately, even in the simplest case of a one-dimensional system with one phonon mode (one atom in a unit cell) and one extra quasiparticle in the chain the corresponding Hamiltonian can not be diagonalized exactly and there is no exact solution of such a problem. One possibility is a numerical solution of the problem, which depends on the choice of the parameter values of the considered chain and can not give a complete description of the problem. Variational methods can be also useful, but it is well known, that the results of such methods depend essentially on the choice of the variational function. Another possibility is to study the problem within the perturbation method. Respectively, different perturbation schemes can be used depending which parameter of the system can be considered as a small parameter.

Thus, it has been shown that depending on the strength of the coupling and the lattice nonadiabaticity parameter, the lowest energy state of a quasiparticle is one of the three possible states: (i) an almost free band state, (ii) a large polaron, (iii) a small polaron [10]. In an almost free band state a quasiparticle is delocalized over the whole length of the system, while the latter two states correspond to a quasiparticle localized state of large radius as comparing with the lattice spacing, or trapped within one lattice site, respectively. We remind here, that the lattice nonadiabaticity parameter is determined as the ratio between the Debye energy of phonons and the resonant (exchange) energy in the lattice. In particular, at moderate values of the electron-lattice interaction constant and not too strong lattice nonadiabaticity the adiabatic approximation is valid.

In such a case a large polaron corresponds to the lowest energy of the system [10]. In particular, within this approximation, Davydov has shown that the Hamiltonian of a one-dimensional molecular lattice can be diagonalized in such a way that the lowest order of the electron-lattice interaction is taken into account in the zero-order term of the Hamiltonian [19, 39]. In other words, in the zero order adiabatic approximation the lowest order of the electron-lattice interaction is taken into account exactly. In this case the 'zero order' term of the Hamiltonian leads to the system of coupled nonlinear discrete equations for the wave-function of a quasiparticle and displacements of atoms from their equilibrium positions [19, 38, 39].

In the continuum approximation this system of equations can be reduced to the Davydov system of equations [19]. This system coincides formally with Zakharov system of equations which describes the propagation of Langmuir waves in an ionized plasma. Davydov system of equations, for the case of functions of a quasiparticle and phonons that depend on the running wave coordinate $x - Vt$, can be reduced to the nonlinear Schrödinger equation. This equation admits the soliton solution [19] of a finite radius of a localization. Here $x = na$ is a lattice coordinate, a is the constant of lattice spacing, t is time, V is the velocity of the running wave. Then the lattice deformation, which is proportional to the probability of a quasiparticle presence in the given place of the lattice, is also a localized function. In this respect Davydov's soliton describes a particular type of a large polaron, in which the electron-lattice interaction is taken into account exactly, without linearization of the system. Davydov's soliton, therefore, describes a bound state of a quasiparticle with the self-induced localized lattice distortion. Such a soliton can propagate along the molecular chain with constant velocity V, neglecting effects of the lattice discreteness, and describes a coherent propagation of a quasiparticle, so that the quasiparticle will reach a certain position in the chain, as an example, the opposite end of the chain, with the probability, equal to 1, at some time instant. Thus, Davydov's soliton describes a large polaron with the lowest energy as compared with other solutions of a large polaron type. The width of the Davydov's soliton, l_s, is inversely proportional to the non-linear parameter of the nonlinear Schrödinger equation, which is proportional to the dimensionless electron-lattice coupling, g, namely, $l_s = \pi a/g$. For the values of the chain parameters, that satisfy the condition of adiabatic approximation, this radius of soliton localization is equal to several lattice sites.

Worth mentioning here also is that Davydov's solitons are essentially nonlinear two-component (sometimes called 'two-field') entities, one component of which is a quasiparticle, and another component is a lattice distortion, determined by the displacements of atoms from their equilibrium positions, induced by the presence of the quasiparticle. In the case of self-trapping of a charged particle (electron or hole) Davydov's soliton is called 'electrosoliton' [19, 38, 39]. From the point of view of conducting properties, namely systems which support formation of large polarons in general, and of solitons in particular, are the most important for their technical applications in modern devices. Indeed, there is a wide class of quasi-one-dimensional crystals in which large polarons exist. This include DNA and α-helical polypeptides [18, 19, 30, 38], polydiacetylene [24, 27, 48], conducting platinum chains and conducting polymers [11], salts of transition metals [3, 16, 40, 49], superconducting

cuprates [4, 13, 23, 26, 32], etc. These compounds find numerous applications in microelectronics and nanotechnologies, or play important role in living systems. This explains our interest in studying nonlinear effects in such systems.

In this respect the question arises if the electron-lattice interaction in low-dimensional systems can result in binding two extra electrons in a localized state. This can be compared with the formation of Cooper pairs due to the exchange with virtual phonons. Indeed, it has been shown that in harmonic lattices pairing of two charged quasiparticles (below we call them 'electrons') with opposite spins in a bisoliton state takes place [8, 9]. The difference between bisolitons and Cooper pairs is the space where the localization of electrons takes place, and the size of the localization: while Cooper pairing takes place in the momentum space and the size of Cooper pairs in a real space is very large, bisolitons are localized in the coordinate space and are extended over a few lattice units.

Generally, in the studies of the properties of Davydov solitons and bisolitons the lattices are usually modeled within the harmonic approximation. Going beyond this, it is now firmly established that solitons are formed in rather generic anharmonic lattices [12, 18, 19, 29, 33, 36, 41, 42]. In this case solitons are one-component entities, sometimes called also 'lattice solitons', to be distinguished from two-component Davydov's solitons. In view of the above here we explicitly analyze how the lattice anharmonicity added to the electron-phonon interaction facilitates electron pairing in a one-dimensional lattice and also helps overcoming Coulomb repulsion. It has been shown that anharmonic lattices also favor pairing of electrons (holes) in a singlet localized state [5, 44, 45]. While in harmonic lattices the nonlinearity in the system is due to the electron-lattice interaction, in anharmonic lattices there are two nonlinearities: the nonlinearity of the lattice itself, and the electron-lattice interaction. It is well known that in nonlinear systems the standard principle of superposition does not take place. As a result, the spectrum of the localized solutions in such systems is bigger than in harmonic lattices. We call these localized solutions "bisolectrons" to indicate the difference with bisolitons in harmonic lattices.

The properties of bisolectrons depend on which nonlinearity is dominating in their formation. It appears that the presence of the lattice anharmonicity results in the stabilization of the dynamics of bisolectrons. They have finite values of energy and momentum in the whole interval of bisolectron velocities which can be subsonic and supersonic. Here we consider first the general case of anharmonic lattices, and then to obtain explicit expressions for the parameters of bisolectrons, we consider lattices with cubic anharmonicity and quartic anharmonicity. We also take into account the Coulomb repulsion between the electrons and show that it can modify the envelope of bisolitons and bisolectrons: their envelope can have two maxima at strong enough Coulomb repulsion. We calculate the bisolectron binding energy and critical value of the Coulomb repulsion at which the bisolectron becomes unstable and decays into two independent solectrons. The bisolectron binding energy is estimated for values of chain parameters that are typical for biological macromolecules and some quasi-one-dimensional conducting systems. We show that the Coulomb repulsion in such systems is relatively weak relative to the binding energy and, therefore, binding of two electrons in a singlet localized bisolectron state takes place in such systems.

Finally, we find another type of localized solutions of the corresponding system of nonlinear equations, which can be only supersonic. We show that our analytical results are in a good agreement with the results of numerical simulations in a broad interval of the parameter values of the system and of the strength of the Coulomb repulsion between the electrons.

12.2 Hamiltonian of the System and Dynamic Equations

Let us consider two added excess electrons (holes) in an infinitely long one-dimensional lattice formed by unit cells of mass M placed at equilibrium lattice spacing a. Such a system can be described by the Fröhlich Hamiltonian in the form:

$$\hat{H} = \hat{H}_{\text{el}} + \hat{H}_{\text{lat}} + \hat{H}_{\text{int}} + \hat{H}_{\text{Coul}}. \tag{12.1}$$

Here the electron Hamiltonian is written as

$$\hat{H}_{\text{el}} = \sum_{n,s} \left[E_0 \hat{B}^{\dagger}_{n,s} \hat{B}_{n,s} - J \hat{B}^{\dagger}_{n,s} \left(\hat{B}_{n+1,s} + \hat{B}_{n-1,s} \right) \right], \tag{12.2}$$

where E_0 is the on-site electron energy, J is the electron exchange interaction energy, $\hat{B}^{\dagger}_{n,s}$, $\hat{B}_{n,s}$ are creation and annihilation operators of an electron with spin index $s = 1, 2$ at the lattice site n.

We assume that in the lattice only one phonon mode, namely acoustical, is the most active. The Hamiltonian of such a lattice has the form

$$\hat{H}_{\text{ph}} = \sum_{n} \left[\frac{\hat{p}_n^2}{2M} + \hat{U} \left(\hat{\beta}_n \right) \right], \tag{12.3}$$

where $\hat{\beta}_n$ is the operator of the displacement of the nth unit cell from its equilibrium position and $\hat{p}_n$ is the operator of the canonically conjugated momentum, and $\hat{U}$ is the operator of the potential energy of the lattice, whose properties will be defined below.

The Hamiltonian of electron-lattice interaction for the case, when the on-site electron energy dependence on the longitudinal displacements of unit cells (acoustical mode) dominates the inter-site dependence, is given by the expression

$$\hat{H}_{\text{int}} = \chi \sum_{n,s=1,2} \left(\hat{\beta}_{n+1} - \hat{\beta}_{n-1} \right) \hat{B}^{\dagger}_{n,s} \hat{B}_{n,s}, \tag{12.4}$$

where χ is the electron-lattice coupling constant.

The Coulomb repulsion between the electrons is given by the Hubbard-type Hamiltonian

$$\hat{H}_{\rm Coul} = \sum_{n,m,s=1,2} V_{nm} \hat{B}^{\dagger}_{n,s} \hat{B}_{n,s} \hat{B}^{\dagger}_{m,s} \hat{B}_{m,s}, \tag{12.5}$$

where V_{nm} is the corresponding matrix element of the Coulomb interaction.

In the adiabatic approximation we can set

$$|\Psi(t)\rangle = |\Psi_{\rm el}(t)\rangle |\Psi_{\rm ph}(t)\rangle. \tag{12.6}$$

Here the vector state of the lattice has the form of the product of the operator of coherent displacements of unit cells and vacuum state of the lattice, $|0\rangle_{\rm ph}$,

$$|\Psi_{\rm ph}(t)\rangle = \exp\left\{-\frac{i}{\hbar}\sum_{n}\left[\beta_n(t)\hat{p}_n - p_n(t)\hat{\beta}_n\right]\right\}|0\rangle_{\rm ph}, \tag{12.7}$$

where $\beta_n(t)$, $p_n(t)$ are, respectively, the mean values of the displacements of unit cells from their equilibrium positions and their canonically conjugated momenta in the state (12.6).

The electron state vector for two excess electrons has the form

$$|\Psi_{\rm el}(t)\rangle = \sum_{n_1,n_2,s_1,s_2} \Psi(n_1,n_2,s_1,s_2;t)\hat{B}^{\dagger}_{n_1,s_1}\hat{B}^{\dagger}_{n_2,s_2}|0\rangle_{\rm el}. \tag{12.8}$$

In the absence of the magnetic field, we can represent the two-electron function of two electrons with anti-parallel spins as the product of the symmetric coordinate function and antisymmetric spin function

$$\begin{aligned} \Psi(n_1,n_2,s_1,s_2;t) &= \Psi(n_1,n_2,t)\chi(s_1,s_2), \\ \Psi(n_1,n_2,t) &= \frac{1}{\sqrt{2}}\left[\Psi_1(n_1,t)\Psi_2(n_2,t) + \Psi_2(n_1,t)\Psi_1(n_2,t)\right], \\ \chi(s_1,s_2) &= \frac{1}{\sqrt{2}}\left[\chi_1(s_1,t)\chi_2(s_2,t) - \chi_2(s_1,t)\chi_1(s_2,t)\right]. \end{aligned} \tag{12.9}$$

Here one-electron wave-functions satisfy the normalization condition

$$\sum_{n}|\Psi_j(n,t)|^2 = 1, \quad j = 1,2. \tag{12.10}$$

Using such a state vector, we can calculate the Hamiltonian function $\mathscr{H} = \langle\Psi(t)|\hat{H}|\Psi(t)\rangle$, corresponding to the Hamiltonian operator (12.1). In the absence of magnetic field we can omit spin functions and spin indexes of the corresponding operators.

First we neglect the Coulomb repulsion and will take it into account at later stage. Electron wave functions and lattice displacements are slowly varying in space functions at intermediate values of the electron-lattice coupling and not too strong anharmonicity of the lattice. Therefore, we can use the continuum approximation $n \to x \equiv na$. From the Hamilton function $\mathscr{H}$ we derive a system of coupled equations for the two-electron wave function $\Psi(x_1, x_2, t)$ and lattice site displacements $\beta(x, t)$:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x_1^2} + \frac{\partial^2\Psi}{\partial x_2^2}\right) + \chi a\left(\frac{\partial\beta(x,t)}{\partial x}|_{x=x_1} + \frac{\partial\beta(x,t)}{\partial x}|_{x=x_2}\right)\Psi, \tag{12.11}$$

$$\frac{\partial^2\beta}{\partial t^2} - V_{\text{ac}}^2\frac{\partial^2 U}{\partial\rho^2}\frac{\partial^2\beta}{\partial x^2} - \alpha\frac{\partial^4\beta}{\partial x^2\partial t^2} = \frac{a}{M}\chi\left(\int dx_2\frac{\partial|\Psi|^2}{\partial x_1}|_{x_1=x} + \int dx_1\frac{\partial|\Psi|^2}{\partial x_2}|_{x_2=x}\right). \tag{12.12}$$

Here $\rho(x, t) = -\partial\beta(x, t)/\partial x$ is the local deformation of the lattice and V_{ac} is the linear sound velocity in the chain. In the left hand side of the second equation we have included an extra term proportional to the fourth derivative of the lattice displacement to take into account a nonlinear dispersion of the lattice if any (see, e.g., comments in [20]). We will ignore this term when considering harmonic lattices and subsonic solutions.

The potential energy of the lattice $U(\rho)$ has a minimum in the equilibrium lattice. We assume that it is increasing function of the lattice compression, ($\rho > 0$), induced by electrons (see [20–22]):

$$\frac{\partial U(\rho)}{\partial\rho}|_{\rho=0} = 0, \qquad \frac{\partial^2 U(\rho)}{\partial\rho^2} > 0. \tag{12.13}$$

Below we will consider separately cases of harmonic and anharmonic lattices.

12.3 Bisolitons in Harmonic Lattices

Let us consider first the electron pairing in a harmonic lattice:

$$U(\rho) = \frac{1}{2}w\rho^2. \tag{12.14}$$

Substituting this potential into (12.11) and (12.12), we obtain the system of coupled equations in the form

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \chi a\rho(x, t)\right]\Psi_j(x, t) = E_0\Psi_j(x, t), \quad j = 1, 2, \tag{12.15}$$

$$\left(\frac{\partial^2}{\partial t^2} - V_{\rm ac}^2 \frac{\partial^2}{\partial x^2}\right) \rho(x,t) + \frac{\chi a}{M} \frac{\partial^2}{\partial x^2} \sum_{j=1}^{2} |\Psi_j(x,t)|^2 = 0. \tag{12.16}$$

We are interested in the localized solutions of the equations and introduce the running wave coordinate

$$\xi = (x - x_0 - Vt)/a, \tag{12.17}$$

so that $\rho(x,t) = \rho(\xi)$, $\Psi_j(x,t) = \Phi_j(\xi) \exp\left(imVx/\hbar - i\phi(t)\right)$. For the localized one-electron functions in the approximation we can set $\Phi_2(\xi) = \Phi_1(\xi + l)$, and omit below index j. From (12.15) we get the expression for the lattice deformation

$$\rho(\xi) = \frac{\chi}{w(1-s^2)} \left[|\Phi(\xi)|^2 + |\Phi(\xi + l)|^2\right], \quad s^2 = \frac{V^2}{V_{\rm ac}^2}. \tag{12.18}$$

Substituting this result into (12.16), we obtain the nonlinear Schödinger equation for the electron wave function

$$\left[\frac{d^2}{d\xi^2} + \varepsilon_l + 2g[\Phi^2(\xi) + \Phi^2(\xi + l)]\right] \Phi(\xi) = 0, \tag{12.19}$$

where

$$g = \frac{\chi^2}{2Jaw(1-s^2)}, \quad \varepsilon_l = \frac{E - E_0}{J}, \tag{12.20}$$

and

$$\varepsilon_l = \int \left[\left(\frac{d\Phi}{d\xi}\right)^2 - 2g\Phi^2(\xi)\left(\Phi^2(\xi) + \Phi^2(\xi + l)\right)\right] d\xi. \tag{12.21}$$

At large distances between the center of mass coordinates, $la >> a$, two electrons move independently, so that $\Phi(\xi + l) = 0$ in the region, where $\Phi(\xi) \neq 0$. In this case we have from (12.19)

$$\left[\frac{d^2}{d\xi^2} + \varepsilon_\infty + 2g\Phi_\infty^2(\xi)\right] \Phi_\infty(\xi) = 0, \tag{12.22}$$

from where we find a soliton solution

$$\Phi_\infty = \Phi_s = \frac{1}{2}\sqrt{g}\,\mathrm{sech}\left(\frac{g\xi}{2}\right), \tag{12.23}$$

which has the eigen-energy

$$\varepsilon_\infty = -\frac{g^2}{4}. \tag{12.24}$$

At $l = 0$ we get from (12.19) that one-electron functions are the solutions of the equation:

$$\left[\frac{d^2}{d\xi^2} + \varepsilon_0 + 4g\Phi_0^2(\xi)\right]\Phi_0(\xi) = 0. \tag{12.25}$$

From above equation we get [8, 9, 19]

$$\Phi_0 = \Phi_{bs} = \sqrt{\frac{g}{2}}\,\mathrm{sech}(g\xi). \tag{12.26}$$

Thus, at $l = 0$ the electrons form a bound state, according to (12.26), called bisoliton, with the eigen-energy

$$\varepsilon_0 = -g^2. \tag{12.27}$$

Comparing the solutions (12.23) and (12.26), we see, that the amplitude of a bisoliton is higher, than the amplitude of a soliton, and width of the localization, $l_{bs} = \pi/g$, is twice the width of the soliton localization, $l_s = \pi/(2g)$. The envelopes of the wave functions of an isolated soliton and of a bisoliton are shown in Fig. 12.1.

The binding energy of a bisoliton, $E_{bind} = E_\infty(V) - E_0(V)$ is [8]

$$E_{bind} = \frac{Jg_0^2}{2}\frac{1 - 5s^2}{(1 - s^2)^3}, \quad g_0 = \frac{\chi^2}{2Jaw}. \tag{12.28}$$

Here $E_\infty(V)$ and $E_0(V)$ are the total energies of the system with account of the deformation energy of the lattice with two solitons on a large distance from one

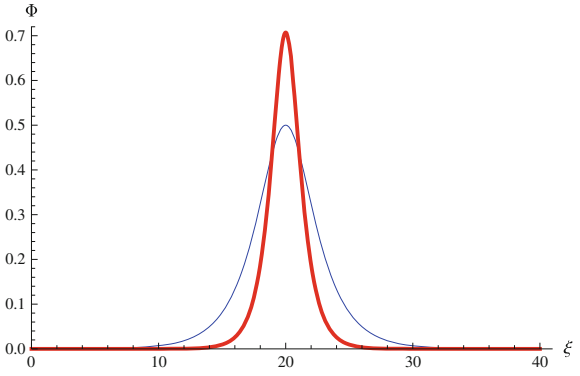

Fig. 12.1 Soliton (*thin blue line*) and bisoliton (*thick red line*) envelope functions (12.23) and (12.26) respectively with the center of mass position at $\xi = 20$ at nonlinearity parameter $g = 1$

another (two independent electro-solitons) and with two electrons bound in a bisoliton state, respectively. From (12.28) we conclude, that the bisoliton in harmonic lattices is stable at small velocities, when the inequality takes place $s^2 < 1/5$. This restriction is the result of the excess of the effective mass of a bisoliton as comparing with the sum of the effective masses of two independent solitons.

12.4 Bisolectrons in Anharmonic Lattices

In this section we will consider binding of electrons in a singlet state in anharmonic lattices. In this case it is convenient to re-write (12.11)–(12.12) in the following form:

$$\frac{d^2\Phi_j}{d\xi^2} + \sigma\rho\Phi_j = \lambda_j\Phi_j, \quad j = 1, 2, \tag{12.29}$$

$$\frac{dF}{d\rho} = D(\Phi_1^2 + \Phi_2^2), \tag{12.30}$$

where F is the effective anharmonic part of the lattice potential

$$F = U(\rho) - \frac{1}{2}s^2\rho^2, \quad s^2 = \frac{V^2}{V_{ac}^2}, \tag{12.31}$$

and the dimensionless parameters are introduced:

$$\lambda_j = -\frac{E_j}{J}, \quad \sigma = \frac{\chi a}{J}, \quad D = \frac{\chi a}{MV_{ac}^2}, \tag{12.32}$$

with E_j being the electron eigen-energy, and Φ_j being the envelope function of the corresponding 'one-electron' wave functions Ψ_j in the two-electron state.

We can rewrite (12.29) in the following form

$$\left(\frac{d\Phi_j}{d\xi}\right)^2 = \lambda_j\Phi_j^2 - \sigma Q_j, \tag{12.33}$$

where

$$Q_j(\xi) = \int_{-\infty}^{\xi} \rho(x)d\Phi_j^2(x), \quad j = 1, 2. \tag{12.34}$$

For localized solutions the corresponding functions attain some maximum values, which we denote as $\Phi_{j,0}$ and ρ_0, respectively. In one-dimensional systems the deformational potential has at least one bound state, which can be occupied by two electrons with opposite spins. When the Coulomb repulsion is very weak, the minimum

energy state corresponds to the case when the maxima of 'one-electron' functions coincide, as we have seen above for the case of harmonic lattices (see also [8, 9]), so that

$$\lambda_1 = \lambda_2, \qquad \Phi_1(\xi) = \Phi_2(\xi), \tag{12.35}$$

and we can omit index j.

In the general case the maximum values of the 'one-electron' wave functions are shifted along the lattice at some value l_0 due to the Coulomb repulsion, which will be considered below.

From (12.33) we obtain the expression for the electron eigen-energies:

$$\lambda = \sigma \frac{Q(0)}{\Phi_0^2}. \tag{12.36}$$

From (12.30) we get the equation which determines the lattice deformation

$$\frac{d\rho}{d\xi} = \pm 2\sqrt{\lambda - \sigma G(\rho)}\,\frac{dF/d\rho}{d^2F/d\rho^2}, \tag{12.37}$$

where

$$G(\rho) = \rho - \frac{F(\rho)}{dF/d\rho}, \tag{12.38}$$

and

$$\lambda = \sigma G(\rho_0). \tag{12.39}$$

Integrating (12.37), we get the implicit expression for the dependence of the lattice deformation on the running wave coordinate:

$$\xi(\rho) = \pm\frac{1}{2\sqrt{\sigma}} \int_{\rho(\xi)}^{\rho_0} \frac{d^2F/d\rho^2}{dF/d\rho} \frac{1}{\sqrt{G(\rho_0) - G(\rho)}} d\rho. \tag{12.40}$$

Using the normalization condition for "one-electron" wave function, we find the expression for the maximum value

$$\Phi_0 = \sqrt{\frac{1}{2D}\left(\frac{dF}{d\rho}\right)\Big|_{\rho=\rho_0} G(\rho_0)}. \tag{12.41}$$

To get the explicit solutions we have to specify the lattice potential. Below we will consider cubic and quartic anharmonic potentials, and we will assign subscript c or q to the functions:

$$U_c(\rho) = \frac{1}{2}\rho^2 + \frac{\alpha}{3}\rho^3, \quad U_q(\rho) = \frac{1}{2}\rho^2 + \frac{\beta}{4}\rho^4, \tag{12.42}$$

respectively.

Substituting these expressions into (12.31), we get

$$F_c(\rho) = \frac{\alpha}{2}\rho^2\left(\frac{2}{3}\rho + \delta_c\right), \quad F_q(\rho) = \frac{\beta}{4}\rho^2\left(\rho^2 + 2\delta_q\right), \tag{12.43}$$

and from (12.38) we find

$$G_c = \frac{\rho}{6}\frac{4\rho + 3\delta_c}{\rho + \delta_c}, \qquad G_q = \frac{\rho}{4}\frac{3\rho^2 + 2\delta_q}{\rho^2 + \delta_q}, \tag{12.44}$$

where the dynamically modulated inverse anharmonic stiffness coefficients are introduced:

$$\delta_c = \frac{1 - s^2}{\alpha}, \qquad \delta_q = \frac{1 - s^2}{\beta}. \tag{12.45}$$

Substituting the explicit form of function G_v into (12.40), we can rewrite the expression in the following form

$$\xi_v(\rho) = \pm\frac{1}{2\sqrt{\sigma}}\int_{\rho(\xi)}^{\rho_{0(v)}} \frac{K_v(\rho, \rho_{0(v)})}{\rho\sqrt{\rho_{0(v)} - \rho}}d\rho, \quad v = c, q \tag{12.46}$$

where the kernel of the integral for both types of anharmonic potentials K_v in view of the explicit form of G_v is very close to unity (see numerical solution in [44, 45]). From (12.46) after integration we find that the deformation of the lattice is given by the soliton solutions of the B-KdV equation [12, 18, 19, 29, 33, 36, 41, 42] which coincides with the solution of the Davydov system of nonlinear equations [19, 38]:

$$\rho_v(\xi) = \rho_{0(v)}\mathrm{sech}^2(\kappa_v\xi), \tag{12.47}$$

the width of which, κ, is determined by the maximum value of the deformation

$$\kappa_c = \sqrt{\frac{\sigma\rho_{0(c)}}{2}}\frac{\sqrt{4\rho_{0(c)}\left(\rho_{0(c)} + 2\delta_c\right)/3 + \delta_c^2}}{2\rho_{0(c)} + \delta_c}, \tag{12.48}$$

for the lattice with cubic anharmonic potential, and

$$\kappa_q = \frac{1}{2}\sqrt{\frac{\sigma\rho_{0(q)}\left(3\rho_{0(q)}^2 + 2\delta_q\right)}{\rho_{0(q)}^2 + 2\delta_q}} \tag{12.49}$$

for the lattice with quartic anharmonic potential.

These expressions can be approximated by the following one:

$$\kappa_v \approx \sqrt{\frac{\sigma\rho_{0(v)}}{2}}. \tag{12.50}$$

In its turn, $\rho_{0(v)}$ is determined by the corresponding equation:

$$\rho_{0(c)}\left(\frac{4}{3}\rho_{0(c)} + \delta_c\right)^2 = g_c^2\theta_c(\rho_{0(c)}) \tag{12.51}$$

for the lattice with cubic anharmonic potential, and

$$\rho_{0(q)}\left(\frac{8}{5}\rho_{0(q)}^2 + \delta_q\right)^2 = g_q^2\theta_q(\rho_{0(q)}) \tag{12.52}$$

for the lattice with quartic anharmonic potential.

Here g_v is a constant, determined below:

$$g_c^2 = \frac{D^2\sigma}{\alpha^2}, \quad g_q^2 = \frac{D^2\sigma}{\beta^2}, \tag{12.53}$$

with

$$\theta_c(\rho_{0(c)}) = \frac{4\rho_{0(c)}(\rho_{0(c)} + 2\delta_c) + 3\delta_c^2}{6(\rho_{0(c)} + \delta_c)^2}, \tag{12.54}$$

$$\theta_q(\rho_{0(q)}) = \frac{3\rho_{0(q)}^4 + 7\delta_q\rho_{0(q)}^2 + 2\delta_q^2}{4\left(\rho_{0(q)}^2 + \delta_q\right)^2}, \tag{12.55}$$

for the lattices with cubic and quartic anharmonic potentials, respectively. The numerical solutions of (12.51) and (12.52) are shown in Fig. 12.2 for two different values of the coupling constant $g_v = 0.05$ and $g_v = 0.2$, respectively.

It follows from Fig. 12.2, that (i) the maximum lattice deformation depends on the soliton velocity; (ii) the soliton amplitude increases and its width decreases with the velocity increasing, attaining some finite values at the sound velocity, $V = V_{ac}$ (i.e., $\delta = 0$); (iii) the soliton amplitude increases with the electron-lattice coupling

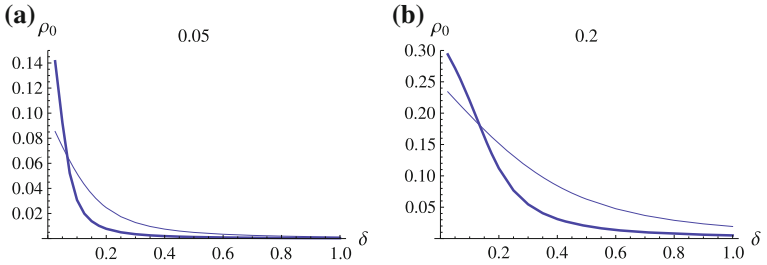

Fig. 12.2 Maximum value of the lattice deformation as a function of the dynamically modulated inverse anharmonic stiffness coefficient δ, in lattices with cubic (*thin line*) and quartic (*thick line*) anharmonicity for the value $g_v = 0.05$ **a** and **b** $g_v = 0.2$

increasing; (iv) the quartic anharmonicity is dominant at small values of δ (large velocities), while cubic anharmonicity is dominant at larger values of δ (small velocities).

From (12.30) we obtain

$$\Phi^2(\xi) = \frac{1}{2D}\frac{dF(\rho)}{d\rho}. \tag{12.56}$$

Using explicit expression for F from (12.43), we find the bisolectron wave function

$$\Phi_c(\xi) = \sqrt{\frac{\rho_{0(c)}}{2D}}\,\mathrm{sech}(\kappa_c\xi)\sqrt{1 - s^2 + \alpha\rho_{0(c)}\mathrm{sech}^2(\kappa_c\xi)}, \tag{12.57}$$

for the lattice with cubic anharmonic potential, and

$$\Phi_q(\xi) = \sqrt{\frac{\rho_{0(q)}}{2D}}\,\mathrm{sech}(\kappa_c\xi)\sqrt{1 - s^2 + \beta\rho_{0(q)}^2\mathrm{sech}^4(\kappa_q\xi)}, \tag{12.58}$$

for the lattice with quartic anharmonic potential, respectively.

Finally, we write down the energy and the momentum of the system, described by the Hamiltonian in (12.1)–(12.4), in the bisolectron state (12.6)-(12.8):

$$E_{\mathrm{tot}}^{(\mathrm{bs})}(V) = mV^2 + E^{(bs)}(V) + W(V), \tag{12.59}$$

$$P_{(\mathrm{bs})}(V) = \left[2m + M\sqrt{\frac{2}{\sigma}}\int_0^{\rho_0} K(\rho, \rho_o)\frac{\rho}{\sqrt{\rho_0 - \rho}}d\rho\right]V \approx \tag{12.60}$$

$$\approx \left[2m + \frac{4}{3}M\sqrt{\frac{2}{\sigma}}\rho_0^{3/2}\right]V.$$

Here we count the energy from the electron energy E_0, $m = \hbar^2/2Ja^2$ is the effective band mass of an electron, $E^{(\mathrm{bs})}(V) = -2\lambda J$ is the bisoliton energy, and W is the energy of the lattice deformation:

$$W(V) = 2MV_{ac}^2 \int_{-\infty}^{0} \left(F(\rho) + s^2\rho^2 \right) d\xi, \tag{12.61}$$

or, in terms of the F and G functions given by expressions (12.31), (12.38), respectively:

$$E^{(\mathrm{bs})}(V) = -2DG(\rho_0)MV_{ac}^2, \tag{12.62}$$

$$W(V) = \frac{MV_{ac}^2}{\sqrt{\sigma}} \int_0^{\rho_0} \frac{d^2F/d\rho^2}{dF/d\rho} \frac{F(\rho) + s^2\rho^2}{\sqrt{G(\rho_0) - G(\rho)}} d\rho. \tag{12.63}$$

Using now the bisolectron solutions (12.47), (12.57) for the cubic anharmonicity, we obtain

$$E_c^{(\mathrm{bs})}(V) = -DMV_{ac}^2 \rho_{0(c)} \frac{4\rho_{0(c)} + 3\delta_c}{3(\rho_{0(c)} + \delta_c)}, \tag{12.64}$$

$$W_c(V) \approx \frac{MV_{ac}^2}{3\sqrt{2\sigma}} \rho_{0(c)}^{3/2} \left(\frac{8}{15}\alpha\rho_{0(c)} + 1 + s^2 \right). \tag{12.65}$$

For the solutions (12.47), (12.58) in the quartic anharmonic lattice we have

$$E_q^{(\mathrm{bs})}(V) = -\frac{1}{2} DMV_{ac}^2 \rho_{0(q)} \frac{3\rho_{0(q)}^3 + 2\delta_q}{\rho_{0(q)}^2 + \delta_q}, \tag{12.66}$$

$$W_q(V) \approx 8 \frac{MV_{ac}^2}{\sqrt{2\sigma}} \rho_{0(q)}^{3/2} \left[\frac{1}{3} \left(s^2 + \frac{1}{2}\delta\beta \right) + \frac{2}{35}\beta\rho_{0(q)}^2 \right]. \tag{12.67}$$

Two important conclusions follow from the above expressions. First of all, comparing the bisolectron energies with the energies of solectrons (see [20–22]), we conclude, that there is positive binding energy of the bisolectron in the whole interval of velocities $V^2 \le V_{ac}^2$

$$E_{\mathrm{bind}(v)}^{(\mathrm{bs})}(V) = 2E_{\mathrm{tot}(v)}^{(\mathrm{s})}(V) - E_{\mathrm{tot}(v)}^{(\mathrm{bs})}(V), \quad v = c, q, \tag{12.68}$$

which means that an anharmonic lattice soliton can capture two electrons with opposite spins and that such a bisolectron state is energetically favorable relative to two independent solectrons (lattice soliton bound with one electron). Here $E_{\mathrm{tot}(v)}^{(\mathrm{bs})}(V)$ is the total energy of the system in the bisolectron state with account of the energy of

the lattice deformation, and $E^{(s)}_{\mathrm{tot}(\nu)}(V)$ is the energy of the system with one electron in a soliton state with account of the energy of the lattice deformation.

Secondly, we see, that the bisolectron energy and the energy of the lattice deformation take finite values at the velocity of the bisolectron equal to the velocity of the sound in the chain, namely:

$$E^{(\mathrm{bs})}_{\mathrm{tot(c)}}(V_{ac}) = mV_{ac}^2 - \frac{2}{3}\chi a\rho_{0(c)} + \frac{16}{45}\chi a\alpha\rho_{0(c)}^2, \tag{12.69}$$

$$E^{(\mathrm{bs})}_{\mathrm{tot(q)}}(V_{ac}) = mV_{ac}^2 - \frac{3}{2}\chi a\rho_{0(q)}^2 + \frac{8}{35}\chi a\beta\rho_{0(q)}^3, \tag{12.70}$$

where the values $\rho_{0(\nu)}$ are calculated at $V = V_{ac}$.

At small velocities the bisolectron energy increases with the velocity increasing, according to the law:

$$E^{(\mathrm{bs})}_{\mathrm{tot(c)}}(V) = mV^2 - \frac{1}{3}\chi a\rho_{0(c)}\left(1 - 2s^2 - \frac{1}{15}\alpha\rho_{0(c)} + 7\alpha\rho_{0(c)}s^2\right), \tag{12.71}$$

for the lattice with cubic anharmonic potential, and

$$E^{(\mathrm{bs})}_{\mathrm{tot(q)}}(V_{ac}) = mV^2 - \frac{1}{3}\chi a\rho_{0(q)}\left(1 - 2s^2 + 3\beta\rho_{0(q)}^2 s^2 - \frac{129}{35}\beta\rho_{0(q)}^2\right) \tag{12.72}$$

for the lattice with quartic anharmonic potential. Recall, in these expressions the value of the maximum lattice deformation is function of the velocity, $\rho_{0(\nu)} = \rho_{0(\nu)}$ (V), according to (12.51) and (12.52), respectively

From the above two equations we can calculate the bisolectron band bottom energy level and bisolectron effective mass in the effective mass approximation for the lattice with cubic anharmonic potential

$$E^{(\mathrm{bs})}_{0(c)} = -\frac{2}{3}Jg^2\left(1 - \frac{1}{15}\alpha\frac{2Jg^2}{\chi a}\right), \tag{12.73}$$

$$M_c^{(\mathrm{bs})} = 2m + \frac{4}{3}\frac{Jg^2}{V_{ac}^2}\left(1 - 7\alpha\frac{Jg^2}{\chi a}\right), \tag{12.74}$$

and for the lattice with quartic anharmonic potential

$$E^{(\mathrm{bs})}_{0(q)} = -\frac{2}{3}Jg^2\left(1 - \frac{129}{35}\beta 4g^2\frac{J^2}{\chi^2 a^2}\right), \tag{12.75}$$

$$M_q^{(\mathrm{bs})} = 2m + \frac{4}{3}\frac{Jg^2}{V_{ac}^2}\left(1 - 6\beta\frac{J^2g^4}{\chi^2 a^2}\right). \tag{12.76}$$

Here g is the dimensionless electron-lattice coupling constant

$$g \equiv \frac{\chi^2}{2Jw}. \tag{12.77}$$

12.5 Bisolectrons with Account of the Coulomb Repulsion

Let us now take into account the Coulomb repulsion between the electrons. The total energy of the system (12.59) in the bisolectron state with account of the Coulomb repulsion is

$$\mathscr{E}^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(V) = E^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(V) + E_{\mathrm{Coul}}. \tag{12.78}$$

In the systems, whose parameters satisfy the condition of the adiabatic approximation (intermediate value of the electron-lattice coupling and relatively small non-adiabaticity parameter) the bisolectron is extended over a few lattice sites. Therefore, the energy of the Coulomb repulsion can be written as

$$E_{\mathrm{Coul}} \approx \frac{e^2}{4\pi\varepsilon l a}, \tag{12.79}$$

where e is the effective electron charge with account of its screening in the lattice due to the surrounding and complex structure of a unit site, and $\varepsilon = \varepsilon_{\mathrm{m}}\varepsilon_0$ is the dielectric constant of the lattice, which contains the dielectric constant ε_{m} of the medium.

Above we have obtained the soliton solutions for two electrons with anti-parallel spins, bound with the lattice soliton, in the approximation of a very weak Coulomb repulsion. In such a case both "one-electron" wave-functions have maximum values at the same position in the lattice. In the general case the corresponding maximum values are shifted along the lattice at some value l_0, which is determined by the balance between the Coulomb repulsion between the electrons and their attraction due to the interaction with the lattice:

$$\Phi_j(\xi) = \Phi_j(\xi \pm l_0/2) f_j(l_0), \tag{12.80}$$

where $f_j(l_0)$ takes into account the change of "one-electron" wave functions due to the Coulomb repulsion. For localized states extended over few lattice sites the repulsion is expected to be weak: $f_j(l_0) \approx 1 + \varepsilon(l_0)$, where here $\varepsilon \ll 1$ is a smallness parameter. Therefore, in the lowest order approximation with respect to ε the maxima of 'one-electron' functions coincide at $\xi = 0$, as was considered in the previous section.

According to (12.80), in the presence of the Coulomb repulsion we have the following expressions for the wave-functions for the cubic anharmonicity (see (12.57))

$$\Phi_{j(c)}(\xi) = \sqrt{\frac{\rho_{0(c)}}{2D}}\,\mathrm{sech}\left(\kappa_c(\xi \pm \frac{l}{2})\right) \tag{12.81}$$

$$\times \sqrt{1 - s^2 + \alpha\rho_{0(c)}\mathrm{sech}^2\left(\kappa_c(\xi \pm \frac{l}{2})\right)},$$

and for a lattice with quartic anharmonicity (see (12.58))

$$\Phi_{j(q)}(\xi) = \sqrt{\frac{\rho_{0(q)}}{2D}}\,\mathrm{sech}\left(\kappa_q(\xi \pm \frac{l}{2})\right) \tag{12.82}$$

$$\times \sqrt{1 - s^2 + \beta\rho_{0(q)}^2\mathrm{sech}^4\left(\kappa_q(\xi \pm \frac{l}{2})\right)}.$$

The distance between the maxima of the 'one-electron' wave-functions, l, can be determined from the condition of the minimum of the total energy of the system with account of the Coulomb repulsion. To calculate it, let us consider for simplicity the case of a bisolectron at rest, $V = 0$. Substituting function (12.81) (or (12.82)) and corresponding lattice deformation (12.47) into the Hamiltonian $\mathscr{H}$ and expanding the result with respect to l in the assumption $l < \mu = 2\pi/\kappa_v$, we obtain after the integration the total energy of the system including the Coulomb repulsion (12.79):

$$\mathscr{E}^{(\mathrm{bs})}_{\mathrm{tot}(v)}(0) = \frac{2}{3}J\frac{\kappa_v}{D}\rho_{0(v)} - \frac{4}{3}\frac{\chi a}{\kappa_v D}\rho_{0(v)}^2\left(1 - l^2\kappa_v^2\right) \tag{12.83}$$

$$+ wa^2\rho_{0(v)}^2\left[\frac{2}{3} + \frac{1}{2}\varsigma_v\rho_{0(v)}^2 - l^2\kappa_v^2\left(\frac{1}{3} + \frac{1}{2}\varsigma_v\rho_{0(v)}^2\right)\right] + \frac{e^2}{4\pi\varepsilon la},$$

where $\varsigma_c \equiv \alpha$, and $\varsigma_q \equiv \beta$, and the energies are counted from the energy of the electron band bottom E_0. Expression (12.62) can be represented in the general form

$$\mathscr{E}^{(\mathrm{bs})}_{\mathrm{tot}(v)}(0) = E^{(\mathrm{bs})}_{\mathrm{tot}(v)}(0) + \frac{1}{2}\zeta_v l^2 + \frac{e^2}{4\pi\varepsilon la}, \tag{12.84}$$

where the first term is the bisolectron energy in the absence of the Coulomb repulsion, the second term is due to modification of the wave functions, and the last term is the Coulomb repulsion.

Minimizing this expression with respect to l, we get the equilibrium distance between the maxima of one-electron functions:

$$l_0 = \left(\frac{e^2}{4\pi\varepsilon a\zeta_v}\right)^{1/3}, \tag{12.85}$$

where we used the notation

$$\zeta_q = \left[\frac{4}{3} \frac{\chi a \rho_{0(q)}^2 \kappa_q}{D} - w a^2 \rho_{0(q)}^2 \kappa_q^2 \left(\frac{1}{3} + \frac{1}{2} \beta \rho_{0(q)}^2 \right) \right]. \tag{12.86}$$

Expression (12.85) can be approximated as

$$l_{0(v)} = \left(\frac{3De^2}{4\pi\varepsilon\chi a^2 \rho_{0(v)}^2 \kappa_v} \right)^{1/3}. \tag{12.87}$$

Substituting these results into (12.78), we obtain the final expression for the total energy of the system at $V = 0$

$$\mathscr{E}_{\mathrm{tot}(v)}^{(\mathrm{bs})}(0) = E_{\mathrm{tot}(v)}^{(\mathrm{bs})}(0) + \frac{3}{2} \left(\frac{e^2}{4\pi\varepsilon a} \right)^{2/3} \zeta_v^{1/3} + \frac{e^2}{4\pi\varepsilon l_0 a}. \tag{12.88}$$

Here l_0 is given by (12.87).

Such a state is stable with respect to the decay of the bisolectron into two solectrons, if the bisolectron binding energy $\mathscr{E}_{\mathrm{bind}(v)}^{(\mathrm{bs})}(0)$ is positive

$$\mathscr{E}_{\mathrm{bind}(v)}^{(\mathrm{bs})}(0) \equiv 2\mathscr{E}_{\mathrm{tot}(v)}^{(\mathrm{s})}(0) - \mathscr{E}_{\mathrm{tot}(v)}^{(\mathrm{bs})}(0) > 0, \tag{12.89}$$

therefore, when the inequality is valid

$$2E_{\mathrm{tot}(v)}^{(\mathrm{s})}(0) - E_{\mathrm{tot}(v)}^{(\mathrm{bs})}(0) + \frac{3}{2} \left(\frac{e^2}{4\pi\varepsilon a} \right)^{2/3} \zeta_v^{1/3} > 0. \tag{12.90}$$

12.6 Comparison with Numerical Simulations

In this section we compare the above obtained analytical results with the results obtained numerically in [25, 46] for a discrete lattice with Morse interaction with two added excess electrons, described by the Hubbard Hamiltonian. The Morse potential

$$U^{\mathrm{Morse}}(r) = D \left[\left(1 - e^{-B(r-a)} \right)^2 - 1 \right], \tag{12.91}$$

can be approximated near the minimum with high degree of precision by the anharmonic potential U_c (see (12.42)) (for more details see [5]).

The parameter values used in the simulations were: $\eta = 2.5a$, $J_0 = 0.02\ (2D)$, $\tau = J_0/(\hbar\,\Omega_{\mathrm{Morse}}) = 20$, for different values of the Hubbard parameter $\bar{U} =$

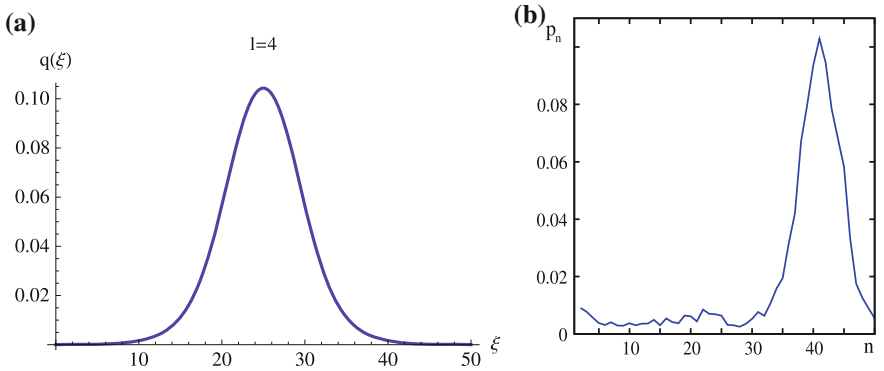

Fig. 12.3 **a** Bisolectron density $q(x = na)$ according to the analytical result (12.81) at $l = l_0 = 4$. **b** Results of the numerical simulations for the electron density P_n at $\bar{U} = 20$

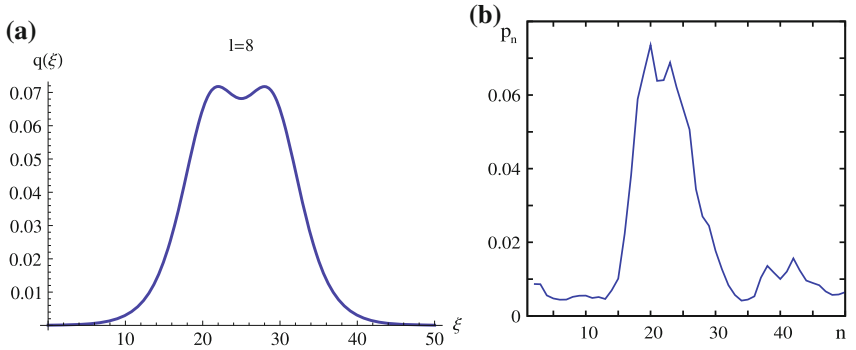

Fig. 12.4 **a** Bisolectron density $q(x = na)$ according to the analytical result (12.81) at $l = l_0 = 8$. **b** Results of the numerical simulations for the electron density P_n at $\bar{U} = 60$

$U/\hbar\Omega_{\text{Morse}}$, namely $\bar{U} = 20, 60, 70, 100$, the lowest of which, $\bar{U} = 20$, for the parameters of alpha-proteins corresponds to $U = 0.004 - 0.02\,\text{eV}$, and the upper value $\bar{U} = 100$, respectively, correspond to $U = 0.02 - 0.1\,\text{eV}$.

In left panels of Figs. 12.3 and 12.6a we show the charge density function within our analytical model for various values of the Coulomb repulsion, which determines the distance between the maxima of one-electron functions. We define the charge density function in elementary charge units in the usual way as $q(\xi) = \Phi_1^2(\xi) + \Phi_1^2(\xi)$, where $\Phi_i(\xi)$ are functions determined by expressions (12.81) and $l = l_0$ as given by the relation (12.87). The results of the numerical simulations for the electron density and the velocity distribution of solectron pairs with Hubbard repulsion on the Morse lattice are shown in right panels (b) of Figs. 12.3, 12.4, 12.5 and 12.6 (a previous version of these figures was published in [5]).

Although the numerical and analytical results are obtained in slightly different models of the anharmonic lattice and the Coulomb repulsion, there is a good

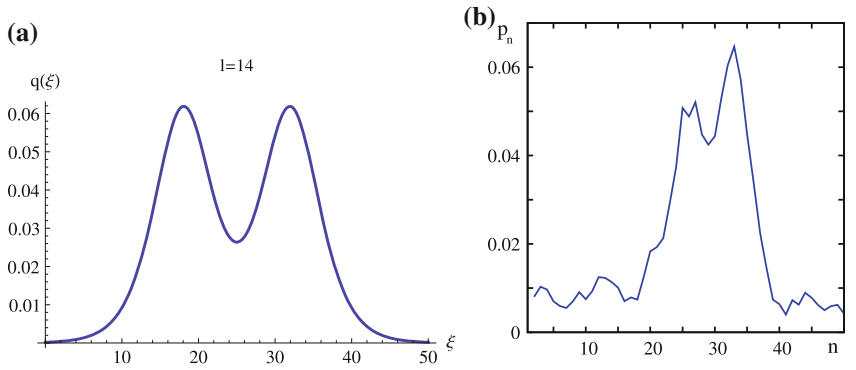

Fig. 12.5 **a** Bisolectron density $q(x = na)$ according to the analytical result (12.81) at $l = l_0 = 14$. **b** Results of the numerical simulations for the electron density p_n at $\bar{U} = 70$

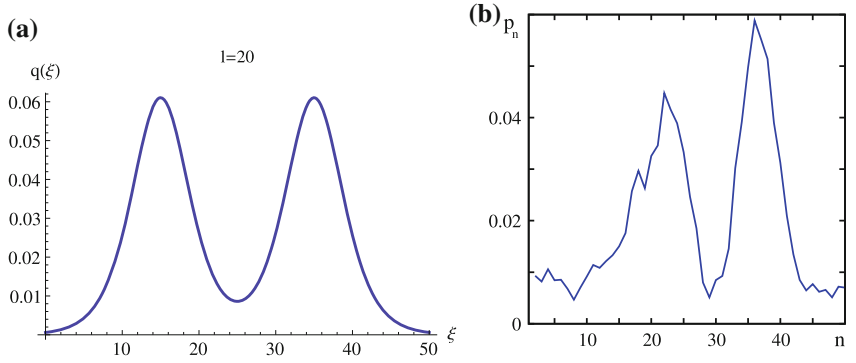

Fig. 12.6 **a** Bisolectron density profile $q(x = na)$ according to the analytical results (12.81) at $l = l_0 = 20$. **b** Results of the numerical simulations for the electron density p_n at $\bar{U} = 100$

qualitative agreement in both approaches. In particular, we see that electrons are localized in the bisolectron state, the profile of which depends on the strength of the Coulomb repulsion with the tendency of splitting one maximum into two maxima with increasing the Coulomb repulsion.

Notice that the parameter values used in the numerical simulations, correspond to relatively high non-adiabaticity of the system and strong anharmonicity. Nevertheless, comparison of the figures corresponding to four different values of the Hubbard term in numerical simulations and, respectively, Coulomb term in the analytical model shows that our analytical model gives rather good results even for quite a strong electron repulsion. In the lowest order of the continuum approximation used in our model, the functions are smooth with one or two maxima depending on the strength of the Coulomb repulsion. The dynamics of the bisolectron and account of the lattice discretness manifested in the presence of the Peierls-Nabarro potential [6,

7] will modify the functions profile, and will lead to some radiation of sound waves, which we can see in the results of the numerical modeling in Figs. 12.4, 12.5 and 12.6.

12.7 Supersonic Bisolectrons

In this section we look for supersonic bisolectrons. First of all, we notice that according to the Hamiltonian (12.2), the dispersion law of the electron band with the electron states $\Psi(n,t) = A\exp(ikn - i\varepsilon(k)\tau)$ is given by the equation

$$\varepsilon(k) = 4j\sin^2\frac{k}{2}, \quad j = \frac{J}{MV_{ac}^2}, \tag{12.92}$$

where k is the dimensionless wave-vector (quasi-momentum), $k \in [-\pi, \pi]$. Here and below we will use the dimensionless time $\tau = V_{ac}t/a$ and measure energies in units of MV_{ac}^2.

The dimensionless electron group velocity is

$$v \equiv \frac{V_g}{V_{ac}} = \frac{d\varepsilon(k)}{dk} = 2j\sin k, \tag{12.93}$$

from where we see that it attains the maximum value $v_{max} = 2j$ at $k = \pi/2$. Therefore, the supersonic regime of the electron motion can take place in systems with large enough electron band width $j > 1/2$.

Let us represent the electron wave function in the form of the modulated envelope $\Psi(x,\tau) = \Phi(x,\tau)\exp[ikx - i(\varepsilon(k) + \varepsilon_b(k))\tau]$ where $\varepsilon_b(k)$ is the corresponding eigen-energy of the state. Now the equations of motion become

$$\frac{\partial\Phi(x,\tau)}{\partial\tau} + 2j\sin k\frac{\partial\Phi(x,\tau)}{\partial x} = 0, \tag{12.94}$$

$$j\cos(k)\frac{\partial^2\Phi(x,\tau)}{\partial x^2} + 2\chi_0\rho(x,\tau)\Phi(x,\tau) + \varepsilon_b(k)\Phi(x,\tau) = 0, \tag{12.95}$$

$$\frac{\partial^2\rho(x,\tau)}{\partial\tau^2} - \frac{\partial^2 u'(\rho)}{\partial x^2} - \frac{1}{12}\frac{\partial^4\rho(x,\tau)}{\partial x^2\partial\tau^2} + 2\chi_0\frac{\partial^2\Phi^2(x,\tau)}{\partial x^2} = 0, \tag{12.96}$$

where

$$u = \frac{U}{MV_{ac}^2}, \quad \chi_0 = \frac{\chi a}{\hbar V_{ac}}, \tag{12.97}$$

and the prime denotes a derivative of the function with respect to the argument.

We have included into (12.96) the additional term with the fourth order derivative in order to take into account the lattice discreteness within the same approximation as the lattice anharmonicity at supersonic velocities (comp. (12.12) and see the discussion there). This equation is known as the improved Boussinesq equation.

It is easy to see that, for the stationary wave functions, (12.94) defines the electron band energy dispersion law, while the potential of the stationary Schrödinger equation (12.95) is the self-consistent deformational potential to be found from (12.96). We are interested in the bound electron states, therefore, the electron eigen energy $\varepsilon_b(k)$ has to be negative, which is possible only if $\cos(k)$ is positive, according to (12.95). Therefore, such states are possible for the corresponding quasi-momentum values in the interval $0 \le k < \pi/2$. The quasi-momentum is determined by the dimensionless soliton velocity according to the relation

$$k = \mathrm{Arc}\cos\sqrt{1 - \frac{v^2}{4j^2}}, \tag{12.98}$$

which follows from (12.92).

Another way to take into account the lattice discreteness is to generalize the equation (12.96) to the ill-posed Boussinesq equation (see comments in [12]):

$$\frac{\partial^2\rho(x,\tau)}{\partial\tau^2} - \frac{\partial^2 u'(\rho)}{\partial x^2} - \frac{1}{12}\frac{\partial^4\rho(x,\tau)}{\partial x^4} + 2\chi_0\frac{\partial^2\Phi^2(x,\tau)}{\partial x^2} = 0. \tag{12.99}$$

Improved and ill-posed Boussinesq equations (12.96) and (12.99) correspond to lattices with nonlinear dispersions

$$\omega_1^2(k) = \frac{k^2}{1 + k^2/12}, \qquad \omega_2^2(k) = k^2(1 - k^2/12), \tag{12.100}$$

respectively. The two dispersions in the admissible interval of quasi-momentum $[0, \pi/2]$ are very close, as we can see from Fig. 12.7.

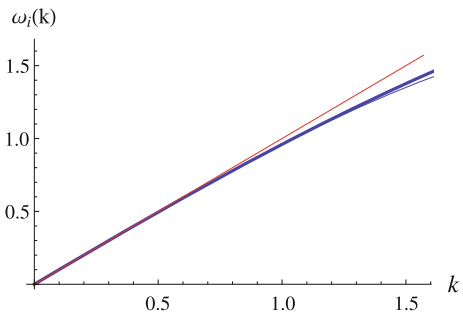

Fig. 12.7 Phonon energy dispersions for the improved (*thick line*) and ill-posed (*thin line*) Boussinesq equations in the interval $[0, \pi/2]$. *Red line* (the *top curve*) shows linear dispersion

For the class of functions, depending on the running wave coordinate $\zeta = x - x_0 - v\tau$, (12.94)–(12.99) take the form

$$\lambda \frac{d^2\Phi(\zeta)}{d\zeta^2} + 2\chi_0\rho(\zeta)\Phi(\zeta) + \varepsilon_b(k)\Phi(\zeta) = 0, \tag{12.101}$$

$$\mu \frac{d^2\rho(\zeta)}{d\zeta^2} + (1 - v^2)\rho(\zeta) + \frac{du_{anh}}{d\rho} = 2\chi_0\Phi^2(\zeta), \tag{12.102}$$

where u_{anh} is the anharmonic part of the lattice potential, $u = u_h + u_{anh}, u_h \equiv \rho^2/2$. Here

$$\lambda = j\cos(k), \quad \mu = \mu_{1,2}, \quad \mu_1 = \frac{v^2}{12}, \quad \mu_2 = \frac{1}{12}. \tag{12.103}$$

Indexes 1 and 2 refer to the improved and ill-posed Boussinesq equations, respectively.

From the system of (12.101) and (12.102) we find, as in Sect. 12.4,

$$\zeta = \pm\sqrt{\frac{\mu}{2}} \int_{\rho}^{\rho_0} \frac{dr}{r\sqrt{Q(r)}}, \tag{12.104}$$

where the function Q is defined in the interval $0 \le \rho \le \rho_0$ by the relation:

$$Q(r) = 2\frac{\chi_0}{\rho^2} \int_0^{\rho} \Phi^2(r)dr + \frac{v^2 - 1}{2} - \frac{1}{\rho^2}u_{anh}(\rho). \tag{12.105}$$

It follows from (12.104) that the kernel function Q has to be positive and convex for all values of ζ. This requirement determines several types of solutions, as described below.

1. Supersonic lattice solitons $v^2 > 1$ in an un-doped chain (i.e., in the absence of an extra electron), which corresponds to $\Phi = 0$, $\chi_0 = 0$.
2. Subsonic and weakly supersonic self-trapped electrons in the bisolectron state in the chain. In this case the first term in the r.h.s. of the function (12.105) is the leading one, and the type of the solution is determined by the asymptotics of the electron wave function depending on ρ. Let us consider the parameter L which is determined as the limit

$$\mathscr{L} \equiv \lim_{\rho\to 0} \frac{1}{\rho^2} \int_0^{\rho} \Phi^2(r)dr. \tag{12.106}$$

If $\Phi^2(\rho) \propto \rho$ at $\rho \to 0$, then the value $\mathscr{L}$ is finite, and, therefore, the first term in (12.105) is important. In this case the solution can be subsonic if $u_{anh} = 0$. The value Q can be positive also at $v^2 = 1$ if $u_{anh} \neq 0$. In this case the solution

has finite values of energy and momentum for the positive lattice anharmonicity (see [44, 45]). This solution can be supersonic for strong lattice anharmonicity u_{anh}.

3. Supersonic bisolectron state. It is valid at a sufficiently fast decay of the electron wave functions in the limit (faster, than the linear decay, considered above), such that the following inequality is fulfilled:

$$2\chi_0 \int_0^{\rho} \Phi^2(r)dr < u_{anh}(\rho). \tag{12.107}$$

In this case the lattice anharmonicity u_{anh} is responsible for the soliton formation. The envelope of such a soliton is modified by the presence of two electrons due to the integral term in expression (12.105). The presence of this integral term increases the maximum value of the chain deformation. Such a lattice soliton creates the potential well for the excess electrons and results in their binding and trapping. Namely this case corresponds to the capture of electrons by the anharmonic lattice soliton and formation of a bisolectron (lattice-polaron l-p mode in [50]).

The wave functions in the class of localized functions with a bell-shaped profile, can be chosen in the form

$$\Phi^2(\zeta) \cong C_p \rho^p(\zeta) \tag{12.108}$$

with positive constants $C_p > 0$ to be determined from the normalization condition of the wave-function Φ.

1. At $p = 1$ we reconstruct analytically the solutions, found in Sect. 12.4 for the lattices with cubic and quartic anharmonicities at some fixed relation between the parameter values. Namely, for the case of the cubic lattice anharmonicity this relation reads as $\lambda\alpha = 6\mu\chi_0$, where α is a anharmonicity coefficient in (12.42).
2. At $p > 1$ we find

$$\varepsilon_b(k) = -jp^2v^2\cos(k), \quad v^2 = \frac{v^2 - 1}{4\mu}, \tag{12.109}$$

which takes place only at $v^2 > 1$. Here parameter p has to be found from the normalization condition of the wave-function.

We can find explicitly analytical solution of the system of equations for the ansatz (12.108) at $p = 2$:

$$\Phi_{bis}^{(ss)} = \frac{3}{\chi_0}\kappa^2\sqrt{\lambda\left(\frac{\alpha}{\chi_0} - \mu\right)}\,\mathrm{sech}^2(\kappa\zeta), \tag{12.110}$$

$$\rho_{bis}^{(ss)} = \frac{3\lambda}{\chi_0}\kappa^2\mathrm{sech}^2(\kappa\zeta). \tag{12.111}$$

From the normalization condition we obtain the relation between the width of the bisolectron and its velocity

$$\kappa^2 = \frac{v^2 - 1}{4\mu\left[1 - 3(\gamma - 1)\right]}, \tag{12.112}$$

or, equivalently,

$$v^2 = 1 + 4\mu\kappa^2\left[1 - 3(\gamma - 1)\right], \tag{12.113}$$

where

$$\gamma = \frac{\alpha\lambda}{2\mu\chi_0}. \tag{12.114}$$

In the case of the arbitrary bisolectron velocity it is difficult to find analytical solutions explicitly. They can be found numerically by solving (12.101) and (12.102) or their equivalent discrete equations. Although the system of equations does not belong to the class of complete integrable equations, it is still very close to a such one, and the corresponding soliton ansatz is a good approximation for its solution. Therefore, we expect, that numerically found solutions are close to the solutions found above for the particular velocity (12.113). To a large extent this conclusion is supported by the numerical simulations of the dynamics of two electrons in the anharmonic Morse lattice [14, 15, 25, 28, 46, 47],where the trapping of two electrons by the supersonic lattice soliton has been observed (see also [14, 15].

12.8 Conclusion

We have shown that in one-dimensional crystal lattices the anharmonicity of the inter-site interactions favors not only self-trapping of an extra electron, but also pairing of two electrons with opposite spins in a single lattice soliton deformation well, resulting in the formation of a stable bisolectron state. Such a bisolectron is the bound state of the lattice soliton and two self-trapped electrons in a singlet bisoliton state. This conclusion generalizes the concepts of polarons and bipolarons [1, 2, 31, 34, 35], and illustrates the existence of bisolitons not only in harmonic one-dimensional systems [8, 9, 17], but in anharmonic lattices too. Our analytical model explains the results of the numerical simulations for lattices with anharmonic Morse potential describing the inter-site interactions, with two extra electrons in it [28, 43, 46, 47]. We have found explicitly the expressions for the lattice deformation and two-electron wave-functions for lattices with cubic and quartic anharmonicities. We also calculated the energies of the bisolectrons for these two types of anharmonicities and shown that bisolectrons can move with the velocities up to the velocity of the sound in the lattice, and the corresponding energy and momentum are finite in the

whole interval of bisolectron velocities. We have also found the conditions for the existence of supersonic bisolectrons for particular values of their velocity.

We have studied the role of the Coulomb repulsion in the formation of bisolectrons in anharmonic lattices. We have shown that with account of the Coulomb repulsion between the electrons their envelope function in a bisolectron state can have one or two maxima, the distance between which is determined by the balance of the gain of energy due to binding to the lattice deformation and loss of energy due to the Coulomb repulsion. The results of the analytical study of two electrons in a lattice with cubic anharmonicity with account of their Coulomb repulsion are in good agreement with the numerical simulations of two electrons in an anharmonic Morse lattice with account of Hubbard electron-electron repulsion in a broad range of parameter values.

The results obtained here are valid for systems, whose parameter values satisfy adiabaticity conditions, i.e., for systems with moderate values of the electron-lattice coupling and not too large nonadiabaticity parameter (the ratio between characteristic phonon energy and electron band width). This is a large class of low-dimensional compounds, including biological macromolecules (DNA and α-helical polypeptides)[18, 19, 30, 38], conducting polymers [11], and low-dimensional crystals, such as polydiacetylene [24, 27, 48], conducting platinum chains [11], salts of transition metals (PbSe,PbTe,PbS) [3, 16, 40, 49], high-temperature superconducting cuprates [4, 13, 23, 26, 32], etc. These compounds find numerous applications in microelectronics and nanotechnologies, or play important role in living systems. This explains our interest in studying nonlinear effects in such systems. We also think that our results apply to muscovite mica, and cover some of the properties of 'quodons' [37], which are widely discussed in the present book.

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