Spinless strong-coupling solitons in a discrete Peierls model

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We construct doubly periodic solutions in a one-dimensional exactly integrable discrete Peierls transition model. We consider spinless strong-coupling solitons on a background of the periodic structure. We find their electrical charge and energy as functions of the total particle number density in the system.

It has been established in papers devoted to quasi-one-dimensional conductors (such as MX_3, M = Nb, X = Se, S, and so on) that in Peierls models with a number ρ of electrons per atom an important role in determining the nature of the ground state and the excitation spectrum is played by particle-like structures such as solitons which have a definite charge and spin (see, e.g., Refs. 1–3). To describe the properties of Peierls dielectrics, an exactly integrable discrete model of a Peierls transition was constructed and solved in Ref. 4 this model included as limiting cases all continuum models considered earlier (see Refs. 1–3).

We consider in the present paper a discrete, exactly sol uble model[4] corresponding to a continuum model of a composite type dielectric.[2] It was shown in Ref. 2 that the Peierls effect in such systems may lead to the occurrence of a strong self-trapping; the most interesting manifestation of such systems may be the existence of bipolarons (spinless charged solitons). We analyze here, in the framework of an exactly soluble discrete model, the conditions for the existence of spinless charged solitons and their physical characteristics.

As in Ref. 4, we consider a one-dimensional chain of N atoms positioned at points x_n. We assume $N_e \leqslant 2N$ electrons per atom. The energy of the system consists of the energy of the electrons ΣE_i in the self-consistent field of the atoms and the potential energy $U(x_n)$ of the atoms:

$$W=\sum_i E_i+U(x_n).$$

We neglect the kinetic energy of the atoms (their mass $M\to\infty$). The electron spectrum is determined by the strong coupling Hamiltonian (i.e., by a discrete Schrödinger equation):

$$c_n\Psi_{n+1}+c_{n-1}\Psi_{n-1}=E\Psi_n,$$

where $n = 0,1,\ldots$ numbers the N atoms, with periodic boundary conditions $\Psi_{n+N}=\Psi_n$. The jump integrals c_n ($c_{n+N}=c_n$) can be expressed in terms of the coordinates by the formula $c_n=\exp(x_n-x_{n-1})$. It is convenient to introduce also the displacement of the nth atom relative to its average position na: $x_n=na+u_n$. The potential energy is chosen in the form of a sum of integrals of the Toda lattice:[4]

$$U(x_n)=-PI_0+\sum_{l=1}\varkappa_l I_{2l}=-PI_0+\varkappa I_2+\varkappa_2 I_4+\ldots,$$

$$I_0=-a=\frac{1}{N}\sum_n \ln c_n,\qquad I_2=\frac{1}{N}\sum_n c_n^2,$$

$$I_4=\frac{1}{N}\sum_n\left(c_n^2c_{n-1}^2+\frac{1}{2}c_n^4\right),\tag{1}$$

where a is the average distance between the atoms, P the pressure, $\varkappa$ a real positive constant, and $\varkappa_2$ a real positive or negative constant. The properties of the model considered depend strongly on the number and the degree of occupation $\rho(1<\rho<2)$ of the electron bands in the metal phase and the number q of forbidden bands does not exceed $4l-2$, where l is the number of integrals in (1). In the general case of arbitrary l a multi-band picture was considered in Ref. 5. It was shown there that the state with the maximum possible number of bands is unstable, except the two-band state for $l = 1$ (model I in Ref. 4).

Earlier, in Refs. 3, 4, 6, the case was studied when only one term, $\varkappa I_2$ is retained in the energy functional (1). Refs. 3 and 4 were the first to study completely for such a functional all possible spin excitations, assuming that the number of electrons with spin down, $\rho/2$, differs from the number of electrons with spin up, $(\rho/2)+m$, and $m\to 0$ (m is the spin moment). Excitations of the domain-wall or symmetric-polaron (bound state of a single electron and two walls) type were obtained in the limit of a half-filled band, $|\rho-1|\ll e^{-1/\lambda}$, and of the domain-wall type in the Fröhlich limit, $|\rho-1|\gg e^{-1/\lambda}$, where λ is the dimensionless electron-phonon interaction constant, defined below in (9a).

In contrast to Refs. 3 and 6 we consider specifically spin states in an exactly integrable, discrete Peierls-transition model when we retain in the functional of the lattice deformation energy (1) the two terms $\varkappa I_2$ and $\varkappa_2 I_4$. This leads to the fact that, in addition to the cases described above, bound states of two electrons and two domain walls or simply a bound state of two walls without the localization of an extra electron are also possible.

In the present paper we study a stable spectrum with four forbidden bands (see Fig. 1). The structure of the spectrum is symmetric under the substitution $E\to -E$. Moreover, we assume that the electron Fermi levels $\mu_\uparrow$ and $\mu_\downarrow$ pass through the forbidden bands of the potential in the fig-

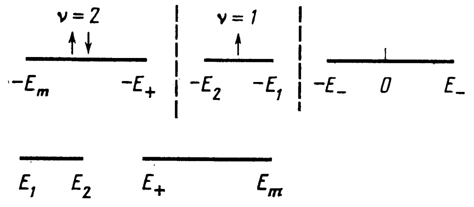

FIG. 1.

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ure. When $\rho, \rho+m<1$ (the electron band is less than half full) the bands $E>E_+, E_2>E>E_1$, and $E_->E>-E_-$ are empty and the band $E<-E_+$ is two-fold occupied. The occupation of the band $-E_2<E<-E_1$ may vary depending on the position of the levels $\mu_\uparrow$ and $\mu_\downarrow$. (The case $1<\rho<2$, $1<\rho+m<2$ differs only by the replacement of electrons by holes.) For the multiplicity of the occupation of the states of this band we have

$$\nu=\begin{cases}0, & -E_2>\mu_\uparrow>-E_+, \quad -E_2>\mu_\downarrow>-E_+,\\ 1, & -E_->\mu_\uparrow>-E_1, \quad -E_2>\mu_\downarrow>-E_+,\\ 2, & -E_->\mu_\uparrow>-E_1, \quad -E_->\mu_\downarrow>-E_1.\end{cases}$$

In contrast to the case $\varkappa_2=0$ (see Ref. 3) when for $\nu=0$ the empty band $(-E_2,-E_1)$ is shifted and combined with the empty band lying above it $(-E_-,E_-)$, for $\nu=2$ the completely filled band $(-E_2,-E_1)$ is combined while conserving its finite width corresponding to the number of particles with the completely filled band lying below it $(-E_m,-E_+)$. In our case, for a definite value of $\varkappa_2\neq 0$, the existence of additional bands $(-E_2,-E_1)$ is possible even for $\nu=0$ or $\nu=2$. In the limit in which we are interested they shrink to localized levels.

We find below the ground state of such a system, the electron spectrum, and the lattice deformation. In the limit as $m\to 0$ we obtain a formula for the deformation of the spin excitation against the background of the periodic superstructure. We evaluate the electrical charge of the soliton and find the connection between the phase shift of the deformation at the soliton and the magnitude of the electrical charge. We use the mathematical formalism and some results from Ref. 4.

We use the spectrum symmetry by virtue of which the square of the wave function Ψ_n^2 depends solely on $E^2=\lambda$. We introduce the notation

$$\lambda_1=E_m^2,\ \lambda_2=E_+^2,\ \lambda_3=E_-^2,\ \lambda_-=E_1^2,\ \lambda_+=E_2^2.$$

The function Ψ_n^2 is completely determined once we specify the points $\lambda_1,\lambda_2,\lambda_3,\lambda_+,\lambda_-,\gamma_1,\gamma_2$, where $\lambda_2\geqslant\gamma_1\geqslant\lambda_+,\lambda_-\geqslant\gamma_2\geqslant\lambda_3$. The boundaries of the bands determine the hyperelliptic Riemann surface Γ:

$$y^2=\lambda\tilde{R}(\lambda),\quad \tilde{R}(\lambda)=(\lambda-\lambda_1)(\lambda-\lambda_2)(\lambda-\lambda_3)(\lambda-\lambda_+)(\lambda-\lambda_-).$$

We use the relations

$$i\,dp={}^1/_2(\lambda^2+r_1\lambda+r_2)[\lambda\tilde{R}(\lambda)]^{-1/2}d\lambda, \tag{2}$$

where the coefficients r_1 and r_2 are found from the conditions

$$\int_{\lambda_2}^{\lambda_+}dp=\int_{\lambda_-}^{\lambda_3}dp=0$$

to introduce the quasi-momentum. By analogy with Ref. 4 we get self-consistency equations determining the boundary points λ_k:

$$P=-\frac{2}{\pi}i\int_\lambda\frac{d\lambda}{[\tilde{R}(\lambda)]^{1/2}}\left(\lambda^2+\frac{s_1}{2}\lambda+\frac{s_2}{2}-\frac{s_1^2}{8}\right),$$

$$\varkappa=\frac{2}{\pi}i\int_\lambda\frac{d\lambda}{[\tilde{R}(\lambda)]^{1/2}}\left(\lambda+\frac{s_1}{2}\right),\quad \varkappa_2=\frac{2}{\pi}i\int_\lambda\frac{d\lambda}{[\tilde{R}(\lambda)]^{1/2}},$$

$$\rho=\frac{2}{\pi}\int_{\lambda_1}^{\lambda_2}dp,\quad m=\frac{\nu}{\pi}\int_{\lambda_+}^{\lambda_-}dp,\quad \int_\lambda\ldots=\int_{\lambda_1}^{\lambda_2}\ldots+\frac{\nu}{2}\int_{\lambda_+}^{\lambda_-}\ldots, \tag{3}$$

$$s_1=-(\lambda_1+\lambda_2+\lambda_3+\lambda_++\lambda_-),\quad s_2=\sum_{k\neq l}\lambda_k\lambda_l.$$

We consider now the case of low spin density $m\to 0$. The band (λ_+,λ_-) then shrinks to a localized level λ_0 which is determined from the self-consistency condition (3):

$$\Lambda_0(\varphi,r)=\nu/2-\varkappa_2[(\lambda_1-\lambda_0)(\lambda_2-\lambda_0)(\lambda_0-\lambda_3)]^{1/2},$$

$$\varphi=\arcsin[(\lambda_0-\lambda_3)/(\lambda_2-\lambda_3)]^{1/2},\quad r=[(\lambda_1-\lambda_2)/(\lambda_1-\lambda_3)]^{1/2}. \tag{4}$$

We have introduced here Heuman's Λ_0 function.[7] Using the definition of $\Lambda_0(\varphi,r)$ we note easily that for $\nu=0$ Eq. (4) has a solution different from λ_3 only when $\varkappa_2<0$. And, on the other hand, for $\nu=2$ there is a solution $(\lambda_0\neq\lambda_2)$ only when $\varkappa_2>0$. In the case $\nu=1$ there are solutions for both signs of the constant $\varkappa_2$.

In order to consider the properties of a single soliton we must calculate the quantities x_n and c_n up to terms of first order in the density m. As the whole calculation is a repeat of the corresponding calculations of Ref. 6 in which the case $\nu=1$ was considered, we only give the final results:

$$c_n^2=\bar{c}^2\bar{\theta}(n-n_0+2)\bar{\theta}(n-n_0-1)/\bar{\theta}(n-n_0)\bar{\theta}(n-n_0+1). \tag{5}$$

Here

$$\bar{\theta}(l-n_0)=\theta_3\left[\frac{\rho}{2}(l-n_0)+\frac{\alpha}{2}\middle|g\right]e^{-l/\xi}+\theta_3\left[\frac{\rho}{2}(l-n_0)-\frac{\alpha}{2}\middle|g\right]e^{l/\xi},$$

$$\alpha=\frac{J_2}{J},\quad \frac{1}{\xi}=\frac{1}{2J}(K_1J_2-K_2J_1),$$

$$g=\exp\left[-\pi\frac{K(k)}{K(k')}\right],\quad \bar{c}=e^{-a},$$

$$J=\int_{\lambda_3}^{\lambda_2}\frac{d\lambda}{[\lambda R(\lambda)]^{1/2}},\quad K_1=\int_{\lambda_+}^{\lambda_2}\frac{\lambda\,d\lambda}{[\lambda R(\lambda)]^{1/2}},\quad J_2=\int_{\lambda_3}^{\lambda_-}\frac{d\lambda}{[\lambda R(\lambda)]^{1/2}},$$

$R(\lambda)=(\lambda-\lambda_1)(\lambda-\lambda_2)(\lambda-\lambda_3)$, and $\theta(v|g)$ is Jacobi's theta function. It follows from Eq. (5) that the change in the phase of the deformation c_n^2 on an isolated polaron equals

$$\varphi=2\pi J_2/J=2\pi F(\beta,k)/K(k),$$
$$\beta=\arcsin[\lambda_2(\lambda_0-\lambda_3)/\lambda_0(\lambda_2-\lambda_3)]^{1/2}. \tag{6}$$

We find the electrical charge of the polaron from the formula

$$q=\lim_{m\to 0}e\langle\rho_n-\rho_n^\infty\rangle/m,$$

where ρ_n^∞ is the asymptotic single-periodic solution in the presence of a single soliton $(\rho_n^\infty=\rho_n^{-\infty})$. Carrying out calculations analogous to those performed in Ref. 6 we finally have

$$q^{(\nu)}=2e\{F(\beta,k)/K(k)-\nu/2\}\equiv 2e\{1-\nu/2-F(\eta,k)/K(k)\}, \tag{7}$$

where

$$\eta=\arcsin\left[\frac{(\lambda_1-\lambda_3)(\lambda_2-\lambda_0)}{(\lambda_1-\lambda_0)(\lambda_2-\lambda_3)}\right]^{1/2},\quad k=\left[\frac{\lambda_1(\lambda_2-\lambda_3)}{\lambda_2(\lambda_1-\lambda_3)}\right]^{1/2}.$$

Comparing Eqs. (6) and (7) we see that the soliton charge is connected with the phase change of the function c_n^2 through the relation

$$q^{(\nu)}=(e/\pi)(\varphi-\pi\nu). \tag{8}$$

We consider to begin with the formulae obtained in the Fröhlich limit $|\rho-1|\gg\exp(-1/\lambda)$. In that limit the expressions for $\lambda_1,\lambda_2,\lambda_3$ (which depend on $\varkappa_2$) found in the same way as in Ref. 4 are equal to

$$\lambda_1\approx 4\bar{c}^2,\quad \frac{\lambda_2}{\lambda_1}\approx\frac{\lambda_3}{\lambda_1}\approx\sin^2\left(\frac{\pi}{2}|\rho-1|\right),$$

$$\lambda_2-\lambda_3\approx 64\bar{c}^2\cos^2\left(\frac{\pi}{2}|\rho-1|\right)e^{-2/\lambda_{\rm eph}}. \tag{9}$$

We have introduced here $\lambda_{\rm eph}$—the dimensionless electron-phonon interaction constant:

$$\lambda_{\rm eph}=\lambda/\cos\left(\frac{\pi}{2}|\rho-1|\right)$$

$$=\left[(\pi\varkappa\bar{c}+2\bar{c}^3\pi\varkappa_2)\cos\left(\frac{\pi}{2}|\rho-1|\right)\right]^{-1}. \tag{9a}$$

We use (9) and Eq. (4) which we managed to solve only approximately, to determine the local level. We restrict ourselves to the case where when the interaction is switched on ($\varkappa_2\neq 0$) the local level is shifted relative to the case $\varkappa_2=0$ by an amount $\delta\lambda$ which is much less than the total bandwidth, i.e., $\delta\lambda/(\lambda_2-\lambda_3)\ll 1$. When $\nu=1$, the presence of $\varkappa_2\neq 0$ leads only to an unimportant correction as compared to the results of Ref. 6. We give therefore only the expressions for the electrical charge and for the polaron energy:

$$q^{(1)}\approx\frac{e}{\pi}\left\{-16\frac{e^{-2/\lambda_{\rm eph}}}{\lambda}+8e^{-2/\lambda_{\rm eph}}/\mathrm{tg}^2\left(\frac{\pi}{2}|\rho-1|\right)\right.$$
$$\left.+32\varkappa_2\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right)e^{-2/\lambda_{\rm eph}}\right\},$$

$$E_s\approx\frac{2}{\pi}\Delta_0(1+\alpha),\qquad \Delta_0=(\lambda_2-\lambda_3)^{1/2},$$

$$\alpha\approx 2^5\varkappa_2\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right)e^{-2/\lambda_{\rm eph}}. \tag{10}$$

As the expression for $\nu=0$ and $\nu=2$ are similar in structure, we give for simplicity only the formulae for the charge, deformation, and soliton energy for the case $\nu=2$. One can determine the phase from its connection (8) with the charge:

$$q^{(2)}\approx-\frac{4e}{\pi}\left(\frac{\delta\lambda_2}{\lambda_2-\lambda_3}\right)^{1/2},\qquad E_s\approx\frac{2}{\pi}(\delta\lambda_2)^{1/2}(1-\beta_0),$$

$$\beta_0\approx\frac{\pi}{32}\varkappa_2\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right)e^{-2/\lambda_{\rm eph}},$$

$$\delta\lambda_2\approx 2^8\pi^2\bar{c}^2\cos^2\left(\frac{\pi}{2}|\rho-1|\right)e^{-6/\lambda_{\rm eph}}\left\{\frac{1}{\lambda_{\rm eph}^2}\right.$$
$$+16\varkappa_2\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right)$$
$$\left.\times\left[-\frac{1}{\lambda_{\rm eph}}+16\varkappa_2\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right)\right]\right\}, \tag{11}$$

$$\Delta_n\approx 16e^{-2/\lambda_{\rm eph}}\mathrm{tg}^{-1}\left(\frac{\pi}{2}|\rho-1|\right)\cos\left(\frac{\pi}{2}|\rho-1|\right)\left(\frac{\delta\lambda_2}{\lambda_2-\lambda_3}\right)^{1/2}$$
$$\times\left\{\mathrm{th}\frac{n}{\xi}\sin\left[\pi\rho\left(n-n_0+\frac{1}{2}\right)\right]\sin\frac{\varphi}{2}\right.$$
$$\left.-\cos\left[\pi\rho\left(n-n_0+\frac{1}{2}\right)\right]\cos\frac{\varphi}{2}\right\}.$$

In the general case the magnitude of the phase can take any value. In the Fröhlich limit $\varphi\to\pi$ for $\varkappa=1$ and $\varphi\to 2\pi$ for $\nu=2$. It follows from Eqs. (10) and (11) for the electrical charge that it is localized in a finite region with a characteristic dimension ξ and $q^{(1)}\to 0$, $q^{(2)}\to 0$, i.e., there is almost complete screening of the charge introduced in the system.

We note that in order that there exist a local level inside the band (λ_2,λ_3) the constant $\varkappa_2$ must take the values

$$\varkappa_2>\lambda_{\rm eph}^{-1}/8\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right),$$
$$\varkappa_2<e^{2/\lambda_{\rm eph}}/32\bar{c}^3\cos^2\left(\frac{\pi}{2}|\rho-1|\right). \tag{12}$$

We now consider the limit of a half-filled band $|\rho-1|\ll e^{-1/\lambda}$. For the boundaries of the bands of the spectrum we have in this case

$$\lambda_1\approx 4\bar{c}^2,\quad \lambda_2\approx 64\bar{c}^2e^{-2/\lambda},\quad \lambda_3/\lambda_2\approx 16\exp(-8e^{-1/\lambda}/|\rho-1|), \tag{13}$$

where

$$1/\lambda\approx\pi\varkappa\bar{c}+2\pi\varkappa_2\bar{c}^3.$$

The charge and the energy for the case $\nu=1$ are equal to

$$q^{(1)}\approx e\left\{1-2\delta|\rho-1|\ln\left[1+\mathrm{tg}\left(\frac{\pi}{4}\left(1\pm\frac{\Delta\lambda}{\lambda_2-\lambda_3}\right)\right)\right]\right\},$$

$$\Delta\lambda\approx 2^9\pi\bar{c}^5\varkappa_2e^{-4/\lambda},\qquad \delta=\frac{1}{4}e^{1/\lambda},$$

$$E_s\approx\frac{2}{\pi}\lambda_2^{1/2}+\frac{\varkappa_2}{2}\lambda_2^2,\qquad E_p\approx 2^{3/2}\frac{\lambda_2^{1/2}}{\pi}+\frac{\pi}{2^{3/2}}\lambda_2^{3/2}\lambda_1^{1/2}\varkappa_2, \tag{14}$$

where E_s and E_p are, respectively, the soliton and polaron energies. The plus or minus signs in these expressions are connected with the aforementioned leeway in the choice of the sign of $\varkappa_2$. In the limit $\varkappa_2=0$ the quantities (14) are the smae as the results of Ref. 6.

In the case $\nu=2$ we have for the charge and energy of the soliton and the bipolaron

$$q^{(2)}\approx-2e\delta|\rho-1|\ln\left\{1+\mathrm{tg}\left[\frac{\pi}{4}\left(\frac{\Delta\lambda_2}{\lambda_2-\lambda_3}\right)\right]\right\},$$

$$\Delta\lambda_2\approx 2^{16}\pi^2\varkappa_2^2\bar{c}^8e^{-6/\lambda},$$

$$E_s\approx\frac{2}{\pi}(\Delta\lambda_2)^{1/2}\left(1+\frac{3}{4}\frac{\lambda_2}{\lambda_1}\right),$$

$$E_{bp}\approx\frac{4}{\pi}(\Delta\lambda_2)^{1/2}\left[1-\frac{5}{2}\left(\frac{\lambda_2}{\lambda_1}\right)^{3/2}\right]. \tag{15}$$

For $n=2$ the expression for the deformation equals

$$\Delta_n\approx(-1)^n\left\{\left[\mathrm{th}\,\gamma\left[\frac{1}{\delta}-\frac{1}{\xi}\mathrm{th}\left(\frac{n-n_0}{\delta}\right)\right]\right.\right.$$
$$-\frac{1}{\delta}\mathrm{th}\frac{n}{\xi}\mathrm{th}\left(\frac{n-n_0}{\delta}\right)$$
$$\left.\left.+\frac{1}{\xi}\mathrm{th}\frac{n}{\xi}\right]\left[1-\mathrm{th}\,\gamma\,\mathrm{th}\left(\frac{n-n_0}{\delta}\right)\mathrm{th}\frac{n}{\xi}\right]^{-1}-\frac{1}{\xi}\mathrm{th}\frac{n}{\xi}\right\},$$

where

$$\frac{1}{\xi}\approx\frac{1}{\delta}\frac{\pi}{4}\left(\frac{\Delta\lambda_2}{\lambda_2-\lambda_3}\right)^{1/2},\quad \mathrm{th}\,\gamma\approx\frac{\pi}{4}\left(\frac{\Delta\lambda_2}{\lambda_2-\lambda_3}\right)^{1/2}.$$

In the general case the periodic structure Δ_n describes a lattice of bipolaron kind of spinless solitons with charge $q^{(2)}$.

In the weak coupling limit and under the condition $|\rho-1|\ll\exp(-1/\lambda)$ (limit of rare domain walls) the phase $\varphi\to2\pi$ when $\nu=1$ and $\varphi\to4\pi$ when $\nu=2$. We find the magnitudes of the electrical charge of the polaron $q^{(1)}\to e$ (see (14)) and of the spinless bipolaron $q^{(2)}\to-2e$ (see (15)). It follows from (14) that the charge of the polaron differs only a little from that of a single electron i.e., the charge introduced in the system hardly interacts with the charge wave density. The evaluation of discrete models[4,6] shows that for $\varkappa_2=0$ only the formation of polarons is possible. In the present paper we show that for sufficiently large $\varkappa_2$ (see (12)) a bipolaron state is possible which in that case, as follows from (15) is the most favorable.

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