Variational Approximation to Electron Trapping by Soliton-Like Localized Excitations in One-Dimensional Anharmonic Lattices

Luis A. Cisneros-Ake, Antonmaria A. Minzoni, and Manuel G. Velarde

Abstract Electron trapping by soliton-like (traveling) localized excitations in one-dimensional anharmonic lattices is discussed with particular emphasis on the case of an initially completely delocalized electron.

1 Introduction

Let us consider a one-dimensional (1d) lattice with units interacting with anharmonic interactions. Then for appropriate anharmonic interactions it can be shown that the lattice can exhibit traveling solitary waves or periodic nonlinear waves, with soliton features as defined by Zabusky and Kruskal [1]. One particular such lattice is the Toda lattice where interactions are of exponential form for the repulsive component [2]. Its soliton solutions are known exactly as the system is integrable.

For our purpose here we shall consider Morse interactions [3] which are not significantly different from Toda's in their repulsive component while offering a physically justified attractive component. The latter is physically meaningless in the Toda case. Moreover, though the Morse lattice is non-integrable its computer

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solutions differ little from the solutions of the Toda lattice [4–6] and hence we shall benefit from such significantly useful approximation. Little has been established about the quantization of the Toda or other anharmonic lattices and, moreover, for the purpose of our present communication it is not needed here.

The next item to be introduced in our mathematical model is an electron. As a quantum mechanical object, its (space and time) evolution obeys the corresponding (linear) Schrödinger equation. We shall consider the electron evolution on a lattice using the tight binding approximation (TBA) . If we disregard the lattice dynamics and hence consider a free evolving electron on the discrete lattice space, if we place it at a given site with maximum probability density, then as time proceeds the electron probability density spreads "uniformly" all over the lattice sites though the probability remains normalized to unity. Such delocalization of the electron can be considered as a form of "dust", tiny spots on the lattice sites.

The electron-phonon interaction or, in more general terms the electron-lattice dynamics interaction, is nonlinear and eventually is an exponential nonlinearity [7,8]. Having in mind electron (charge) transfer processes in biomolecules, Davydov [9] was able, using suitable approximations, to reduce the electron-lattice phonon dynamics to soliton-bearing evolution equations. Then he was able to show that the real electric carrier was the compound he called electrosoliton . Unfortunately there is numerical evidence that such electrosolitons do not survive beyond 10 K. This temperature is far from physiological temperatures ca. 300 K [10–13].

Recently, the electron-lattice dynamics was considered for anharmonic (Toda, Morse, etc.) lattices [14–16]. Then the mixed quantum-classical (electron-lattice) evolution problem possesses two distinct nonlinearities. On the one hand, there is the electron-lattice interaction and, on the other hand, we have the lattice intrinsic anharmonicity . The latter already offers a soliton carrier and hence the compound electrosoliton (Davydov concept generalized to anharmonic lattices) together with the lattice soliton defines a dynamic (space and time evolving) bound state of an electron to a lattice soliton which is a new electron (charge) carrier that has been denoted solectron [17]. Thus the latter concept (and quasiparticle) appears as a natural generalization of the original (Landau-Pekar) polaron (for harmonic lattices) and the (Davydov) electrosoliton (also for harmonic lattices) to the case of initially anharmonic lattices, with, let us emphasize it, the genuinely new ingredient of offering a possible charge carrier before injecting, e.g., the electron. Davydov and Zolotaryuk and colleagues also elaborated some results about the same concept including supersonic motions [9, 18–20].

One interesting feature and the motivation for this communication is the following. It has been shown that placing an electron, using TBA, at any lattice site, and a soliton at the same or at another lattice site, as time proceeds the electron is eventually trapped and transported (electron surfing) by the lattice soliton. Moreover, if as noted above the electron is completely delocalized in the lattice as probability density "dust" spots, following Schrödinger equation alone, then as soon as the electron-lattice soliton is switched-on the latter is able to gather the electron probability density thus "reconstruding" the electron (or better said, its maximum probability density) around the soliton itself and trapping it with

subsequent transport, as the soliton is a (generally) supersonic, always moving localized excitation. This phenomenon has been denoted as the "vacuum cleaner effect" [14, 15]. The above phenomena have been shown to occur for temperatures from zero K up to the physiological range (ca. 300 K; for materials other than biomolecules the actual temperature range may be different) [21].

In the present communication we take up the problem from a variational perspective starting with the Lagrangian embracing coupled together the lattice classical dynamics and the quantum (discrete) Schrödinger electron dynamics in the tight binding approximation.

2 Formulation of the Problem and Numerical Results

Let us consider a 1d lattice of N units all with equal mass, M, and interacting with a Morse potential [3] (like equal massless springs operating beyond Hooke's linear elasticity), to which an excess electron is added as a Gaussian probability density centered at site n. Having in mind the TBA the function $c_n(t)$ (or better said $|c_n|^2$) gives the probability of finding the electron at site n, while the function $\xi_n(t)$ gives the distortion of the lattice caused by the polarization of lattice atom-units. The model assumes a hopping probability from site n to site $n+1$ of the form $e^{\alpha(\xi_{n+1}-\xi_n)}$ [7,8]. The coupling parameter α is determined by a quantum mechanical calculation and can in principle be modified by the further electron doping of the material. In this case we will have α to be a given function of site the n, that is $\alpha = \alpha(n)$, which describes the doping. Clearly, such n-dependent coupling between the lattice and the electron changes the probability of hopping. In its absence this probability does not depend on the lattice deformation and the deformation just acts as a trapping potential. The model Lagrangian is given in the form:

$$\begin{aligned} L = &\sum_{n=-\infty}^{\infty} \tfrac{1}{2}\tfrac{p}{V_0}\dot{q}_n^2 + \tfrac{i}{2}\left(\dot{c}_n c_n^* - \dot{c}_n^* c_n\right) \\ &+ p e^{\alpha(q_{n-1}-q_n)}\left(c_{n-1}c_n^* + c_{n-1}^* c_n\right) - \tfrac{p}{2V_0}\left(1 - e^{q_{n-1}-q_n}\right)^2, \end{aligned} \tag{1}$$

where we set

$$\begin{aligned} \xi_n &= \tfrac{1}{\beta} q_n, \quad \tau = \omega_M t = t\sqrt{\tfrac{2D\beta^2}{M}}, \\ \tilde{\alpha} &= \tfrac{\alpha}{\beta}, \quad \tilde{V}_0 = \tfrac{V_0}{2D}. \end{aligned}$$

The quantities β and D parameterize the Morse lattice. V_0 and α account for electron-lattice coupling strength and their tilde has been removed from (1) in the new variables for practical purposes. According to the physical values [9–11,22,23] the non dimensional parameter $p = 2D\tilde{V}_0/(\hbar\omega_M) = V_0/(\hbar\omega_M) \approx 10$ is the ratio between the electronic and mechanical time scales.

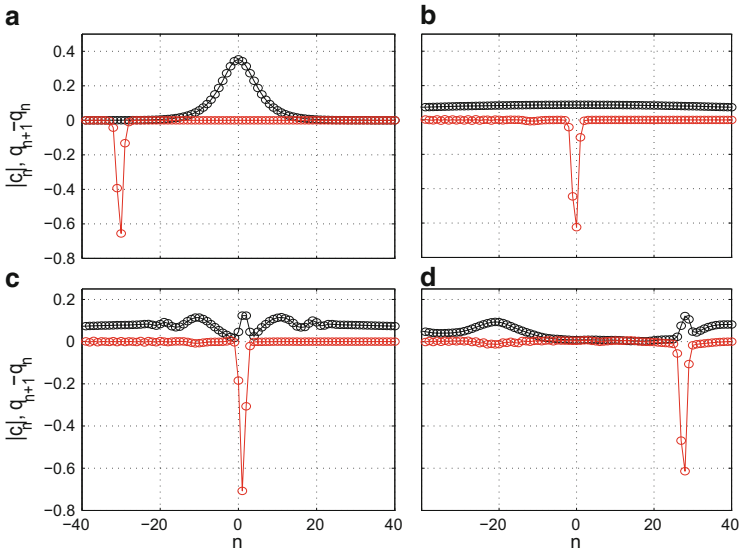

Fig. 1 Numerical evolution of system (2) and (3) for $w = 4$, $v = 0$, $\phi = 0$, $\xi_0 = 0$ and $k = 1.35$, $A = 0.29$, $\xi_1 = -30$, $\xi = 1.5$. Parameter values: $V_0 = 0.5$, $p = 10$ $\alpha = 0$ for $t \leq 20$ and $\alpha = 1.75$ for $t > 20$ in (**a**) $t = 0$, (**b**) $t = 20$, (**c**) $t = 21$ and (**d**) $t = 40$ (*red lines*: soliton; *black lines*: electron)

We thus obtain from (1), and its associated Euler-Lagrange equations , the corresponding non dimensional equations of motion in the form:

$$\frac{dc_n}{d\tau} = ip\left(e^{\alpha(q_{n-1}-q_n)}c_{n-1} + e^{\alpha(q_n-q_{n+1})}c_{n+1}\right), \tag{2}$$

$$\begin{aligned}\frac{d^2q_n}{d\tau^2} &= \left(1-e^{q_n-q_{n+1}}\right)e^{q_n-q_{n+1}} - \left(1-e^{q_{n-1}-q_n}\right)e^{q_{n-1}-q_n} \\ &+\alpha V_0\left[\left(c_{n+1}c_n^* + c_{n+1}^*c_n\right)e^{\alpha(q_n-q_{n+1})}\right. \\ &\left.-\left(c_{n-1}c_n^* + c_{n-1}^*c_n\right)e^{\alpha(q_{n-1}-q_n)}\right].\end{aligned} \tag{3}$$

In Refs. [14, 15] the authors considered as initial condition both a localized and a delocalized electron separated from a (supersonic) compression wave (a localized soliton-like excitation) which was allowed to travel along the lattice. The computer experiment starts with α set to zero, hence no interaction between electron and lattice dynamics. By the time the compression wave reaches the center of the lattice the original electron Gaussian distribution has decreased to 25 % of the original amplitude before α is switched to a nonzero value. Very rapidly a coherent compound localized structure is formed from the small amplitude delocalized electron wave function, which is swept away by the compression wave (Fig. 1). This is the above mentioned "vacuum cleaner effect". In Fig. 1 we reproduce this

process which was obtained integrating numerically Eqs. (2) and (3) with initial conditions:

$$c_n(0) = A\,\mathrm{sech}\left(\frac{n-\xi}{w}\right)\exp\left[i\phi + iv\,(n-\xi_0)\right], \tag{4}$$

$$q_n(0) = \ln\frac{1+e^{2k(n-1-\xi_1)}}{1+e^{2k(n-\xi_1)}}, \tag{5}$$

thus confirming the results of [14, 15]. Note the solectron detaching from the background in Fig. 1c.

It was shown in [16] that the equations

$$i\frac{dc_n}{d\tau} = \mu\,(q_{n+1}-q_n)\,c_n - p\,(c_{n+1}+c_{n-1}), \tag{6}$$

$$K\frac{d^2q_n}{d\tau^2} = (q_{n-1}-2q_n+q_{n+1})\,(1-\beta\,(q_{n+1}-q_{n-1})) + \mu\left(|c_n|^2-|c_{n-1}|^2\right), \tag{7}$$

which are the Davydov analog to (2) and (3) with cubic anharmonicity in the lattice [9], have supersonic (generalized) polaron solutions similar in shape to the ones of (2) and (3) shown in Fig. 1. A similar "vacuum cleaner effect" was observed integrating (6) and (7) using same initial condition as (4) and a similar condition as (5) in the form:

$$q_n(0) = \frac{B}{2}\left[1-\tanh\left(\frac{n-\frac{1}{2}-\xi}{w}\right)\right].$$

Typical results found for a wide range of parameter values and initial conditions (4) and (5) are displayed in Figs. 2–5. We first consider the possibility of vacuum cleaning for the (linear) Davydov model ($\beta = 0$). In Fig. 2 we observe the formation of a right-to-left moving polaron due to the large Peierls-Nabarro (PN) potential (a signature of the lattice discreteness) which stops the left-to-right going waves. The PN potential is obtained at second order approximation in the Poisson summation formula. It is proportional to $\sinh^{-1}(\pi^2/k)$ for Morse interactions and $\sinh^{-1}(\pi^2/w)$ for cubic anharmonicities, according to the wave profile initial conditions (i.c.). PN terms raise due to the discreteness and non-integrability of a problem. In Fig. 3 we show the evolution of the initial conditions and we see no polaron formation but rather a bouncing back of the electron wave function caused by the peaks in the potential. In Fig. 4, very weak vacuum cleaning occurs as compared to the TBA. In Fig. 5 we see new phenomena where the interaction produces a left-to-right traveling compression and a right-to-left moving localized structure. This is due to the fact that for $p = 1$ there is a stronger PN potential which prevents the compression wave trapping process. In the supersonic case solectron formation is found.

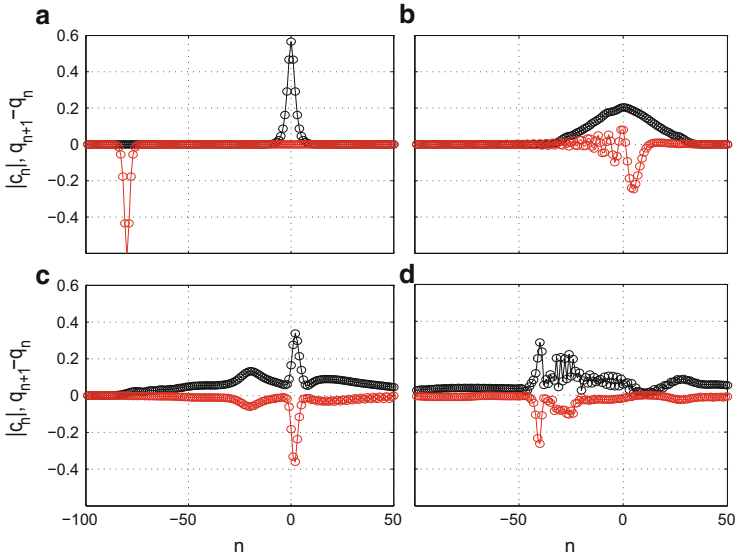

Fig. 2 Numerical evolution of system (6) and (7) for the harmonic (linear) lattice $\beta = 0$ and $p = 1$. The coupling parameter μ is switched on at $t = 14$ from 0 to 1.75. Wave parameter values: $B = 2$, $w = 1.56$, $v = 0$ and $\dot{\xi} = 1$. (**a**) $t = 0$, (**b**) $t = 15$, (**c**) $t = 40$ and (**d**) $t = 70$ (*red lines*: soliton; *black lines*: electron)

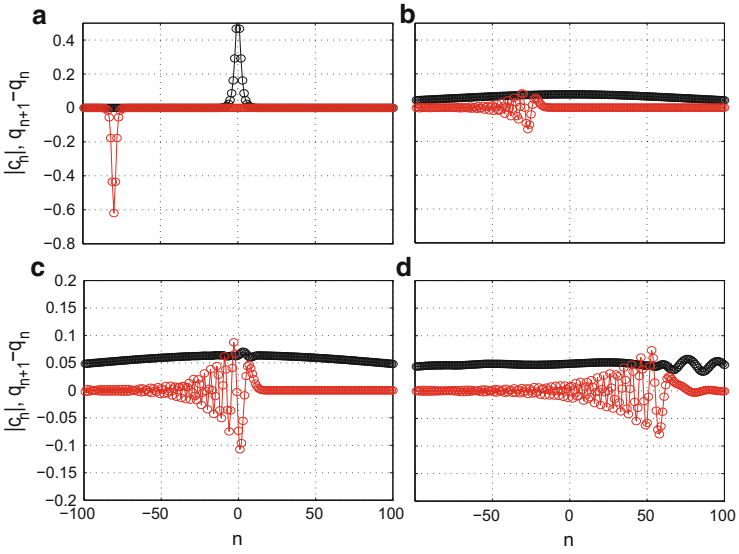

Fig. 3 Numerical evolution of system (6) and (7) for the harmonic (linear) lattice $\beta = 0$ and $p = 10$. The coupling parameter μ is switched on at $t = 14$ from 0 to 1. Wave parameter values as in Fig. 2: (**a**) $t = 0$, (**b**) $t = 15$, (**c**) $t = 25$ and (**d**) $t = 35$ (*red lines*: soliton; *black lines*: electron)

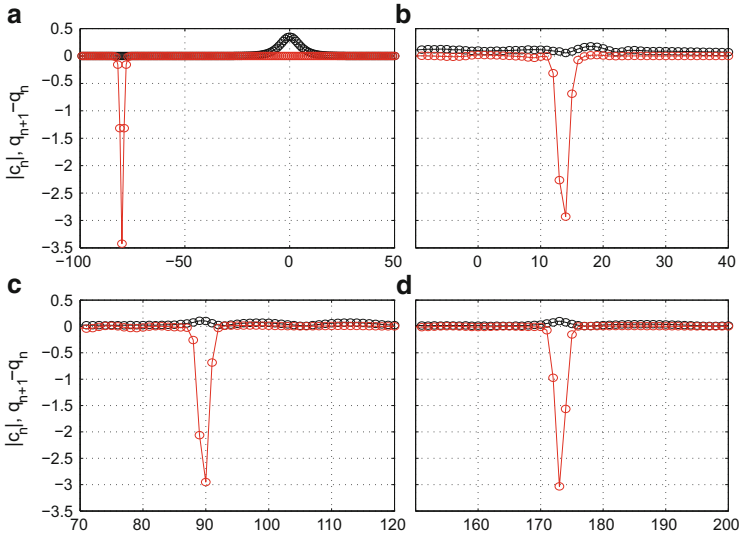

Fig. 4 Numerical evolution of system (6) and (7) for the anharmonic lattice $\beta = 0.5$ with $p = 10$. The coupling parameter μ is switched on at $t = 10$ from 0 to 1.75. Wave parameter values: $B = 6.407$, $w = 0.8385$, $\eta = 4$, $v = 0$ and $\dot{\xi} = 8.48$. (**a**) $t = 0$, (**b**) $t = 11$, (**c**) $t = 20$ and (**d**) $t = 30$ (*red lines*: soliton; *black lines*: electron)

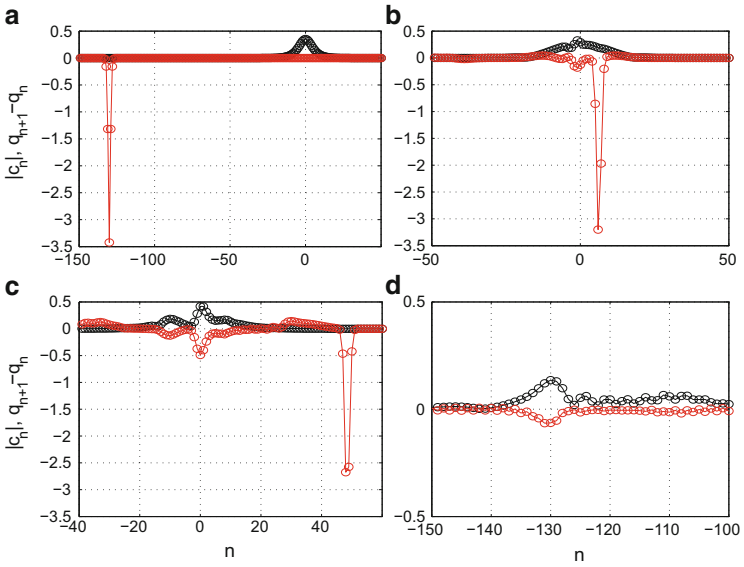

Fig. 5 Numerical evolution of system (6) and (7) for the anharmonic lattice $\beta = 0.5$ with $p = 1$. The coupling parameter μ is switched on at $t = 15$ from 0 to 1.75. Wave parameter values as in Fig. 4: (**a**) $t = 0$, (**b**) $t = 16$, (**c**) $t = 21$ and (**d**) $t = 100$ (*red lines*: soliton; *black lines*: electron)

3 Traveling Polaron/Solectron Solutions

Static polaron solutions were found numerically in [23]. To find traveling polarons/solectrons we proceed as in [16] averaging the Lagrangian in non dimensional variables (1) for the special case of $\alpha = 1$ using the trial functions:

$$c_n = A\,\mathrm{sech}\left(\frac{n-\xi}{w}\right)\exp\left[i\phi + i\,v\,(n-\xi)\right], \tag{8}$$

$$q_n = \ln\frac{1+e^{2k(n-1-\xi)}}{1+e^{2k(n-\xi)}}, \tag{9}$$

$$q_n - q_{n+1} = \ln\left[1+\sinh^2 k\,\mathrm{sech}^2\left(k\,(n-\xi)\right)\right]. \tag{10}$$

Here we take, unlike in [24], the kink/topological soliton/shock wave in $q_n\,(t)$ to satisfy the amplitude width relation for the Toda shock since in the numerics (unlike in [25]) there is very little change in the compression wave due to the presence of the electron. The velocity $\dot{\xi}$ of the localized structure and the width of the electron wave function will be determined as a function of the amplitude of the electron wave function (which is, in turn, given by the initial normalization to probability unity) and the compression width.

We now substitute (8)–(10) in the Lagrangian (1) and to leading order in the Poisson sum we obtain:

$$\begin{aligned} L = {} & \tfrac{2P}{V}k\,(k\coth k - 1)\,\dot{\xi}^2 - \tfrac{2P}{3V}\tfrac{\sinh^4 k}{k} - 2A^2 w\left(\dot{\phi} - v\dot{\xi}\right) \\ & + 2PA^2 h\,(w,k)\cos v, \end{aligned} \tag{11}$$

where

$$h\,(w,k) = \frac{2}{\sinh\frac{1}{w}} + \sinh^2 k\int_{-\infty}^{\infty}\mathrm{sech}^2\left(k\,(x-1)\right)\mathrm{sech}\frac{x}{w}\,\mathrm{sech}\frac{x-1}{w}\,dx,$$

is well approximated, for the range of interest, by the functional fitting:

$$h\,(w,k) = \frac{2}{\sinh\frac{1}{w}}\left(1 + \frac{\sinh^2 k}{1+kw}\right). \tag{12}$$

The modulation equations take the form:

$$\begin{aligned} \delta k:\ & \tfrac{2P}{V}\left(2k\coth k - \tfrac{k^2}{\sinh^2 k} - 1\right)\dot{\xi}^2 - \tfrac{2P}{3V}\tfrac{\sinh^3 k}{k}\left(4\cosh k - \tfrac{\sinh k}{k}\right) \\ & + 2PA^2 h_k\cos v = 0, \end{aligned} \tag{13}$$

which determines the velocity of the compression wave $\dot{\xi}$ as a function of the shock width and the amplitude of the electron wave function.

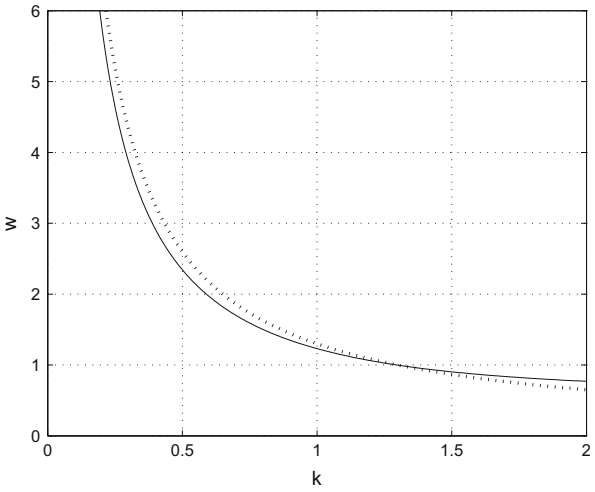

Fig. 6 Dispersion relation $w = w(k)$ obtained from equation (16). *Dotted line*: $w = 1.3/k$

To determine the width of the trapped electron wave function we take the equations:

$$\delta w: \ -2A^2\left(\dot{\phi} - v\dot{\xi}\right) + 2PA^2 h_w \cos v = 0, \tag{14}$$

$$\delta A: \ -4Aw\left(\dot{\phi} - v\dot{\xi}\right) + 4PAh\cos v = 0, \tag{15}$$

and obtain,

$$h_w = \frac{h}{w}, \tag{16}$$

an implicit equation which gives w as a function of k as shown in Fig. 6. It is shown in Fig. 6 that $w = 1.3/k$ is also a good approximation to the solution.

The variation with respect to v gives:

$$\dot{\xi} = \frac{P}{w} h \sin v. \tag{17}$$

We take $\frac{\pi}{2} \leq v < \pi$ which gives $\dot{\xi} > 0$. Solving for v as a function of $\dot{\xi}$ in (17) and using this solution into (13) we obtain a quadratic dependence of $\dot{\xi}$ as a function of k in the form:

$$\begin{aligned} &\tfrac{\sinh^3 k}{3k}\left(4\cosh k - \tfrac{\sinh k}{k}\right) - \left(2k\coth k - \tfrac{k^2}{\sinh^2 k} - 1\right)\dot{\xi}^2 \\ &+VA^2 h_k \sqrt{1 - \left(\tfrac{w\dot{\xi}}{Ph}\right)^2} = 0. \end{aligned} \tag{18}$$

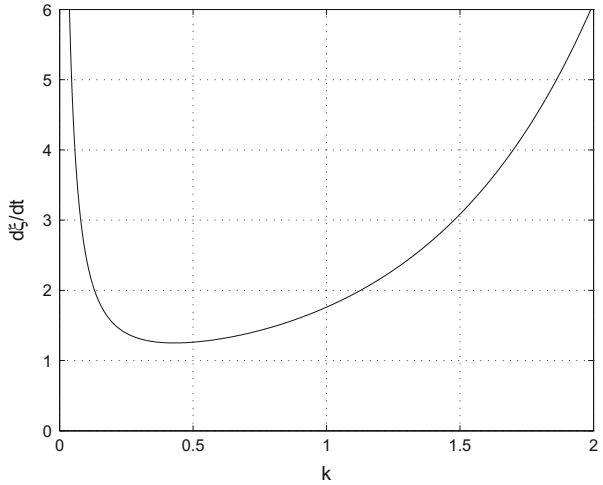

Fig. 7 Zero level curve for velocity $\dot{\xi}$ obtained from (18) for $A = 0.25$ and $V_0 = 0.5$ with $p = 10$.

Notice that for each given pair, A^2 and k, there is only one branch of solutions which represents a polaron, as illustrated in Fig. 7. Unlike the anharmonic one there are no multiple solutions and no sonic solution. This is due to the very small feedback of the electron to the distortion since $h\,(w, k)$ becomes very small as k is large compared to the $\sinh^3 k$ term.

4 Conclusions

When an electron is free to evolve along a lattice, obeying Schrödinger equation, after sometime it becomes completely deslocalized with its probability density uniformly distributed as "dust", tiny spots all over the lattice sites. Needless to say their integration gives probability one. If, however, the electron is coupled to lattice excitations in the form of solitons then we have shown that the latter are able to gather together all probability density spots thus reconstructing to a significantly large extent a localized electron which is carried with the soliton. This is the dynamic process we have denoted as "vacuum cleaner effect". The solution shown here illustrates the trapping of the electron as the consistent ground state for the potential. This in turn shows the supersonic compression wave giving the coherent structure.

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