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Spontaneous localization of electrons in lattices with nonlocal interactions

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We study spontaneously localized electron states in a *D*-dimensional lattice with a nonlocal electron-phonon interaction. We show that, in the adiabatic long-wave approximation, such electron states are described by a modified nonlinear Schrödinger equation with a nonlocal nonlinear interaction which, within certain ranges of the parameter values, admits localized soliton-type solutions. We also calculate nonadiabatic corrections and estimate conditions of the applicability of the adiabatic approximation in one- and two-dimensional cases. We show that the adiabatic approximation is valid at strong enough electron-phonon coupling.

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I. INTRODUCTION

It is well known that self-trapping of electron states in low-dimensional electron-phonon systems can result in very peculiar conducting and optical properties of some materials.[1–3] In general, such self-trappings are described by a complex system of nonlinear equations whose exact solutions are not known and, therefore, this problem has to be studied within various approximations and/or using perturbation methods. In our previous papers,[4–6] we have studied numerically and analytically, within the adiabatic approximation, the conditions for the existence and various properties of the self-trapped electron states in *D*-dimensional electron-phonon lattices ($D=1,2,3,\ldots$). Such systems can be described by a system of partial differential equations involving two fields: the electron wave function and the displacement vector field with *D* components for a *D*-dimensional lattice. Here we continue our investigations further and show that, for stationary configurations, one can eliminate the displacement field and that, if one keeps only the lowest-order terms in the continuum limit, the corresponding equation reduces to the nonlinear Schrödinger equation (NLSE).

In one dimension, the NLSE guarantees the existence of solitonic solutions but in higher dimensions higher-order terms are essential. In particular, these higher-order terms play an important role for the soliton stability as they can prevent a soliton from collapsing. In Ref. 4 it was suggested that if one takes into account the second-order term, the equations for the electron-phonon system which, for simplicity, we consider to be isotropic, reduce to the following modified nonlinear Schrödinger equation (MNLSE) for the electron wave function $\varphi=\varphi(\vec{r},\tau)$:

$$i\frac{\partial\varphi}{\partial\tau}+\Delta\varphi+2g\left(|\varphi|^2+\frac{\alpha}{12}\Delta|\varphi|^2\right)\varphi=0, \qquad (1)$$

where $\vec{r}$ is a *D*-dimensional radius vector, Δ is the Laplacian operator, g is the dimensionless electron-phonon coupling, and α is a constant ($1<\alpha<4$).[4] In this paper, we rederive this equation and show that the extra term in it arises from an expansion of the generic nonlinear nonlocal term describing the electron-phonon interaction.

In general, the modeling of physical systems by various modifications of the NLSE usually requires certain simplifications. The different discrete versions of NLSE's correspond to various approximations in the description of the systems and, in particular, of an electron-phonon system, see e.g., Refs. 7–11. It is known that solitonlike stationary solutions of nonlinear equations can not only be excited by initial pulses that satisfy certain conditions (so called excitation thresholds[8,9,12,13]) but also that they are stable within certain intervals of parameters (see, e.g., Refs. 14–19). In more realistic models, the additional terms due to the higher-order dispersion, nonlinearity saturation or nonlocal interactions should also be taken into account and, sometimes, these extra terms can result in the stabilization of soliton solutions in a wider range of parameter values. One of such cases is the electron-phonon system described below. In this case, the general problem does not have a simple solution even for a one-dimensional case, let alone in higher dimensions, even though it has been studied for several decades.

In our previous paper,[6] we started from a system of partial differential equations describing the stationary electron-phonon system and applied some approximations to integrate the phonon field and to reduce the system of equations to the MNLSE. In this paper, we start from the quantum-mechanical description of the electron-phonon system by the Fröhlich Hamiltonian.[20] Performing the unitary transformations[21] we represent the Hamiltonian in the form of two terms, one of which describes the system in the adiabatic approximation, while the second one describes the nonadiabatic correction. We then show that in the adiabatic approximation the system of equations can be reduced to the MNLSE with a nonlocal nonlinear interaction. It is well known that the nonlocal interactions can not only modify the properties of the solitonlike solutions, but also affect the conditions of their existence. Our construction clearly shows that it is the interaction with the lattice which leads to the nonlocal nonlinear interaction which in turn leads to the MNLSE. We show also that the nonadiabatic part of the Hamiltonian results in an additional term in the expression for the energy of the system.

II. GENERAL MODEL

Consider a D-dimensional lattice with one atom per unit cell with few extra electrons in the conductive band. We neglect the Coulomb repulsion between electrons and take into account the electron-phonon interaction which arises from the electron interaction with the lattice deformation. In this case, electrons interact only with acoustical phonons. Such a system can be described by the Fröhlich Hamiltonian

$$H=\sum_{\sigma,\vec{k}} E(\vec{k})A^{+}_{\sigma,\vec{k}}A_{\sigma,\vec{k}}+\frac{1}{\sqrt{\mathcal{N}}}\sum_{\sigma,\vec{k},\vec{q}} \chi(\vec{q})A^{\dagger}_{\sigma,\vec{k}}A_{\sigma,\vec{k}-\vec{q}} \times(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})+\sum_{\vec{q}} \hbar\omega_{\vec{q}}b^{\dagger}_{\vec{q}}b_{\vec{q}}. \quad (2)$$

Here $A^{\dagger}_{\sigma,\vec{k}}, A_{\sigma,\vec{k}}$ are creation and annihilation operators of the electron with spin projection σ and wave vector $\vec{k}$, which is given by

$$\vec{k}=\sum_{\mu=1}^{D} k_\mu \vec{e}_\mu, \quad k_\mu=\frac{2\pi l_\mu}{N_\mu}, \quad l_\mu=0,\pm1,\ldots,\frac{N_\mu}{2}, \quad (3)$$

where $\mathcal{N}=\Pi_\mu N_\mu$ is the total number of lattice sites; $b^{\dagger}_{\vec{q}}, b_{\vec{q}}$ are creation and annihilation operators of longitudinal-acoustic phonons with wave vector $\vec{q}$ and frequency $\omega_{\vec{q}}$, and, finally, $\chi(\vec{q})$ is the function which describes the electron-phonon coupling. The electron energy dispersion in the nearest-neighbor approximation is given by the following expression:

$$E(\vec{k})=E_L-2J\sum_{\mu=1}^{D}\cos(k_\mu), \quad (4)$$

where E_L is the on-site electron energy and J is the exchange interaction energy.

The Hamiltonian of system (2) commutes with the operator of the number of electrons in the system,

$$\hat{N}=\sum_{\sigma,\vec{k}} A^{\dagger}_{\sigma,\vec{k}}A_{\sigma,\vec{k}}, \quad (5)$$

and with the operator of the total momentum of the system,

$$\hat{\vec{P}}=\sum_{\sigma,\vec{k}} \hbar\vec{k}A^{\dagger}_{\sigma,\vec{k}}A_{\sigma,\vec{k}}+\sum_{\vec{q}} \hbar\vec{q}b^{\dagger}_{\vec{q}}b_{\vec{q}}. \quad (6)$$

The state vector of the system, $|\Psi(t)\rangle$, satisfies the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle=H|\Psi(t)\rangle. \quad (7)$$

The energy of a stationary state depends on the eigenvalue $\vec{p}$ of the operator $\hat{\vec{P}}$ (6), where $\vec{p}$ corresponds to the propagation of an excitation with the group velocity $\vec{v}=dE(\vec{p})/d\vec{p}$. Thus it is natural to use the coordinate system moving with this velocity. This is achieved by performing the state-vector transformation

$$|\Psi(t)\rangle=e^{-i\vec{v}\hat{\vec{P}}t/\hbar}|\phi(t)\rangle, \quad (8)$$

and looking for a stationary solution of Eq. (7). This leads to the stationary Schrödinger equation

$$(H-\vec{v}\hat{\vec{P}})|\phi\rangle=E|\phi\rangle, |\phi(t)\rangle=e^{-iEt/\hbar}|\phi\rangle. \quad (9)$$

For further consideration, it is convenient to choose the following state vector for the system:

$$|\phi\rangle=U|\psi\rangle, \quad (10)$$

where U is an unitary operator of the coherent molecule displacements

$$U=\exp\left[\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q}} (\beta_{\vec{q}}b^{\dagger}_{\vec{q}}-\beta^{*}_{\vec{q}}b_{\vec{q}})\right], \quad (11)$$

with an arbitrary function $\beta_{\vec{q}}$ that will be determined later. Operator (11) describes the ground state of the system, renormalized by the electron-phonon interaction.

Using Eqs. (9) and (10), it is easy to show that $|\psi\rangle$ satisfies the equation

$$\mathcal{H}|\psi\rangle=E|\psi\rangle, \quad (12)$$

where the Hamiltonian is determined by transformation (11)

$$\mathcal{H}=U^{\dagger}(H-\vec{v}\hat{\vec{P}})U. \quad (13)$$

Taking into account the explicit form of the unitary operator (11), we get from Eq. (13) the following expression:

$$\mathcal{H}=\sum_{\vec{k},\sigma}\left\{[E(\vec{k})-\hbar\vec{v}\vec{k}]A^{\dagger}_{\sigma,\vec{k}}A_{\sigma,\vec{k}} +\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q}} \chi(\vec{q})A^{\dagger}_{\sigma,\vec{k}}A_{\sigma,\vec{k}-\vec{q}}\left[b_{\vec{q}}+b^{\dagger}_{-\vec{q}}+\frac{1}{\mathcal{N}}(\beta_{\vec{q}}+\beta^{\dagger}_{-\vec{q}})\right]\right\} +\sum_{\vec{q}} \hbar(\omega_{\vec{q}}-\vec{v}\vec{q})\left[b^{\dagger}_{\vec{q}}b_{\vec{q}}+\frac{1}{\mathcal{N}}(\beta_{\vec{q}}b^{\dagger}_{\vec{q}}+\beta^{*}_{\vec{q}}b_{\vec{q}})\right]+W, \quad (14)$$

where W is the energy of the lattice deformation,

$$W=\frac{1}{\mathcal{N}}\sum_{\vec{q}} \hbar(\omega_{\vec{q}}-\vec{v}\vec{q})|\beta_{\vec{q}}|^2. \quad (15)$$

To partially diagonalize Hamiltonian (14), we perform a unitary transformation, as it was done in Ref. 21 for the one-dimensional case, and introduce new electron creation and annihilation operators determined by the, appropriately chosen, complete orthonormal set of functions $\varphi_\lambda(\vec{k})$,

$$A^{\dagger}_{\sigma,\vec{k}}=\sum_{\lambda}\ \varphi^{*}_{\lambda}(\vec{k})a^{\dagger}_{\sigma,\lambda},\ \ A_{\sigma,\vec{k}}=,\sum_{\lambda}\ \varphi_{\lambda}(\vec{k})a_{\sigma,\lambda}. \quad (16)$$

We now choose the functions $\varphi_{\lambda}(\vec{k})$ in such a way that the part of the Hamiltonian which is independent of the phonon operators (14), and which is quadratic in the electron operators, becomes diagonal in the new representation. This will be the case if we require that the functions $\varphi_{\lambda}(\vec{k})$ solve the equation

$$[E(\vec{k})-\hbar\vec{v}\vec{k}]\varphi_{\lambda}(\vec{k})+\frac{1}{N}\sum_{\vec{q}}\ \chi(\vec{q})(\beta_{\vec{q}}+\beta^{*}_{-\vec{q}})\varphi_{\lambda}(\vec{k}-\vec{q})$$
$$=E_{\lambda}\varphi_{\lambda}(\vec{k}). \quad (17)$$

When Eq. (17) is satified, E_{λ} is interpreted as the eigenenergy of the corresponding state λ and Hamiltonian (14) reduces to the following form:

$$\mathcal{H}=\sum_{\lambda,\sigma}E_{\lambda}a^{\dagger}_{\sigma,\lambda}a_{\sigma,\lambda}+\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q},\lambda,\lambda',\sigma}f_{\lambda,\lambda'}(\vec{q})a^{\dagger}_{\sigma,\lambda}a_{\sigma,\lambda'}$$
$$\times(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})+\sum_{\vec{q}}\ \hbar(\omega_{\vec{q}}-\vec{v}\vec{q})$$
$$\times\left[b^{\dagger}_{\vec{q}}b_{\vec{q}}+\frac{1}{\sqrt{\mathcal{N}}}(\beta_{\vec{q}}b^{\dagger}_{\vec{q}}+\beta^{*}_{\vec{q}}b_{\vec{q}})\right]+W, \quad (18)$$

where we have introduced the functions

$$f_{\lambda,\lambda'}(\vec{q})=\chi(\vec{q})\sum_{\vec{k}}\ \varphi^{*}_{\lambda}(\vec{k})\varphi_{\lambda'}(\vec{k}-\vec{q}), \quad (19)$$

which possess the following symmetry properties:

$$f_{\lambda,\lambda'}(\vec{q})=f^{*}_{\lambda',\lambda}(-\vec{q}). \quad (20)$$

Expression (18) can be represented as the sum of the two terms,

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1, \quad (21)$$

where $\mathcal{H}_0$ is the part of the total Hamiltonian which is diagonal with respect to the new electron operators and represents the adiabatic part of the total Hamiltonian (18):

$$\mathcal{H}_0=\sum_{\lambda,\sigma}\left[E_{\lambda}+\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q}}\ F_{\lambda}(\vec{q})(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})\right]a^{\dagger}_{\sigma,\lambda}a_{\sigma,\lambda}$$
$$+\sum_{\vec{q}}\ \hbar(\omega_{\vec{q}}-\vec{v}\vec{q})\left[b^{\dagger}_{\vec{q}}b_{\vec{q}}+\frac{1}{\sqrt{\mathcal{N}}}(\beta_{\vec{q}}b^{\dagger}_{\vec{q}}+\beta^{*}_{\vec{q}}b_{\vec{q}})\right]+W \quad (22)$$

and $\mathcal{H}_1$, respectively, is the corresponding nondiagonal part:

$$\mathcal{H}_1=\frac{1}{\sqrt{\mathcal{N}}}\sum_{\lambda\neq\lambda',\vec{q}}f_{\lambda\lambda'}(\vec{q})a^{\dagger}_{\sigma,\lambda}a_{\sigma,\lambda'}(b_{\vec{q}}+b^{\dagger}_{-\vec{q}}), \quad (23)$$

i.e., it is the part of the second term of Hamiltonian (18), which contains the products of the electron operators $a^{\dagger}_{\sigma,\lambda}a_{\sigma,\lambda'}$ with $\lambda'\neq\lambda$.

The functions $F_{\lambda}(\vec{q})$ in Eq. (22) are given by

$$F_{\lambda}(\vec{q})=f_{\lambda,\lambda}(\vec{q})=\chi(\vec{q})\sum_{\vec{k}}\ \varphi^{*}_{\lambda}(\vec{k})\varphi_{\lambda}(\vec{k}-\vec{q}). \quad (24)$$

Note that the sum in Eq. (23) should be taken over all states, including the ground state $\lambda=0$, possible bound states in the deformational potential, and the continuous part of the spectrum. Thus, the operator $\mathcal{H}_1$ corresponds to the nonadiabatic part of the electron-phonon interaction and, under certain conditions, can be considered to be small. In the one-dimensional case, for instance, as it has been shown in Refs. 16,22, that this is the case when the inequality $Jg^2>\hbar v_0$ holds (g is the dimensionless electron-phonon coupling constant).

Taking all this into account and assuming that the nonadiabaticity corrections are small, we can represent the state vector and the energy of the system in the form

$$|\psi\rangle=|\psi_0\rangle+|\psi_1\rangle+\cdots, E=E_0+E_2+\cdots, \quad (25)$$

where $|\psi_0\rangle$ is the eigenstate of the adiabatic Hamiltonian $\mathcal{H}_0$ with the eigenenergy E_0; $|\psi_1\rangle$ and E_2 are, respectively, a small correction to the wave function and the energy due to the nonadiabatic part of the Hamiltonian $\mathcal{H}_1$.

III. ADIABATIC APPROXIMATION

Let us now consider the adiabatic approximation, i.e., we use the Hamiltonian $\mathcal{H}=\mathcal{H}_0$ neglecting $\mathcal{H}_1$. In this case the wave function of the ground state, $|\psi\rangle=|\psi_0\rangle$, of the system with few extra electrons, N_e, in the conducting band can be taken in the form

$$|\psi_0\rangle=\prod_{\lambda,\sigma}\ (a^{\dagger}_{\sigma,\lambda})^{n_{\sigma,\lambda}}|0_e\rangle|0_{ph}\rangle, \quad (26)$$

where $n_{\sigma,\lambda}=0,1$ are the occupation numbers of the adiabatic levels λ by electrons with spin σ. Then we have $\Sigma_{\lambda,\sigma}n_{\lambda,\sigma}=N_e$. Substituting Eq. (26) into Eq. (12), we get the following equation:

$$\mathcal{H}_0|\psi_0\rangle=\left\{W+\sum_{\lambda,\sigma}\ n_{\lambda,\sigma}E_{\lambda}+\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q}}\ \left[\left(\hbar(\omega_{\vec{q}}-\vec{v}\vec{q})\beta_{\vec{q}}\right.\right.\right.$$
$$\left.\left.\left.+\sum_{\lambda,\sigma}\ n_{\lambda,\sigma}F^{*}_{\lambda}(\vec{q})\right)b^{\dagger}_{\vec{q}}\right]\right\}|\psi_0\rangle. \quad (27)$$

From Eq. (27) we see then that if we choose the arbitrary coefficients $\beta_{\vec{q}}$ to be given by

$$\beta_{\vec{q}}=-\frac{\sum_{\lambda,\sigma} n_{\lambda,\sigma}F_{\lambda}^{*}(\vec{q})}{\hbar(\omega_{\vec{q}}-\vec{v}\vec{q})}, \tag{28}$$

the terms proportional to $b_{\vec{q}}^{\dagger}$ vanish and, therefore, Eq. (26) is an eigenvector of H_0 with the eigenenergy

$$E_0=W+\sum_{\lambda} n_{\lambda}E_{\lambda}, \tag{29}$$

where n_λ is the occupation number of the energy level E_λ which can be unoccupied or occupied by one or two electrons with opposite spins:

$$n_{\lambda}=\sum_{\sigma} n_{\lambda,\sigma}=0,1,2. \tag{30}$$

Using Eqs. (28) and (24), we note that Eq. (17) reduces to

$$[E(\vec{k})-\hbar\vec{v}\vec{k}]\varphi_{\lambda}(\vec{k})-\frac{1}{\mathcal{N}}\sum_{\vec{q}} G(\vec{q})\Phi(\vec{q})\varphi_{\lambda}(\vec{k}-\vec{q}) =E_{\lambda}\varphi_{\lambda}(\vec{k}), \tag{31}$$

where we have defined

$$G(\vec{q})=\frac{2|\chi(\vec{q})|^2\omega_{\vec{q}}}{\hbar(\omega_{\vec{q}}^2-(\vec{v}\vec{q})^2)}, \tag{32}$$

and

$$\Phi(\vec{q})=\sum_{\lambda} n_{\lambda}\Phi_{\lambda}(\vec{q}), \quad \Phi_{\lambda}(\vec{q})=\sum_{\vec{k}} \varphi_{\lambda}(\vec{k})\varphi_{\lambda}^{*}(\vec{k}-\vec{q}). \tag{33}$$

To proceed further, it is convenient to use the fields defined on the physical lattice sites and related to $\varphi_\lambda(\vec{k})$ by the Fourier transforms,

$$\varphi_{\lambda}(\vec{k})=\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{m}} \varphi_{\lambda}(\vec{m})e^{-i\vec{k}\vec{m}},$$

$$\varphi_{\lambda}(\vec{m})=\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{k}} \varphi_{\lambda}(\vec{k})e^{i\vec{k}\vec{m}}, \tag{34}$$

where $\vec{m}$ corresponds to the lattice sites.

Note that the wave-function normalization condition is automatically satisfied, i.e.,

$$\sum_{\vec{n}} |\varphi_{\lambda}(\vec{n})|^2=N \quad \text{if} \quad \sum_{\vec{k}} \varphi_{\lambda}(\vec{k})\varphi_{\lambda}^{*}(\vec{k})=N. \tag{35}$$

For the problem considered here, $N=1$, since φ_λ are the coefficients of the unitary transformation (16) and condition (35) corresponds to the normalization of the electron wave functions, although we can keep N as a parameter for other physical applications.

Performing the unitary transformation (34) in Eq. (31) at $\vec{v}=0$ and taking into account the energy dispersion relation (4), we get

$$E_L\varphi_{\lambda}(\vec{m})-J\sum_{\mu} [\varphi_{\lambda}(\vec{m}+\vec{a}_{\mu})+\varphi_{\lambda}(\vec{m}-\vec{a}_{\mu})] -\left(\sum_{\vec{n}} F(\vec{m}-\vec{n})\Phi(\vec{n})\right)\varphi_{\lambda}(\vec{m})=E_{\lambda}\varphi_{\lambda}(\vec{m}) \tag{36}$$

where $\vec{a}_\mu$ is the μth component of the unit lattice vector,

$$\Phi(\vec{m})=\sum_{\lambda} n_{\lambda}|\varphi_{\lambda}(\vec{m})|^2, \tag{37}$$

and

$$F(\vec{m}-\vec{n})=\frac{1}{\mathcal{N}}\sum_{\vec{q}} G(\vec{q})e^{i\vec{q}(\vec{m}-\vec{n})}. \tag{38}$$

At zero temperature the ground state of the system with N_e electrons corresponds to the filling of the lowest-energy levels E_λ, where $\lambda=0,\ldots,N_e/2$. We see from Eq. (17) that the adiabatic electronic terms are determined by the lattice configuration $\{\beta_{\vec{q}}\}$ which, according to Eq. (28), depends on the occupied electron states. Thus, substituting Eq. (28) into Eq. (17), we get Eq. (31) or Eq. (36) in the site representation. We see that the problem has been reduced to a system of nonlinear equations for $N_e/2$ occupied electron states. This solution defines the self-consistent states of electrons and lattice distortions. All other virtual adiabatic electronic states are determined by the linear equations [Eqs. (31) or (36)] with the deformational potential of lattice distortions given by

$$V(\vec{m})=\sum_{\vec{n}} F(\vec{m}-\vec{n})\Phi(\vec{n}). \tag{39}$$

Finally, we note that the kernel $F(\vec{m}-\vec{n})$ of the nonlinear term in Eq. (36), according to Eq. (38), is a function of the distance $(\vec{m}-\vec{n})$ and, therefore, Eq.(36) is a nonlinear nonlocal equation for the electron wave function. At this stage, the continuum approximation becomes a useful tool to study analytically Eq. (36). If we assume that the functions $\varphi_\lambda(\vec{n})$ are smooth enough, we can expand $\varphi_\lambda(\vec{m}-\vec{a}_\mu)$ as a Taylor series and obtain a differential equation. But there is also another way to go to the continuum limit. Let us introduce the following functions of the continuum variable $\vec{r}$:

$$\varphi_{\lambda}(\vec{r})=\frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{k}} \varphi_{\lambda}(\vec{k})e^{i\vec{k}\vec{r}}, \tag{40}$$

where $\vec{r}$ is a vector with D components x_μ measured in units of lattice spacing. Note that at $\vec{r}=\vec{m}$ these functions coincide with the functions in the site representation (34), and for Eq. (40) we have[23]

$$\varphi_\lambda(\vec{k})=\frac{1}{\sqrt{}}$$

$$\omega_q^2 = v_0^2\left(q^2 - \frac{1}{12}q^4 + \cdots\right). \tag{51}$$

In this approximation, we can easily consider also a nonzero velocity. From above, we obtain the following expression for the function $G(q)$ (32):

$$G(q) = 2Jg\left(1 - \frac{\alpha}{12}q^2 + \cdots\right), \tag{52}$$

where

$$g = \frac{g_0}{1-s^2}, \quad \alpha = \frac{3-4s^2}{1-s^2}, \quad s^2 = \frac{v^2}{v_0^2}. \tag{53}$$

Note that the second term in Eq. (53) arises as a result of the second terms in the expansions of ω and $\sin(q)$ in Eq. (32). Restricting our attention to the first terms of expansions, gives us, according to Eqs. (43) and (44), the following equation:

$$J\frac{d^2\varphi_\lambda(x)}{dx^2} + i\hbar v\frac{d\varphi_\lambda(x)}{dx} + 2Jg\Phi(x)\varphi_\lambda(x) = \mathcal{E}_\lambda\varphi_\lambda(x), \tag{54}$$

where

$$\Phi(x) = \sum_\lambda n_\lambda|\varphi_\lambda(x)|^2. \tag{55}$$

As one can easily see, in the case of one or two electrons in the ground state, only one adiabatic level is occupied with the occupation number (30) $n_g = 1$ or 2, respectively. Therefore, the corresponding wave function satisfies NLSE,

$$J\frac{d^2\varphi_g(x)}{dx^2} + i\hbar v\frac{d\varphi_g(x)}{dx} + 2Jg|\varphi_g(x)|^2\varphi_g(x) = \mathcal{E}_g\varphi_g(x). \tag{56}$$

The general solution of Eq. (56) is a hyperbolic secant which describes a soliton propagating along the chain. Taking into account the normalization condition for the function $\varphi_g(x)$, we can calculate the eigenenergy (29) of such a localized state and we find

$$\mathcal{E}_g = \frac{Jg^2}{4}. \tag{57}$$

Note that in the case of two electrons the parameter g in Eqs. (56) and (57) has to be substituted by $2g$. In the case of many electrons, the system is governed by a many component, NLSE, which admits exact solutions for few-electron states[21] and for an arbitrary concentration of electrons.[25] Taking into account the fourth-order terms in the expansion [Eqs. (51) and (52)] leads to the following form of the stationary MNLSE:

$$J\frac{d^2\varphi_g(x)}{dx^2} - \frac{J}{12}\frac{d^4\varphi_g(x)}{dx^4} + 2Jg|\varphi_g(x)|^2\varphi_g(x) + \frac{Jg}{2}\left(\frac{d^2}{dx^2}|\varphi_g(x)|^2\right)\varphi_g(x) = \mathcal{E}_g\varphi_g(x). \tag{58}$$

In the limit of the long-wave approximation, the term $d^4\varphi_g(x)/dx^4$ is very small and it can be neglected. Equation (58) then becomes the MNLSE with $\alpha = 3$. This shows that the differential equation obtained using the long-wave approximation is the same as the one obtained in the continuum limit after the exact evaluation of the kernel function (49).

V. TWO-DIMENSIONAL CASE

Let us consider now a two-dimensional lattice and, for simplicity, look for its static solution, $\vec{v} = 0$, with one or two electrons. The equations for a soliton and bisoliton will coincide, the only difference is the multiplier $2g$ for a bisoliton instead of g for a soliton or, equivalently, the bisoliton normalization condition (35) should be $N = 2$ instead of $N = 1$.

From Eq. (32) we get the expression for the function G,

$$G(\vec{q}) = \frac{\chi^2}{4Mv_0^2}\frac{\sin^2(q_x) + \sin^2(q_y)}{\sin^2\frac{q_x}{2} + \sin^2\frac{q_y}{2}} \tag{59}$$

and, in principle, we can proceed as before, i.e., calculate $F(\vec{m} - \vec{n})$. This involves performing the summation

$$S_{\vec{n},\vec{m}} = \sum_{q_x,q_y}\frac{\sin^2(q_x) + \sin^2(q_y)}{\sin^2\frac{q_x}{2} + \sin^2\frac{q_y}{2}}e^{-i\vec{q}(\vec{n}-\vec{m})}. \tag{60}$$

Unfortunately, this cannot be done in a closed form even in the continuum limit. On the other hand, we can evaluate Eq. (60) numerically or use the long-wave approximation as in the one-dimensional case where this approximation has given very reliable results.

The numerical evaluation of (60) shows that $S_{\vec{n},\vec{m}}$ is a decreasing function of the distance $|\vec{n} - \vec{m}|$ and that it is essentially nonzero only when the vector $(\vec{n} - \vec{m})$ is parallel to the lattice axes as it is very small when the vector is aligned along the lattice diagonals. Taking this into account (i.e., keeping only the contributions along the axes), we obtain the following discrete version of the two-dimensional (2D) MNLSE:

$$E_L\varphi_g(\vec{n})-J\sum_{\mu}\left[\varphi_g(\vec{n}+\vec{a}_\mu)+\varphi_g(\vec{n}-\vec{a}_\mu)\right]-2Jg_0\Big\{|\varphi_g(\vec{n})|^2+\frac{1}{5}\sum_{\mu}\Big[(|\varphi_g(\vec{n}+\vec{a}_\mu)|^2+|\varphi_g(\vec{n}-\vec{a}_\mu)|^2)-\frac{3}{8}(|\varphi_g(\vec{n}+2\vec{a}_\mu)|^2$$
$$+|\varphi_g(\vec{n}-2\vec{a}_\mu)|^2)-\frac{1}{4}(|\varphi_g(\vec{n}+3\vec{a}_\mu)|^2+|\varphi_g(\vec{n}-3\vec{a}_\mu)|^2)+\cdots\Big]\Big\}\varphi_g(\vec{n})=\mathcal{E}_g\varphi_g(\vec{n}). \quad (61)$$

If we now take the continuum limit of Eq. (61), in the nearest-neighbor approximation, we recover Eq. (1) with $\alpha=4/3$.

As the long-wave approximation leads to good results for the one-dimensional case, we can try to use it here too and approximate the function $G(\vec{q})$ by the following expression:

$$G(\vec{q})\approx 2Jg_0\frac{q_x^2+q_y^2-\frac{1}{3}(q_x^4+q_y^4)}{q_x^2+q_y^2-\frac{1}{12}(q_x^4+q_y^4)}$$
$$\approx 2Jg_0\left(1-\frac{1}{4}w^2+O(w^4)\right), \quad (62)$$

where

$$w^2=\frac{q_x^4+q_y^4}{q_x^2+q_y^2}=q^2-\frac{2q_x^2q_y^2}{q^2}, \quad q^2=q_x^2+q_y^2. \quad (63)$$

Taking into account the results of the numerical calculation of Eq. (60), we approximate the function $G(\vec{q})$ in Eq. (62) by the expression

$$G(\vec{q})\approx 2Jg_0\left(1-\frac{1}{4}q^2+O(g^4)\right). \quad (64)$$

Substituting this into Eq. (61) we obtain, in the continuum limit, the following form of the MNLSE:

$$J\Delta\varphi_g(\vec{r})+2Jg_0|\varphi_g(\vec{r})|^2\varphi_g(\vec{r})+\frac{1}{2}Jg_0(\Delta|\varphi_g(\vec{r})|^2)\varphi_g(\vec{r})$$
$$=\mathcal{E}_g\varphi_g(\vec{r}), \quad (65)$$

where $\vec{r}$ is the two-dimensional vector in the plane (x,y) and Δ is the two-dimensional Laplacian in the Cartesian coordinate system. The generalization of this equation to higher dimensions is straightforward. Comparing Eq. (65) with Eq. (1) we see that $\alpha=3$. This result confirms the results obtained within the semiclassical approach, which were analyzed in detail in Refs. 4,6 (see also Ref. 19).

Solutions

The solutions of Eq. (1) where studied in detail in Ref. 6. First, it was shown that one can rescale the equation and set $\alpha=1$. The localized solutions were then computed numerically and it was shown that they exist only for certain values of the parameter g. In two dimensions, the stationary localized solutions exist only when $g>g_c\approx 5.85$. The solution of the full system of discrete equations for the electron-phonon lattice was studied in Ref. 4. There it was shown that the stationary localized solution existed only when the coupling constant g was larger than a critical value g_c and it was found numerically that, again, $g_c\approx 5.85$. The fact that critical values of g_c, for both the system of discrete equations and the MNLSE, coincide is not surprising as we have shown that the MNLSE is the continuum limit of the electron-phonon system; when g is slightly larger than g_c, the soliton is very broad and the continuum approximation is very reliable.

In Fig. 1, we show the inverse radius of the soliton, $1/R$, as a function of g for the solution of the MNLSE and of the full electron-phonon system of discrete equations in 2D. Here R is defined as

$$R^2=\sum_{n,m}(n^2+m^2)|\varphi(n,m)|^2=\int d\vec{r}|\vec{r}|^2|\varphi(\vec{r})|^2. \quad (66)$$

One notes that near the critical value of g_c, the solutions are broad and very similar in size. When g increases, the solutions become narrower and the continuum approximation becomes less reliable and finally breaks down. Hence, for larger values of g, the solutions of the two systems become different from each other as one would expect.

In Fig. 2, we present the modulus of the solution of the full system of discrete equations. One notes that the electron density looks radially symmetric.

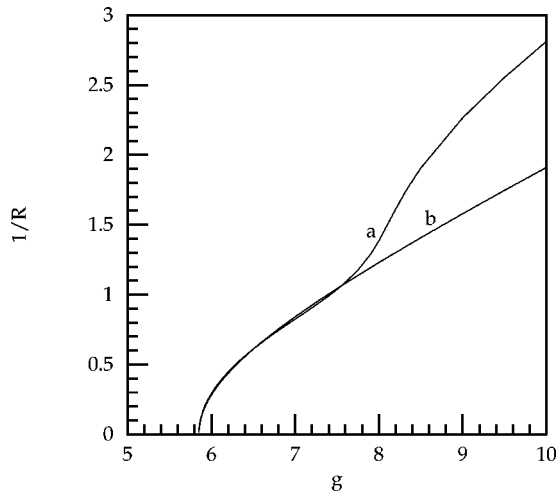

FIG. 1. Inverse radius of localization, $1/R$, as a function of g: (a) Numerical solution of the full system of discrete equations (Ref. 4), (b) Eq. (1) at $\alpha=1$.

VI. NONADIABATIC CORRECTIONS

To calculate the nonadiabatic corrections in Eq. (25), we consider a one-electron case described in the zero adiabatic approximation by the vector state

$$|\psi_0\rangle = a^{\dagger}_{\sigma,g}|0_e\rangle|0_{ph}\rangle. \tag{67}$$

Considering the nonadiabatic term of the Hamiltonian $\mathcal{H}_1$ as a perturbation, the first-order correction to the state vector is given by

$$|\psi_1\rangle = \frac{1}{E-\mathcal{H}_0}\mathcal{H}_1|\psi_0\rangle, \tag{68}$$

and the corresponding energy correction is given by

$$E_2 = \langle\psi_0|\mathcal{H}_1\frac{1}{E_0-\mathcal{H}_0}\mathcal{H}_1|\psi_0\rangle. \tag{69}$$

Here $E_0 = E_g + W$, and in the operator $\mathcal{H}_0$ determined in Eq. (22), the lattice distortion is taken in form Eq. (28).

The norm of the total state reads as

$$\langle\psi|\psi\rangle = \langle\psi_0|\psi_0\rangle + \langle\psi_1|\psi_1\rangle + \cdots = 1 + O(\varepsilon^2). \tag{70}$$

Nonadiabatic corrections are small, provided that

$$\langle\psi_1|\psi_1\rangle = \langle\psi_0|\mathcal{H}_1\frac{1}{(E_0-\mathcal{H}_0)^2}\mathcal{H}_1|\psi_0\rangle \approx \varepsilon^2 \ll 1. \tag{71}$$

It is convenient to introduce the operator

$$\hat{Q} = \int_0^{\infty}\exp\{i(E_0-\mathcal{H}_0+i\epsilon)t\}dt$$

$$= \frac{\epsilon}{(E_0-\mathcal{H}_0)^2+\epsilon^2} + i\frac{E_0-\mathcal{H}_0}{(E_0-\mathcal{H}_0)^2+\epsilon^2}. \tag{72}$$

Then we see that

$$E_2 = \lim_{\epsilon\to 0}\mathrm{Im}\langle\hat{Q}\rangle, \quad \langle\psi_1|\psi_1\rangle = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\mathrm{Re}\langle\hat{Q}\rangle, \tag{73}$$

where

$$\langle\hat{Q}\rangle = \langle\varphi_1|\hat{Q}|\varphi_1\rangle \tag{74}$$

is the expectation value of the operator $\hat{Q}$ on the state

$$|\varphi_1\rangle = \mathcal{H}_1|\psi_0\rangle. \tag{75}$$

Taking into account the explicit form of the nonadiabatic part of the Hamiltonian (23), we find from Eq. (75)

$$|\varphi_1\rangle = \frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q},\lambda\neq g} f^{*}_{g,\lambda}(\vec{q})b^{\dagger}_{\vec{q}}a^{\dagger}_{\sigma,\lambda}|0_e\rangle|0_{ph}\rangle. \tag{76}$$

Using the operator definition (72), (22), and (76), we can calculate Eq. (74) and obtain

$$\langle\hat{Q}\rangle = \frac{1}{\mathcal{N}}\sum_{\vec{q},\vec{q}',\lambda\neq g} f^{*}_{g,\lambda}(\vec{q})f_{g,\lambda}(\vec{q}\,') \times \int_0^{\infty} e^{-i(E_\lambda - E_0 - i\epsilon)t}dt\langle 0_{ph}|b_{\vec{q}'}e^{-i\tilde{H}_{ph}t}b^{\dagger}_{\vec{q}}|0_{ph}\rangle. \tag{77}$$

Here

$$\tilde{H}_{ph} = \sum_{\vec{q}}\hbar\omega_{\vec{q}}b^{\dagger}_{\vec{q}}b_{\vec{q}} - \frac{1}{\sqrt{\mathcal{N}}}\sum_{\vec{q}}[F_g(\vec{q}) - F_\lambda(\vec{q})](b_{\vec{q}} + b^{\dagger}_{-\vec{q}}). \tag{78}$$

The correlation function

$$\mathcal{G}_\lambda(\vec{q},\vec{q}\,';t) = \langle 0_{ph}|b_{\vec{q}'}e^{-i\tilde{H}_{ph}t}b^{\dagger}_{\vec{q}}|0_{ph}\rangle, \tag{79}$$

$$\mathcal{G}_\lambda(\vec{q},\vec{q}';t)=e^{iW_\lambda t-Z_\lambda(t)}\Big[e^{-i\hbar\omega_{\vec{q}}t}\delta_{\vec{q},\vec{q}'}+\frac{1}{\mathcal{N}}f_\lambda(\vec{q})f_\lambda^*(\vec{q}')$$

$$\times(1-e^{-i\hbar\omega_{\vec{q}}t})(1-e^{-i\hbar\omega_{\vec{q}'}t})\Big], \tag{84}$$

where

$$Z_\lambda(t)=\frac{1}{\mathcal{N}}\sum_{\vec{q}}|f_\lambda(\vec{q})|^2(1-e^{-i\hbar\omega_{\vec{q}}t}). \tag{85}$$

Substituting Eq. (84) into Eq. (77), we obtain the following result:

$$\langle\hat{Q}\rangle=\frac{1}{\mathcal{N}}\sum_{\vec{q},\lambda\neq g}|f_{g,\lambda}(\vec{q})|^2\int_0^\infty e^{-i(E_\lambda+\hbar\omega_{\vec{q}}-E_g-W_\lambda-i\epsilon)t-Z_\lambda(t)}dt$$

$$+\frac{1}{\mathcal{N}^2}\sum_{\vec{q},\vec{q}',\lambda\neq g}f_{g,\lambda}^*(\vec{q})f_\lambda(\vec{q})f_{g,\lambda}(\vec{q}')f_\lambda^*(\vec{q}')$$

$$\times\int_0^\infty e^{-i(E_\lambda-E_g-W_\lambda-i\epsilon)t-Z_\lambda(t)}$$

$$\times(1-e^{-i\hbar\omega_{\vec{q}}t})(1-e^{-i\hbar\omega_{\vec{q}'}t})dt. \tag{86}$$

We see that our result is quite complicated as it involves various sums and integrations. In fact, our expression is typical of those that arise when one studies many-phonon processes. The corresponding calculations are not easy and one has to resort to various approximation schemes. Here we note that the second integral in Eq. (86) is small and so we can use the following approximation:

$$Z_\lambda(t)\approx -iW_\lambda t. \tag{87}$$

Thus, from Eq. (77) and relations (73), we obtain

$$E_2=-\frac{1}{\mathcal{N}}\sum_{\vec{q},\lambda\neq g}\frac{|f_{g,\lambda}(\vec{q})|^2}{E_\lambda+\hbar\omega_{\vec{q}}-E_g}, \tag{88}$$

$$\langle\psi_1|\psi_1\rangle=\frac{1}{\mathcal{N}}\sum_{\vec{q},\lambda\neq g}\frac{|f_{g,\lambda}(\vec{q})|^2}{(E_\lambda+\hbar\omega_{\vec{q}}-E_g)^2}. \tag{89}$$

We conclude that the adiabatic approximation is valid provided Eq. (89) is small.

Substituting Eq. (19) in Eq. (89), we rewrite the condition of applicability of the adiabatic approximation in the form of the inequality:

$$\langle\psi_1|\psi_1\rangle=\frac{1}{2\mathcal{N}}\sum_{\vec{q},\lambda\neq g}\frac{G(\vec{q})\hbar\omega_{\vec{q}}|J_{g,\lambda}(\vec{q})|^2}{(E_\lambda+\hbar\omega_{\vec{q}}-E_g)^2}\ll 1, \tag{90}$$

where

$$J_{g,\lambda}(\vec{q})=\int e^{i\vec{q}\vec{r}}\varphi_g^*(\vec{r})\varphi_\lambda(\vec{r})d\vec{r}. \tag{91}$$

To evaluate the energy correction, one thus needs the

$$\langle\psi_1|\psi_1\rangle \leqslant \frac{1}{\mathcal{N}}\sum_{\vec{q}} \frac{Jg\hbar\omega_{\vec{q}}|J_{g,\vec{k}=0}(\vec{q})|^2}{(\mathcal{E}_g+\hbar\omega_{\vec{q}})^2}+\mathcal{F}_b$$

$$\leqslant \frac{Jg\hbar\omega_{q=\beta\kappa}}{(\mathcal{E}_g+\hbar\omega_{q=\beta\kappa})^2}\frac{1}{\mathcal{N}}\sum_{\vec{q}}|J_{g,\vec{k}=0}(\vec{q})|^2+\mathcal{F}_b, \tag{96}$$

where $\mathcal{F}_b$ is the part of sum (89) determined by possible excited bound states.

Note, the sum in the last expression can be rewritten as $\Sigma_{\vec{n}}|\varphi_g(\vec{n})|^2|\varphi_{\vec{k}}(\vec{n})|^2\approx 1$ due to the fact that $|\varphi_{\vec{k}}(\vec{n})|^2\approx 1$ and due to the normalization condition of the function $\varphi_g(\vec{n})$. Finally, at small values of the parameter γ, the condition of applicability of the adiabatic approximation takes the form

$$\langle\psi_1|\psi_1\rangle \leqslant C\frac{Jg\hbar v_0\kappa}{\mathcal{E}_g^2}<1, \tag{97}$$

where C is some numerical constant.

In the 1D case $\mathcal{E}_g$ was given by Eq. (57) and, when $\kappa=g/2$, we recover Eq. (94). In the 2D case, according to (Ref. 4), the energy $\mathcal{E}_g=J\kappa^2$ and the localization parameter $\kappa^2=6(g-g_{cr})/(\alpha I_0)$, where $g_{cr}=5.85, I_0=9.8$, and α is a parameter in MNLSE (1). Substituting these results in Eq. (97), we obtain

$$C\left(\frac{I_0\alpha}{6}\right)^{3/2}\frac{\gamma g}{(g-g_{cr})^{3/2}}\ll 1, \tag{98}$$

or, equivalently,

$$\left(\frac{g-g_{cr}}{g}\right)^3 g>C'\gamma^2\alpha^3. \tag{99}$$

Thus, we conclude that the adiabatic approximation is valid at strong enough electron-phonon coupling. Near the critical value we thus have $g-g_{cr}>C'\alpha^3 g_{cr}^2\gamma^2$, and taking $C'\approx 10$ and $\alpha\approx 2$ we have $g-g_{cr}>3400\gamma^2$. If $\gamma=0.001$, then the adiabatic approximation is valid for values of g very near the critical value g_{cr}, while for $\gamma=0.01$ it can still be used but only for, roughly, $g>6.2$.

Examples of two-dimensional compounds in which the adiabatic approximation is valid, are given by the doped crystals of tungsten oxide (WO_3), such as WO_{3-x},[3] and the monophosphate tungsten bronzes (MPTB) $(PO_2)_4(WO_3)_{2m}$ with alternate stacking of m WO_3 layers.[27] The insulating oxide WO_3 corresponds to the limit of infinite m for the MPTB series. Both classes of substances posses 2D transport properties. In particular, the parameter values for the tungsten oxide are $\hbar\omega=0.07$ eV (Ref. 28) and $J=0.3$–0.5 eV. The *ab initio* band-structure calculation for MPTB (Ref. 27) shows that the bandwidth is ≈ 2 eV, i.e., $J\approx 0.5$ eV. Similar values of the bandwidth have been found in the *ab initio* calculation of the electronic structure of the regular $m=4$ member.[29] Therefore, for this class of compounds $\gamma\approx 10^{-3}$–10^{-2}, which means that in these compounds the adiabatic approximation is valid. This is in agreement with the conclusion that the transport properties of some structural phases of WO_{3-x} are determined by large polarons,[3] and that MPTB crystals exhibit charge density waves instabilities.[27]

VII. CONCLUSION

We have shown that, within the adiabatic approximation, the system of equations that describes a lattice with an electron-phonon interaction can be reduced in a self-consistent way to the nonlocal nonlinear equation (43). For the electron-phonon interaction, given by Eq. (46), this equation reduces, in the long-wave approximation, to the D-dimensional MNLSE (65). Such types of equations arise also in many other physical systems: in nonlinear optics,[15] plasma,[19] photonic crystals,[30,31] electromagnetic energy propagation in superlatices,[32,33] etc. In our previous papers, this latter equation has been shown to admit soliton-type localized solutions which are stable against shrinking and/or dispersion. These solutions exist within a certain range of the values of the nonlinear electron-phonon coupling constant g which depends on the dimensionality of the system. In particular, the variational study of this equation for $D\geqslant 2$ has been carried out in (Ref. 6), where it has been shown that there is a threshold for the stability of localized solutions, $g>g_c$, and that all two-dimensional localized solutions are stable and their total energy is negative. Moreover, Eq. (65) in the 2D case has stationary solutions with a nonzero angular momentum. These results are confirmed by our numerical calculations.

The stabilizing role of the extra terms that arise when the nonlocal nonlinear interactions are taken into account, the interplay between these terms, and the short-range dispersive interactions are important questions. These problems have been discussed also in Refs.[10,19] and some other papers.

We have also calculated the nonadiabatic corrections and estimated the conditions for the applicability of the adiabatic approximation in the one- and two-dimensional cases. We have found that the adiabatic approximation is valid at not very large values of the nonadiabaticity parameter $\gamma\leqslant 1$ (i.e., in systems with broad electron conducting band as compared to the characteristic phonon frequency) and at strong enough electron-phonon coupling.

In future work, we plan to extend our approach to model nanotubes using hexagonal lattices.

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