Spin states in a discrete Peierls model

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We construct doubly periodic solutions in a one-dimensional exactly integrable discrete model of the Peierls transition. We consider solitons on the background of the periodic structure which carry localized spin states. We find their electric charge as a function of the total number density of the particles in the system. We obtain a connection between the electric charge of the soliton and the change in the phase of the deformation of the periodic structure at the soliton.

I. INTRODUCTION

Recently an exactly integrable discrete model of the Peierls transition has been constructed and solved.[1] In the present paper we consider the spin states in this model. We shall assume that the number of electrons per cell with spin below $\rho/2$ differs from the number of electrons with spin above $\rho/2 + c$ (c is the spin angular momentum). Such a situation can be realized in an external magnetic field. In what follows we shall find the ground state of such a system, the electron spectrum, the lattice deformation and we shall obtain in the limit as $c \to 0$ a formula for the deformation of a spin excitation (soliton) on the background of the periodic structure. We shall evaluate the electric charge of the soliton, find a connection between the phase shift of the deformation at the soliton and the magnitude of the electric charge. In particular, we consider the important weak-coupling limit corresponding to the linearized discrete model studied in Refs. 2.

The interest in the solitons considered is not exhausted by the spin excitation problem. As mentioned in Ref. 3 equivalent structures to the spin solitons occur in any systems where there is a weak splitting of the electron bands.

In this case the magnitude of the splitting plays the role of a magnetic field and the quantity $c = n_1 - n_2$, where n_1, n_2 are the electron densities in the split bands is equivalent to a spin angular momentum. Such a statement of the problem is particularly timely for MX_3 type systems ($M = Nb$, Ta; $X = Se$, S). In that case the splitting of the electron bands occurs either due to the fact that the two kinds of conducting chains are not equivalent or because of electron transitions between the chains.

There can thus occur a number of physical situations where the existence of either a rarefield gas or of a periodic structure of objects equivalent to spin solitons in the one-dimensional Peierls model will play an important role. Clearly, the physical properties of such systems will strongly depend on the presence or absence of electric charges q on the solitons and also on the magnitude of the phase change of the charge density wave (CDW) on one soliton.

The spin solitons have been considered before in a continuum model. It was shown in Ref. 4 that in the Peierls-Fröhlich model, valid for systems with a number ρ far from the integers 0,1,2, the charge of the spin soliton equals zero. However, it was shown in Ref. 3 that the appearance of charge is possible due to the effect of almost twofold commensurability. For instance, for $\rho = 1$, $q = 1$ was obtained and when the quantity ρ got away from unity the charge decreased as

$$q \propto e^{-2/\lambda}/(\rho-1)^2.$$

Here λ is the dimensionless electron-phonon interaction constant. In the framework of the Peierls-Fröhlich model the effect of phonon dispersion on the nature of the spin excitations was taken into account in Ref. 5. The magnitude of the soliton charge which is caused by the phonon dispersion was found:

$$q \propto e^{-2/\lambda}/\lambda;$$

the phase changes of the CDW with the passage of the soliton then differs from π by an amount $\alpha = q\pi$.

The discrete model considered in the present paper contains as limiting cases all Peierls models studied before and also, clearly, takes into account the dispersion of the phonon spectrum. We shall use the mathematical formalism and many results from Ref. 1.

II. GROUND STATE

We consider a one-dimensional chain of atoms situated at the points x_n. At each atom there are $\rho + c \leqslant 2$ electrons. The energy of the system consists of the energy ΣE_i of the electrons in the self-consistent field of the ions and the potential energy $U(x_n)$ of the atoms:

$$W = \sum_i E_i + U. \tag{1}$$

The spectrum of the electrons is determined by the equation

$$c_n\psi_{n+1} + c_{n-1}\psi_{n-1} = E\psi_n, \quad c_n = \exp(x_n - x_{n+1}), \tag{2}$$

and we choose the potential energy as a sum of so-called Langmuir chain integrals:

$$\begin{gathered} U(x_n) = -PI_0 + \varkappa I_2, \\ I_0 = \frac{1}{N}\sum \ln c_n = -a, \quad I_2 = \frac{1}{N}\sum_n c_n^2, \end{gathered} \tag{3}$$

where a is the average distance between the atoms, and P the pressure. The extremals of the functional are found in a simi-

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lar way as in Ref. 1. The specturm of the system is symmetric with respect to the substitution $E \to -E$ and contains four forbidden bands (Fig. 1). When $\rho, \rho + c \leqslant 1$ the band $(-E_m, -E_+)$ is doubly occupied, and the band $(-E_2, -E_1)$ singly; when $\rho > 1$ the bands $(-E_m, -E_+)$, $(-E_2, -E_1)$, $(-E_-, +E_-)$ are doubly occupied and the band (E_1, E_2) singly. The ground state of the system contains two zero modes. We use the symmmetry of the spectrum by virtue of which the square of the wave function ψ_n^2 depends only on $E^2 = \lambda$. We introduce the notation $\Lambda_1 = E_m^2, \Lambda_2 = E_+^2, \Lambda_3 = E_-^2, \Lambda_+ = E_2^2, \Lambda_- = E_1^2$. The function ψ_n^2 is completely determined by the value of 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 band edges Λ_i determine the hyperelliptical Riemann surface Γ:

$$y^2 = \lambda \tilde{R}(\lambda),$$
$$\tilde{R}(\lambda) = (\lambda - \Lambda_1)(\lambda - \Lambda_2)(\lambda - \Lambda_3)(\lambda - \Lambda_+)(\lambda - \Lambda_-). \tag{4}$$

The Riemann surface of function (4) is a surface of the second kind in the two-dimensional complex (y, Λ) space. One can represent it as being two sheets of the E-plane which are joined with cuts along the allowed bands. There are four independent cycles: a_1 and a_2 over the forbidden bands and b_1 and b_2 shown in Fig. 2.

As usual the holomorphic differentials on Γ are determined as follows:

$$\omega_i = \frac{A_i \lambda + B_i}{[\lambda \tilde{R}(\lambda)]^{1/2}} d\lambda, \qquad i = 1, 2. \tag{5}$$

We find their coefficients from the conditions

$$\oint_{a_k} \omega_i = \delta_{ik}. \tag{6}$$

The integrals of the ω_k along the b_l cycles are determined by the matrix of the Riemann coefficients B_{kl}:

$$B_{kl} = \oint_{b_k} \omega_l. \tag{7}$$

We bear in mind the definition of the qth order θ-function:

$$\theta(v_1, v_2, \ldots, v_q) = \sum_{m_1 \in Z} \cdots \sum_{m_q \in Z} \exp\left\{ \sum_{k,l=1}^{q} \pi i B_{kl} m_k m_l + 2\pi i \sum_{k=1}^{q} v_k m_k \right\},$$

where $Z = 0, \pm 1, \pm 2, \ldots$.

We introduce the quasimomentum differential using the relation

$$i\,dp = \frac{\lambda^2 + r_1 \lambda + r_2}{2[\lambda \tilde{R}(\lambda)]^{1/2}} d\lambda. \tag{8}$$

The coefficients r_1 and r_2 are found from the condition

$$\oint_{a_k} dp = 0, \qquad k = 1, 2. \tag{9}$$

The quasimomentum $p > 0$ and takes on values from 0 to π. The function ψ_n^2 has the form[6]

$$\psi_n^2(\lambda) = r_n \exp\left\{ 2in \int_{\Lambda_1}^{\lambda} dp \right\} \frac{\theta^2(A_k(\lambda) + nU_k - V_k)}{\theta^2(A_k(\lambda) - V_k)}, \tag{10}$$

where

$$A_k(\lambda) = \int_{\Lambda_1}^{\lambda} \omega_k, \qquad U_k = \frac{1}{2\pi} \int_{b_k} dp,$$

$$V_k = \int_{\Lambda_2}^{\gamma_1} \omega_k + \int_{\Lambda_-}^{\gamma_2} \omega_k + \frac{k}{2}, \qquad k = 1, 2.$$

We also write down an expression for x_n and c_n in a similar way as in Ref. 6:

$$\exp(4x_n) = \exp(-4nI_0) \frac{\theta^2((n-1)U_k + \Phi_k)\,\theta^2(U_k + \Phi_k)}{\theta^2((n+1)U_k + \Phi_k)\,\theta^2(-U_k + \Phi_k)}, \tag{11}$$

$$c_n^2 = \bar{c}^2 \frac{\theta((n-1)U_k + \Phi_k)\,\theta((n+2)U_k + \Phi_k)}{\theta((n+1)U_k + \Phi_k)\,\theta(nU_k + \Phi_k)}, \tag{12}$$

where $\Phi_k = V_k + \frac{1}{2}$, $\bar{c} = \exp(-a)$.

By analogy with Ref. 1 we write down the conditions for self-consistency which determine the boundary points of the spectrum Λ_i:

$$\int_{\lambda} \frac{d\lambda}{[\tilde{R}(\lambda)]^{1/2}} = 0, \tag{13}$$

$$\frac{2i}{\pi} \int_{\lambda} \frac{\lambda\, d\lambda}{[\tilde{R}(\lambda)]^{1/2}} = \varkappa, \tag{14}$$

$$-\frac{2i}{\pi} \int_{\lambda} \frac{\lambda^2 - s\lambda/2}{[\tilde{R}(\lambda)]^{1/2}} d\lambda = P, \tag{15}$$

$$\frac{2}{\pi} \int_{\Lambda_1}^{\Lambda_2} dp = \rho, \tag{16}$$

$$\frac{1}{\pi} \int_{\Lambda_+}^{\Lambda_-} dp = c, \tag{17}$$

where

$$s = \Lambda_1 + \Lambda_2 + \Lambda_3 + \Lambda_-, \qquad \int_{\lambda} = \int_{\Lambda_1}^{\Lambda_2} + \frac{1}{2} \int_{\Lambda_+}^{\Lambda_-}.$$

We now get expressions for the electron density distribution in the system.

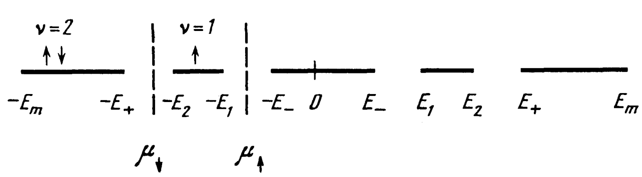

FIG. 1.

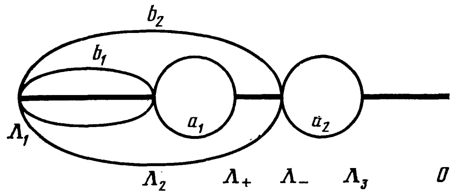

FIG. 2.

Using the results of Ref. 1 we have

$$\rho_n=\sum_\lambda \frac{(\lambda-\gamma_1(n))(\lambda-\gamma_2(n))}{\langle(\lambda-\gamma_1(n))(\lambda-\gamma_2(n))\rangle}, \tag{18}$$

$$\frac{dp}{d\lambda}=\frac{1}{2}\frac{\langle(\lambda-\gamma_1(n))(\lambda-\gamma_2(n))\rangle}{[\lambda\tilde{R}(\lambda)]^{1/2}}. \tag{19}$$

Similar to what was done in Ref. 7 we get from Eqs. (3) and (18), (19) the connection between the quantities $\gamma_1(n)$, $\gamma_2(n)$ and the c_n:

$$\begin{aligned}\gamma_n&=\gamma_1+\gamma_2=s/2-c_n^2-c_{n-1}^2,\\ \Gamma_n&=\gamma_1(n)\gamma_2(n)\\ &=c_{n+1}^2c_n^2+c_{n-1}^2c_{n-2}^2+(c_n^2+c_{n-1}^2)^2\\ &\quad-\frac{s}{2}(c_n^2+c_{n-1}^2)-\sum_{i>j}\frac{\Lambda_i\Lambda_j}{2}-\frac{s^2}{8}.\end{aligned} \tag{20}$$

Substitution expression (19) into Eq. (18) and using (20) we get

$$\rho_n-\bar{\rho}=-\frac{1}{\pi}\int_\lambda\frac{\lambda\,d\lambda}{[\lambda\tilde{R}(\lambda)]^{1/2}}(\gamma_n-\bar{\gamma})+\frac{1}{\pi}\int_\lambda\frac{d\lambda}{[\lambda\tilde{R}(\lambda)]^{1/2}}(\Gamma_n-\bar{\Gamma}). \tag{21}$$

III. SINGLE-ELECTRON AND SPIN EXCITATIONS

1. We consider now the case of low spin density ($c\to 0$). The (Λ_+,Λ_-) band then contracts into a localized level Λ_0 which is determined from the self-consistency condition (13):

$$\Lambda_0(\varepsilon|r)={}^1/_2,\quad \varepsilon=\arcsin\left(\frac{\Lambda_0-\Lambda_3}{\Lambda_2-\Lambda_3}\right)^{1/2},\quad r=\left(\frac{\Lambda_1-\Lambda_2}{\Lambda_1-\Lambda_3}\right)^{1/2}. \tag{22}$$

We have introduced here the Heuman lambda function

$$\Lambda(\varepsilon|r)=\frac{2}{\pi}[K(r)E(\varepsilon|r')-(K(r)-E(r))F(\varepsilon|r')],$$

where K, F, and E are elliptical integrals of the first and second kind. Explicit expressions for Λ_1, Λ_2, and Λ_3 are for this limit found in Ref. 1.

In order to find out what the general expressions for c_n and x_n become in the limit of a single soliton we must evaluate the quantities (5), (7), (10) up to terms of first order in the density c. Performing the appropriate elementary calculations we have

$$c=(K_1I_2-K_2I_1)\left(2I\ln\frac{1}{\Lambda_+-\Lambda_-}\right)^{-1}, \tag{23}$$

$$\begin{aligned}&B_{11}=iB_0+O(c),\quad B_0=\frac{K'(k)}{K(k)},\quad k=\left[\frac{\Lambda_1(\Lambda_2-\Lambda_3)}{(\Lambda_1-\Lambda_3)\Lambda_2}\right]^{1/2},\\ &B_{12}=B_{21}=B_{11}-iI_2\pi\left(I\ln\frac{1}{\Lambda_+-\Lambda_-}\right)^{-1},\\ &B_{22}=B_{11}-iI_2\left(I\ln\frac{1}{\Lambda_+-\Lambda_-}\right)^{-1}+iI_1\left(I\ln\frac{1}{\Lambda_+-\Lambda_-}\right)^{-1},\\ &U_1=\rho/2,\ U_2=\rho/2+c,\quad V_2-V_1={}^1/_2+O(c),\end{aligned} \tag{24}$$

$$K_i=\frac{1}{2}\oint_{a_i}\frac{\lambda\,d\lambda}{[\lambda R(\lambda)]^{1/2}},\quad I_i=\frac{1}{2}\oint\frac{d\lambda}{[\lambda R(\lambda)]^{1/2}},\quad i=1,2,$$

$$I=\int_{\Lambda_3}^{\Lambda_2}\frac{d\lambda}{[\lambda R(\lambda)]^{1/2}},\quad R(\lambda)=(\lambda-\Lambda_1)(\lambda-\Lambda_2)(\lambda-\Lambda_3).$$

Substituting (23), (24) into (11) we can after a few calculations get

$$c_n^2=\bar{c}^2\tilde{\theta}(n-1-n_0)\tilde{\theta}(n+2-n_0)/\tilde{\theta}(n+1-n_0)\tilde{\theta}(n-n_0). \tag{25}$$

Here

$$\tilde{\theta}(m-n_0)=\theta_3\left(\frac{\rho}{2}(m-n_0)-\frac{\alpha}{2}\,\Big|\,q\right)\times e^{m/\xi}+\theta_3\left(\frac{\rho}{2}(m-n_0)+\frac{\alpha}{2}\right)e^{-m/\xi},$$

$$\alpha=\frac{I_2}{I_1},\quad \xi^{-1}=\frac{K_1I_2-K_2I_1}{2I},\quad q=\exp\left[-\frac{\pi K(k')}{K(k)}\right],$$

where $\theta_3(v|q)$ is Jacobi's theta function. It is clear from (25) that the change in the phase of the deformation c_n at an isolated polaron equals

$$\varphi=2\pi\frac{I_2}{I}=2\pi\frac{F(\beta|k)}{K(k)},\quad \beta=\arcsin\left[\frac{\Lambda_2(\Lambda_0-\Lambda_3)}{(\Lambda_2-\Lambda_3)\Lambda_0}\right]^{1/2}. \tag{26}$$

Similarly, Eq. (11) becomes

$$e^{2x_n}=e^{-2n\alpha}\tilde{\theta}(n-n_0-1)\tilde{\theta}(-n_0+1)/\tilde{\theta}(n+1-n_0)\tilde{\theta}(-n_0+1). \tag{27}$$

We now find the magnitude of the polaron electric charge. Following Ref. 3 we write

$$q=e\lim_{c\to 0}\frac{\langle\rho_n-\rho_n^\infty\rangle}{c}, \tag{28}$$

where ρ_n^∞ is the asymptotic single-period solution when there is a single soliton present (it is clear from (25), (27) that $\rho_n^{+\infty}=\rho_n^{-\infty}$). We have from (18), (19)

$$\begin{aligned}\rho_n&=\frac{1}{\pi}\int_\lambda\left\{\frac{A_n}{[(\lambda-\lambda_+)(\lambda-\lambda_-)]^{1/2}[\lambda R(\lambda)]^{1/2}}+\left[\frac{\lambda-\lambda_+}{\lambda-\lambda_-}\right]^{1/2}\frac{\lambda+B_n}{[\lambda R(\lambda)]^{1/2}}\right\}d\lambda,\\ i\frac{dp}{d\lambda}&=\frac{\langle A_n\rangle}{2[(\lambda-\lambda_+)(\lambda-\lambda_-)]^{1/2}[\lambda R(\lambda)]^{1/2}}+\frac{1}{2}\left[\frac{\lambda-\lambda_+}{\lambda-\lambda_-}\right]^{1/2}\frac{\lambda+\langle B_n\rangle}{[\lambda R(\lambda)]^{1/2}}\end{aligned} \tag{29}$$

$$A_n=(\lambda_+-\gamma_1(n))(\lambda_+-\gamma_2(n)),\quad B_n=\lambda_+-\gamma_1(n)-\gamma_2(n).$$

From (17) it follows that

$$\langle A_n\rangle=2[\lambda_+R(\lambda_+)]^{1/2}c. \tag{30}$$

Using (8) and (29) we find

$$\langle B_n\rangle-\langle B_n^\infty\rangle=-\langle A_n\rangle F/I, \tag{31}$$

where

$$F=\int_{\Lambda_3}^{\Lambda_2}\frac{d\lambda}{(\lambda-\Lambda_0)\,[\lambda R(\lambda)]^{1/2}}.$$

Substituting Eqs. (30), (31) into (29) and (28) and evaluating the integrals in (29) we finally have

$$q=e\left[\frac{2F(\beta|k)}{K(k)}-1\right]=e\left[1-\frac{2F(\eta|k)}{K(k)}\right],$$
$$\eta=\arcsin\left[\frac{\Lambda_1-\Lambda_3}{\Lambda_1-\Lambda_0}\,\frac{\Lambda_2-\Lambda_0}{\Lambda_2-\Lambda_3}\right]^{1/2}. \tag{32}$$

Comparing Eq. (26) with (32) we find that the soliton charge is connected with the change in phase of the function c_n as follows:

$$q=e(\varphi-\pi)/\pi. \tag{33}$$

2. We consider the formulae obtained above with the limit corresponding to the linearized model:

$$c_n\approx\bar{c}[1-\varepsilon(u_{n+1}-u_n)],\quad x_n=na+u_n. \tag{34}$$

It is shown in Ref. 1 that this limit corresponds to small ε or, in dimensionless variables to the inequality

$$P\gg\bar{c},\quad \varkappa\bar{c}\gg\lambda\quad(\lambda^{-1}=\pi\varkappa\bar{c}).$$

The quantity $\lambda/\sin(\pi\rho/2)=\lambda_{\rm ep}$ corresponds to the usual definition of the dimensionless electron-phonon coupling constant. The linearized model corresponds also to the weak coupling limit $\lambda_{\rm ep}\ll 1$. The following relations were obtained in Ref. 1:

$$|\rho-1|\gg e^{-1/\lambda}\quad\begin{cases}\Lambda_2/\Lambda_1\approx\Lambda_3/\Lambda_1\approx\sin^2(\pi|\rho-1|/2), & \Lambda_1=4\bar{c}^2\\ \Lambda_2-\Lambda_3=64\bar{c}^2\cos^2\dfrac{\pi|\rho-1|}{2}\exp\left(-\dfrac{2}{\lambda_{\rm ep}}\right)\end{cases}, \tag{35}$$

$$|\rho-1|\ll e^{-1/\lambda}\begin{cases}\Lambda_1=4\bar{c}^2, & \Lambda_2=64\bar{c}^2e^{-2/\lambda}\\ \Lambda_3/\Lambda_2=16\exp(-8e^{-1/\lambda}/|\rho-1|)\end{cases}. \tag{36}$$

In the limit $|\rho-1|\ll e^{-1/\lambda}$ we have from (22), (32), (36)

$$\Lambda_0=(\Lambda_2+\Lambda_3)/2,$$
$$q=e[1-2\ln(\sqrt{2}+1)\delta|\rho-1|],\quad 4\delta=e^{1/\lambda}. \tag{37}$$

Equations (37) are similar to those obtained in Ref. 3.

In the limit $|\rho-1|\gg e^{-1/\lambda}$ we get from (22), (32)

$$\Lambda_0=\frac{\Lambda_2+\Lambda_3}{2}+\frac{\Lambda_2-\Lambda_3}{2}\left[-\frac{4\exp(-2/\lambda_{\rm ep})}{\lambda_{\rm ep}}+2\exp(-2/\lambda_{\rm ep})\right],$$
$$q\approx\left[-\frac{16}{\pi}\frac{\exp(-2/\lambda_{\rm ep})}{\lambda}+\frac{8}{\pi}\frac{\exp(-2/\lambda_{\rm ep})}{\mathrm{tg}^2(\pi|\rho-1|/2)}\right]e. \tag{38}$$

It follows from (38) that when $\lambda\ll|\rho-1|^2$

$$q\approx-\frac{16}{\pi}\frac{\exp(-2/\lambda_{\rm ep})}{\lambda}e, \tag{39}$$

and when $\lambda\ll|\rho-1|^2$

$$q\approx\frac{32}{\pi^3}\frac{\exp(-2/\lambda_{\rm ep})}{|\rho-1|^2}. \tag{40}$$

Equation (40) is the same as the expression obtained in the continuum model in Ref. 3 and Eq. (39) gives the same kind of λ-dependence as the charge obtained in Ref. 5 in the continuum model taking the phonon dispersion close to the Fermi surface into account. It is clear form (33) that the change in phase on the soliton varies within wide limits such that $\varphi\to 2\pi$ as $\rho\to 1$ and $\varphi\approx\pi$ as $\rho\to 0$:

$$|\rho-1|\ll e^{-1/\lambda}:\quad \varphi=\pi(q/e+1)=2\pi[1-\ln(\sqrt{2}+1)\delta|\rho-1|],$$
$$|\rho-1|\gg e^{-1/\lambda}: \tag{41}$$

$$\varphi=\pi\left(\frac{q}{e}+1\right)$$
$$=\pi\left[1+\frac{8}{\pi}\frac{\exp(-2/\lambda_{\rm ep})}{\mathrm{tg}^2(\pi|\rho-1|/2)}-\frac{16}{\pi}\frac{\exp(-2/\lambda_{\rm ep})}{\lambda_{\rm ep}}\right]. \tag{42}$$

We obtain an expression for the deformation $\Delta_n=u_{n+1}-u_n$. When $|\rho-1|\ll e^{-1/\lambda}$ we have $\xi=\sqrt{(2)}\delta$ and

$$\Delta_n=\frac{(-1)^n}{\sqrt{2}\,\delta}\left[\frac{\mathrm{th}[(n-n_0)/\delta]}{\sqrt{2}-\mathrm{th}[(n-n_0)/\delta]\,\mathrm{th}(n/\sqrt{2}\,\delta)}-\mathrm{th}\frac{n}{\sqrt{2}\,\delta}\right]. \tag{43}$$

Formula (43) gives an expression for the deformation of a polaron located at a distance n_0 from the closest domain wall. As $n_0\to-\infty$ we get from (43)

$$\Delta_n=\frac{(-1)^n}{\sqrt{2}\,\delta}\left[\frac{1}{\sqrt{2}-\mathrm{th}(n/\sqrt{2}\,\delta)}-\mathrm{th}\frac{n}{\sqrt{2}\,\delta}\right]. \tag{44}$$

Equation (44) is the same as the one obtained in Ref. 8. As $|\rho-1|\gg e^{-1/\lambda}$ we get from (25)

$$\frac{1}{\xi}\approx\frac{4\exp(-2/\lambda_{\rm ep})}{\mathrm{tg}(\pi|\rho-1|/2)}, \tag{45}$$

$$\Delta_n\approx 16\exp(-2/\lambda_{\rm ep})\frac{\cos^2(\pi|\rho-1|/2)}{\sin(\pi|\rho-1|/2)}\left\{\mathrm{th}\frac{n}{\xi}\sin\left[\pi\rho\left(n-n_0+\frac{1}{2}\right)\right]\sin\frac{\varphi}{2}-\cos\left[\pi\rho\left(n-n_0+\frac{1}{2}\right)\right]\cos\frac{\varphi}{2}\right\}. \tag{46}$$

In the limit as $n_0\to\pm\infty$ it follows from (44) that

$$\Delta_n\propto\cos[\pi\rho(n-n_0+{}^1/_2)\pm\varphi/2],$$

so that the phase change at the polaron equals $\varphi=\pi(q/e+1)$, as should be the case.

IV. CONCLUSION

We considered in the present paper spin states in an exactly soluble discrete model of the Peierls transition. We noted in the Introduction that such states can occur in various physical systems. We found the ground state of the system, the electron spectrum, the wavefunctions, the deformation in the system [Eqs. (8), (9), (13) to (17), (10) to (12)], and the electron density distribution (21) for arbitrary spin angular momentum. The electron state spectrum has in the ground state five allowed and four forbidden bands; depending on the magnitudes of the densities ρ, c two or four allowed bands are occupied and the upper occupied allowed band is always occupied singly.

In the limit as $c \to 0$ two of the allowed bands present, (E_1, E_2) and $(-E_2, -E_1)$ (see Fig. 1) contract into localized levels $\pm E_0$, determined from condition (22). In the weak coupling limit we wrote down explicit expressions, (37) and (38), for the quantity E_0 for arbitrary electron density $\rho(0<\rho<2)$. We obtained the shape (25) of an isolated soliton on the background of the periodic superstructure of the ground state and the magnitude (26) of the change in the phase φ of the CDW at a single soliton. In the general case the magnitude of φ can take on any value. In the weak coupling limit under the condition $|\rho - 1| \ll \exp(-1/\lambda)$ (limit of rare domain walls) the quantity $\varphi \approx 2\pi$ and is given by Eq. (41) while under the condition $|\rho - 1| \gg \exp(-1/\lambda)$ (Fröhlich limit) we get $\varphi \approx \pi$, (42). We found the magnitude (32) of the electric charge q of the polaron. In the weak coupling limit when $|\rho - 1| \ll \exp(-1/\lambda)$ we get $q \approx 1$, see (37); when $|\rho - 1| \gg \exp(-1/\lambda)$ we have $q \approx 0$, see (38); when $|\rho - 1| \lesssim \lambda^{1/2}$ see Eqs. (39) and (40). We showed in the general case that there exists the exact relation (33)—$q = e(\varphi - \pi)/\pi$—between the electric charge of the polaron and the amount by which the phase of the CDW changes when it passes through a single polaron.

The charge of the polaron is, as is clear from Eqs. (21), (43), (46), localized in a finite region with characteristic size ξ. The magnitude of the charge can in the general case have any value $0 \leqslant q \leqslant 1$. We recall that by the magnitude of the charge we mean the quantity $q = \Sigma(\rho_n - \rho_n^\infty)$ which is composed not only of the magnitude of the charge brought into the system by the electron, but also of a contribution caused by the redistribution of the electron density in the system. The polaron charge therefore differs from the single-electron charge; it is partly screened by the redistributed charge in the CDW. The interaction of an external electron, carrying an uncompensated spin, reduces mathematically in the CDW to a change in the phase of the CDW at the polaron. It is clear from the theory that the case $\rho = 1$ is a special one. In that case the phase change $\varphi = 2\pi$, i.e., the polaron, in fact, does not interact with the CDW as at the polaron the phase of the CDW is not changed (modulo 2π). This leads to the fact that there does not occur a redistribution of the electron density and that the charge of the external electron is not screened: $q = e$ in agreement with the general formula $q = e(\varphi - \pi)/\pi$. Another limiting case occurs when $|\rho - 1| \gg \exp(-1/\lambda)$. Now the interaction of the soliton with the CDW is a maximum (the phase changes in the region of the polaron almost by half a period) and there occurs almost complete screening of the charge: $q \approx 0$.

The theory described here can in practice be applied to linear polymers such as, for instance, alloyed trans-polyacetylene. One can produce a spin density by putting the system in an external strong magnetic field. We indicated in the Introduction that objects like spin solitons can appear also in systems with a split electron spectrum.

The physical properties of actual systems will depend to a large extent on the presence or absence of electric charge at the spin solitons. In the general case both the Fröhlich conducticity and the current of the charged spin solitons will contribute to the magnitude of the electric conductivity. If for some reason in the system the Fröhlich conductivity is pinned, only the charged spins polarons will contribute to the current. One can judge the magnitude of the polaron charge using the ratio of the magnitude of the transferred spin current to the magnitude of the transferred electric charge. The presence or absence of electric charge can be established in experiments about the scattering of spin solitons by charged and uncharged impurities.

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