Quantization and soliton charge in the Peierls model

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(Submitted 28 October 1988; resubmitted 20 January 1989)
Zh. Eksp. Teor. Fiz. **96**, 229–236 (July 1989)

An analysis is made of semiclassical quantization of solitons (kinks, polarons, bipolarons) in the model of a Peierls insulator with a degenerate or a nondegenerate ground state. The electric current and the charge of quantum excitations are calculated and it is found that the latter differs from the local charge of classical excitations.

It is known[1–6] that polaron states (solitons, polarons, bipolarons, etc.) having a localized electron level lying well inside the band gap form in one-dimensional electron–phonon systems as a result of electron self-trapping (for a review see Ref. 5). In the case of topological solitons the electric charge of excitations may be fractional and its value is a continuous function of the parameters of the system.[6–9] The charge is given by

$$q=\int dx[\rho(x)-\rho_0],$$

where $\rho(x)$ is the density of the electric charge and ρ_0 is the density far from a soliton. The charge is localized in a finite region of the order of the soliton size. The fractional value of the charge is due to the fact that introduction of an additional particle into the system results, because of self-trapping, in a local deformation of the lattice and in an associated redistribution of the electron density which gives rise to partial screening of the electric field of the new particle. The integral charge of this particle can be assumed to be partly localized at an exciton and partly distributed uniformly over the whole length of a one-dimensional chain. The question arises whether the uniformly distributed part of the charge contributes to the electric current generated by the motion of a soliton under the action of an external electric field, i.e., whether the soliton charge defined in the usual way is the ratio of the electric current to the velocity of an excitation, $q=j/v$, is identical with the familiar local static charge. Moreover, the very concept of a local electric charge is meaningful only in the case of a classical description of the lattice deformation $\Delta(x)$. If a quantum description is adopted, all the states become delocalized and, therefore, the local charge cannot be defined at all.

1. CURRENT AND CHARGE OF A KINK IN THE PEIERLS MODEL WITH A DEGENERATE OR A NONDEGENERATE GROUND STATE

We shall carry out a semiclassical quantization of solitons and calculate their charge, defined as the ratio of the electric current to the velocity of an excitation. We shall confine ourselves to solitons in the model of a Peierls insulator with a mixed state.[5,6] The deformation $\Delta(x)$ consists of a spontaneous deformation $\Delta_2(x)$ caused by the Peierls effect and a constant contribution Δ_1 due to the molecular structure of a polymer. It is assumed that the deformations Δ_1 and Δ_2 are "orthogonal" $[\Delta(x)=\Delta_1+i\Delta_2(x)]$. This situation may be encountered[5,10,11] in polymers of the $(AB)_x$ type. The local static charge of such solitons is calculated in Ref. 3.

The classical soliton solutions are associated with extended states in quantum theory. We shall use the lowest order of a semiclassical expansion to allow for quantum fluctuations in the vicinity of the classical solution. We shall quantize solitons using a canonical Hamiltonian procedure analogous to that used in Refs. 12 and 13. We shall describe the deformation $\Delta(x,t)$ in the form

$$\Delta(x,t)=\Delta(x-X(t))+\sum q_n(t)\eta_n(x-X(t)),$$

where $X(t)$ is the coordinate of a soliton, $\Delta(x)$ is the classical soliton solution, and η_n are normal modes of fluctuations of nonzero energy in the vicinity of the classical solution. We shall consider only the contribution associated with the zeroth mode. In the canonical Hamiltonian formalism the variable X defining the soliton position transforms into a dynamic coordinate, which is an implicit collective coordinate associated with the translation symmetry of the system.

The Langrangian of the system is

$$\mathscr{L}=\int dx\left(\Psi^+ i\frac{\partial}{\partial t}\Psi-\Psi^+\hat{H}\Psi+\frac{\dot{\Delta}_2^2}{g^2\omega^2}-\frac{\Delta^2}{g^2}\right),$$

$$\hat{H}=\begin{pmatrix}-i\dfrac{\partial}{\partial x} & \Delta\\ \Delta^* & i\dfrac{\partial}{\partial x}\end{pmatrix},\qquad \Psi=\begin{pmatrix}\Psi_+\\ \Psi_-\end{pmatrix},$$

$$\Delta(x,t)=\Delta_1+i\Delta_2(x,t), \tag{1}$$

where $\Psi(x,t)$ is the electron field; g is the electron–phonon coupling constant; ω is the frequency of phonons with a wave vector $2k_F$ (k_F is the Fermi wave vector); the Fermi velocity is assumed to be unity; $v_F=1$; $\dot{f}=\partial f/\partial t$;

$$\Delta_2(x,t)=\Delta_2\,\mathrm{th}[\Delta_2(y)],\quad x-X(t)=y. \tag{2}$$

For a given value of $X(t)$, variation of Eq. (1) in respect of $\Psi(x,t)$ may yield the Schrödinger equation for the wave functions $\Psi(x,t)=\Phi(y,t)$. Then the Langrangian is written in the form

$$\mathscr{L}=\int dx\left[\Phi^+ i\frac{\partial}{\partial t}\Phi-\Phi^+ i\frac{\partial}{\partial x}\Phi\dot{X}(t)-\Phi^+\hat{H}\Phi-\frac{\Delta_2^2}{g^2}\right]+\frac{M\dot{X}^2}{2}. \tag{3}$$

 0038-5646/89/070128-05$04.00

where

$$M=2\int dx\left(\frac{\partial\Delta}{\partial x}\right)^2\Big/g^2\omega^2.$$

Equation (3) does not contain $X(t)$ and depends only on $\dot{X}(t)$. The canonical momentum, which is conjugate to the coordinate $X(t)$, is equal to—as expected—the total conserved momentum of the system:

$$P=\frac{\delta\mathscr{L}}{\delta\dot{X}}=\sum_\mu\int\Phi_\mu^\cdot\left(-i\frac{\partial}{\partial y}\right)\Phi_\mu\,dy+M\dot{X}$$
$$=-\int dy\left(\frac{\delta\mathscr{L}}{\delta\dot\Psi}\frac{\partial\Phi}{\partial y}-\frac{\delta\mathscr{L}}{\delta\dot\Delta}\frac{\partial\Delta}{\partial y}\right)=T_{01},$$

where the summation is carried out over the occupied electron states μ with the wave functions $\Psi_\mu(x,t)$ and T_{01} is a component of the energy-momentum tensor.

It should be noted that the electric current and charge in a chain, defined as the variational derivatives of the Langrangian with respect to the vector potential, are

$$j=\sum_\mu\int\Psi_\mu^+\sigma_z\Psi_\mu\,dx,\quad q=\sum_\mu\int\Psi_\mu^+\Psi_\mu\,dx$$

(σ_2 is a Pauli matrix). The classical Hamiltonian is obtained from the Langrangian in the usual way:.

$$H=P\dot{X}-\mathscr{L}=\int\sum_\mu\left(\Phi_\mu^+i\frac{\partial}{\partial t}\Phi_\mu+\Phi^+\hat{H}\Phi\right)dy$$
$$+\frac{(P-P_{el})^2}{2M}+\frac{\Delta^2}{g^2},\tag{4}$$

where

$$P_{el}=\sum_\mu\int\Phi_\mu^+\left(-i\frac{\partial}{\partial y}\right)\Phi_\mu\,dx.$$

The Hamiltonian of Eq. (4) is indepenent of $X(t)$. The soliton is quantized by replacing the coordinate X and the momentum P with the operators $\hat{X}$ and $\hat{P}=-i\partial/\partial X$, which obey the familiar commutation relations. As a result, the solution becomes a delocalized quantum particle with a wave function $\exp(iPX)$.

We shall consider a state with a given momentum P (this can be done because $\hat{P}$ commutes with the Hamiltonian). Variation of Eq. (4) with respect to Φ and the condition that the energy of the system should be minimal yield the following equations for the wave functions:

$$i\frac{\partial}{\partial t}\Phi(y,t)-iv\frac{\partial}{\partial y}\Phi(y,t)-\hat{H}(y)\Phi(y,t)=0,\tag{5}$$

where $v=(P-P_{el})/M=\partial H/\partial P$ is the soliton velocity.

Equation (5) is identical with the Schrödinger equation of the steady-state classical problem of a soliton moving at a constant velocity v. Therefore, we shall calculate the current using the exact solutions for the wave functions $\Psi_\mu(x,t)$. For the states in a continuous spectrum, we have

$$\begin{gathered}\psi_+=(A+iB\Delta_2\,\text{th}\,\xi)\exp(-i\lambda t+ipx),\\ \psi_-=(C-iB\Delta_2\,\text{th}\,\xi)\beta\exp(-i\lambda t+ipx),\\ A=[\Delta_1+(\lambda+p)\beta]B,\quad C=[\Delta_1+(\lambda-p)/\beta]B,\\ \lambda^2=p^2+\bar\Delta^2,\ \bar\Delta^2=\Delta_1^2+\Delta_2^2,\ \beta=\left(\frac{1-v}{1+v}\right)^{1/2},\quad\xi=\frac{x-vt}{(1-v^2)^{1/2}},\\ |B|^2={}^1/_4(1+v)\{L\lambda[\lambda+\Delta_1(1-v^2)^{1/2}-pv]-\Delta_2(1-v^2)^{1/2}\}^{-1}.\end{gathered}\tag{6}$$

A discrete level is described by the function

$$\begin{gathered}\psi_+=-\psi_-=\Delta_2^{1/2}\exp(-i\lambda_0t+ip_0x)/2\beta^{1/2}\,\text{ch}\,\xi,\\ \lambda_0^2=p_0^2+\Delta_1^2,\quad\lambda_0=-\Delta_1/(1-v^2)^{1/2}.\end{gathered}\tag{7}$$

Equations (6) and (7) are deduced from the corresponding expressions for a soliton at rest[6] by the substitution $x\to(x-vt)/(1-v^2)^{1/2}$. The coefficients A, B, C, and D are found by substitution of Eq. (6) into the Schrödinger equation.

The electric current associated with the motion of electrons at a discrete level is usually found from Eq. (7):

$$j_0=v\nu_0,\tag{8}$$

where ν_0 is the multiplicity of the occupancy of the discrete level. The contribution of the continuous spectrum is found from the system of equations (6):

$$j_1=\sum\frac{-p[\varepsilon+pv-\Delta_1(1-v^2)^{1/2}]-\Delta_2v(1-v^2)^{1/2}/L}{\varepsilon[\varepsilon+pv-\Delta_1(1-v^2)^{1/2}]-\Delta_2(1-v^2)^{1/2}/L}.\tag{9}$$

The summation is carried out over the continuum states with $\lambda=-\varepsilon<0$. At low values of v, expansion of Eq. (9) yields (to within the first order in v)

$$j_1=\sum\frac{-p}{\varepsilon}+\frac{v\Delta_2}{L}\sum\frac{-1}{\varepsilon(\varepsilon-\Delta_1)}+\frac{v\Delta_2}{L}\sum\frac{p^2}{\varepsilon^2(\varepsilon-\Delta_1)^2}.\tag{10}$$

[Since a localized level λ_0 splits off from the valence band, the term with the wave number p_0 should be omitted from the sum in Eq. (10).] The second and third sums in Eq. (10) converge rapidly and can be calculated readily employing the substitution $\Sigma\to(L/\pi)\int dp$ (we allow here for the spin degeneracy):

$$\frac{v\Delta_2}{L}\sum\left(-\frac{1}{\varepsilon(\varepsilon-\Delta_1)}+\frac{p^2}{\varepsilon^2(\varepsilon-\Delta_1)^2}\right)$$
$$=\frac{\Delta_2^2}{\Delta_1^2}\left(1+\frac{2}{\pi}\arcsin\frac{\Delta_1}{\Delta}\right)$$
$$-\frac{\Delta_2\bar\Delta}{\Delta_1^2}-\frac{2}{\pi}\frac{\Delta_2}{\Delta_1}.\tag{11}$$

The first sum in Eq. (10) must be calculated rigorously. Going over from summation to integration we have to include corrections of the next order in L^{-1}, which contribute to the current in the zeroth order in L^{-1}. The allowed values of the wave number p can be found by adopting symmetric boundary conditions[1)] for the wave function $\Psi(x,t)$:

$$\Psi(x+L,\ t)=\Psi(x,\ t).\tag{12}$$

The wave function $\Psi(x,t)$ can be represented in the form

$$\Psi(x,\ t)=C_1\Psi_p(x,\ t)+C_2\Psi_{-p}(x,\ t),\tag{13}$$

where $\Psi_{\pm p}$ are the wave functions of Eq. (6) with the wave number $\pm p$ corresponding to one value of the parameter λ. To the left and right far from a soliton the wave function $\Psi(x,t)$ is described by Eqs. (6) and (13), where tanh ξ is replaced by ∓ 1, respectively. The functions $\Psi(x,t)$ and $\Psi(x+L,t)$ are related by a translation matrix T acting in the basis (Ψ_p, Ψ_{-p})

$$\Psi(x+L)=T\Psi(x,\ t), \tag{14}$$

where T is a 2×2 matrix the elements of which are readily obtained by the substitution of Eq. (13) into Eq. (14):

$$T=\begin{pmatrix} t_1 & t_2^* \\ t_2 & t_1^* \end{pmatrix}\frac{1}{p(\lambda+\Delta_1-i\Delta_2 v)}$$

$$t_1=(\lambda+\Delta_1+i\Delta_2)p\cos(pL)+i[\lambda^2+\lambda(\Delta_1+i\Delta_2)+i\Delta_2(\Delta_1+i\Delta_2)]\sin(pL),$$

$$t_2=i[\Delta_2 p\cos(pL)-(\bar{\Delta}^2+\lambda\Delta_1)\sin(pL)]. \tag{15}$$

The eigenvalues Λ of the matrix T are found from the equation

$$\Lambda^2-2\Lambda Q+\det T=0, \tag{16}$$

where

$$Q=\frac{1}{2}\operatorname{Tr}T=\frac{\lambda+\Delta_1}{\lambda+\Delta_1-i\Delta_2 v}\left[\cos(pL)-\frac{\Delta_2}{p}\sin(pL)\right].$$

The symmetric boundary conditions (12) correspond to the value $\Lambda = 1$, the substitution of which in Eq. (16) yields the equation for the determination of the values of the wave number p:

$$\cos(pL)-\frac{\Delta_2}{p}\sin(pL)=\frac{1}{2}\left(\frac{\lambda+\Delta_1}{\lambda+\Delta_1-i\Delta_2 v}+\frac{\lambda+\Delta_1-i\Delta_2 v}{\lambda+\Delta_1}\right). \tag{17}$$

If $v = 0$, Eq. (17) gives the allowed values of p for the case of a soliton at rest. Expanding Eq. (17) in powers of the velocity v, we find that terms of the first order in v vanish and, ignoring the terms of the second order in v, we find that the conditions for quantization of the wave number are the same as for a soliton at rest:

$$pL+\operatorname{arctg}(\Delta_2/p)=\pm\operatorname{arctg}(\Delta_2/p)+2\pi n.$$

Therefore, the first term in the expression for the current given by Eq. (10) vanishes to within v^2. The summation is carried out using the expression

$$\sum_n=2\int dp\frac{\partial n}{\partial p}.$$

Therefore, the current in a system with a moving soliton is

$$j=v\left[\nu_0+\frac{\Delta_2^2}{\Delta_1^2}\left(1+\frac{2}{\pi}\arcsin\frac{\Delta_1}{\bar{\Delta}}\right)-\frac{\Delta_2\bar{\Delta}}{\Delta_1^2}-\frac{2}{\pi}\frac{\Delta_2}{\Delta_1}-\frac{2\Delta_1}{\bar{\Delta}}\right]. \tag{18}$$

The corresponding charge is

$$q=\frac{j}{v}=\nu_0+\frac{\Delta_2^2}{\Delta_1^2}\left(1+\frac{2}{\pi}\arcsin\frac{\Delta_1}{\bar{\Delta}}\right)-\frac{\Delta_2\bar{\Delta}}{\Delta_1^2}-\frac{2}{\pi}\frac{\Delta_2}{\Delta_1}-\frac{2\Delta_1}{\bar{\Delta}}. \tag{19}$$

[In the case of an antikink with a deformation $\Delta(x,t)=\Delta_1-i\Delta_2\tanh\xi$ we have to modify Eqs. (18) and (19) by the substitution $\Delta_1\to-\Delta_1$.]

We can see that the charge (19) differs considerably from the local charge q_0 of a classical soliton at rest:

$$q_0=\nu_0-1+\frac{2}{\pi}\arcsin\frac{\Delta_1}{\bar{\Delta}}.$$

In the limiting cases we have

$$\begin{aligned}&\Delta_1\to 0:\ q_0=\nu_0-1,\ q=\nu_0-1/2,\\&\Delta_2\to 0:\ q_0=\nu_0-2,\ q=\nu_0-2.\end{aligned} \tag{20}$$

Note that current and charge of a quantum soliton considered in the lowest order of the semiclassical approximation are identical with the current and charge of a classical soliton moving at a constant velocity. We can see that the contribution to the current comes not only from the local soliton charge [representing the second term in Eq. (10)], but also from the charged background [third term in Eq. (10)]. It follows from Eq. (20) that in the case of a pure Peierls insulator ($\Delta_1 = 0$) introduction of an additional electron into the system ($\nu_0 = 1$) does not result in full compensation of the electric charge of the particle, in contrast to the classical limit, but the charge of the excitation (particle) becomes half-integral: $q = e/2$.

2. POLARON AND BIPOLARON CURRENT AND CHARGE IN THE PEIERLS MODEL

The results obtained above are readily generalized to excitations of the polaron and bipolaron type. By analogy with a kink, we shall show that the lowest semiclassical approximation is that of classical polarons and bipolarons moving at a constant velocity. The general solution for the deformation describing a pair of coupled domain walls (including the polaron and bipolaron states) is given by an expression which generalizes the results of Ref. (6):

$$\begin{aligned}&\Delta(x,\ t)=\bar{\Delta}-\tilde{\Delta}[\operatorname{th}(\xi+a/2)-\operatorname{th}(\xi-a/2)],\\&\tilde{\Delta}=\bar{\Delta}\operatorname{th}a,\quad \xi=\bar{\Delta}(x-vt)/(1-v^2)^{1/2}.\end{aligned} \tag{21}$$

For simplicity, we shall consider the case of a pure Peierls insulator ($\Delta_1=0$). The parameter a is found from the self-consistency conditions, which are of the same form as for $v=0$ (Ref. 6). The wave functions are found from the Schrödinger equations of the type given by Eq. (5).

In the case of states in a continuous spectrum, we obtain

$$\begin{aligned}&V=[A+iB\tilde{\Delta}\operatorname{th}(\xi-a/2)+F\tilde{\Delta}\operatorname{th}(\xi+a/2)]\exp(ipx-i\lambda t),\\&U=[C+iD\tilde{\Delta}\operatorname{th}(\xi+a/2)+G\tilde{\Delta}\operatorname{th}(\xi-a/2)]\exp(ipx-i\lambda t),\end{aligned} \tag{22}$$

where

$$V=[\psi_+(x)+\psi_-(x)]/\sqrt{2},\qquad U=(\psi_+-\psi_-)/\sqrt{2},$$

$$A=2(p-\lambda v)\,[1+(1-v^2)^{1/2}-p(p-i\Delta)v/\lambda]^{-1}B,$$

$$C=A(p-i\tilde{\Delta})/\lambda,$$

$$D=B\{(p-i\tilde{\Delta})/\lambda-v/[1+(1-v^2)^{1/2}]\}\{1-((p-i\tilde{\Delta})/\lambda)v/[1+(1-v^2)^{1/2}]\}^{-1},$$

$$F=iv[1+(1+v^2)^{1/2}]^{-1}D,\quad G=iv[1+(1+v^2)^{1/2}]^{-1}B,$$

$$|B|^2=(1/2L)\,(p^2-p\lambda v-\tilde{\Delta}^2pv/\lambda+\tilde{\Delta}^2+pv\tilde{\Delta}^2/\lambda-2\tilde{\Delta}/L)^{-1}.$$

The states in the discrete spectrum are then described by

$$U=\left[\frac{1}{\mathrm{ch}(\xi+a/2)}\pm\frac{iv}{1+(1-v^2)^{1/2}}\frac{1}{\mathrm{ch}(\xi-a/2)}\right]B\exp(-i\lambda_0 t+ip_0 x),$$
$$V=\left(\pm\frac{i}{\mathrm{ch}(\xi-a/2)}+\frac{v}{1+(1-v^2)^{1/2}}\frac{1}{\mathrm{ch}(\xi+a/2)}\right)B\exp(-i\lambda_0 t+ip_0 x), \tag{23}$$

where

$$\lambda_0=\pm\frac{\bar\Delta}{(1-v^2)^{1/2}\,\mathrm{ch}\,a},\qquad p_0=v\lambda_0,\quad |B|^2=\frac{\bar\Delta}{8}\frac{1+(1-v^2)^{1/2}}{(1-v^2)^{1/2}}.$$

Substituting the resultant quantities of Eqs. (22) and (23) into the expression for the current[4] we find, to within $O(v)$, that

$$j=\nu_0 v+\sum_\lambda\left[\frac{p}{\lambda}+\frac{p}{\lambda}\frac{1}{p^2+\bar\Delta^2}\frac{2\bar\Delta}{L}-\frac{v}{p^2+\bar\Delta^2}\frac{2\bar\Delta}{L}+\frac{2\bar\Delta}{L}v\frac{p^2}{\lambda^2}\frac{\lambda^2+\bar\Delta^2-\bar\Delta^2}{(p^2+\bar\Delta^2)^2}\right], \tag{24}$$

where the summation is carried out over the occupied states of the continuous spectrum. We note that since a localized level splits off from the valence band, the term with the wave number p_0 should be dropped from Eq. (24).

The final expression for the current is

$$j=v[\nu_0-2/\mathrm{ch}\,a-2\,\mathrm{th}\,a/(1+\mathrm{th}\,a)]. \tag{25}$$

We shall now consider the limiting cases. The case $a\to\infty$ corresponds to a pair of kinks which are not coupled and the current in the system is then $j=(\nu_0-1)v$, in agreement with the results obtained in Sec. 1 for a kink and antikink, each of which carries a current $j_1=(\nu_1-\frac{1}{2})v$, $j_2=(\nu_2-\frac{1}{2})v$, so that $j=j_1+j_2=(\nu_0-1)v$, where $\nu_0=\nu_1+\nu_2$ is the number of electrons at localized levels.

In the other limit when $a\to 0$ we have $j=(\nu_0-2)v$. In this case introduction of one electron at a local level into the system splits off two electrons from the valence band so that $\nu_0=3$ and the current is, as expected, given by $j=v$.

In the case of a polaron formed on introduction of one electron into the system ($\nu_0=3$ for the same reason as above; $\cosh a=\sqrt{2}$) gives a result different from the familiar local charge of a classical polaron ($q_{\mathrm{cl}}=e$):

$$q=(\sqrt{2}-1)e/(\sqrt{2}+1). \tag{26}$$

We have thus considered in a consistent manner the main type of excitations in the Peierls model. The results demonstrate that the motion of classical or quantum solitons gives rise to two types of vacuum current: 1) a current associated directly with a moving local vacuum charge; 2) a current distributed uniformly over the whole length of the chain and governed by the parameters of a given state. It is remarkable that the vacuum currents of both types exist both in the case of topological excitations (kinks) and in the case of polarons and bipolarons. Therefore, the observed effects cannot be attributed to the one-dimensional nature of the system. In the case of classical solitons the density of the uniform vacuum current is of the order of $1/L$, whereas in the quantum case (when the state as a whole is delocalized) the densities of all types are of the order of $1/L$. Of physical meaning is the integrated current

$$j=\int j(x)\,dx=qv.$$

In the case of classical solitons the uniform vacuum current cannot be found from the continuity equation

$$d\rho/dt+\mathrm{div}\,\mathbf{j}=0,$$

which gives only the local currents and charges.

Obviously, the results are in conflict with the usual ideas about the gradient invariance. We can show that in the presence of an electromagnetic field the wave functions are transformed in a guage-invariant manner and, in particular, the wave functions in a constant vector potential A acquire a factor $\exp[i(e/c)Ax]$, which ensures a correct periodicity in A. In an attempt to interpret the results in terms of the one-particle Hamiltonian for a soliton, where obviously we should have $j=eqv$, we obtain a gradient-noninvariant theory for a fractional value of q. This may mean that a one-particle long-wavelength approximation is invalid for a quantum soliton, i.e., the electron continuum must always be allowed for.

APPENDIX

We can find the allowed values of the quasimomentum p by substituting in Eq. (12) the periodic boundary conditions for the functions ψ_+ and ψ_-. We shall adopt here the periodic boundary conditions for the total wave function Ψ, which in the case of a half-filled energy band is

$$\Psi(n,t)=\psi_+(n,t)(i)^n+\psi_-(n,t)(-i)^n. \tag{A1}$$

The periodic conditions for $\Delta(x)$ in the case of a chain with one soliton $\Delta(x+L,t)=\Delta(x,t)$ require that the number of sites in the chain should be odd: $N=2n+1$. The periodicity conditions of of the wave functions of Eq. (A1) are $\Psi(n,t)=\Psi(n=N,t)$, and they lead to the relationship

$$\begin{pmatrix}\psi_+(n+N,t)\\ \psi_-(n+N,t)\end{pmatrix}=\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}\begin{pmatrix}\psi_+(n,t)\\ \psi_-(n,t)\end{pmatrix}=T\begin{pmatrix}\psi_+(n,t)\\ \psi_-(n,t)\end{pmatrix}. \tag{A2}$$

The matrix T had been calculated earlier [Eq. (15)]. In the case of Eq. (A2) we obtain the following equations for determination of quasimomentum p:

$$1+\det T+i(t_{22}-t_{11})=0$$

or to within $O(v)$,

$$\cos(pN)+\frac{\varepsilon^2-\varepsilon\Delta_1-\Delta_2^2}{p\Delta_2}\sin(pN)=\frac{\varepsilon-\Delta_1}{\Delta_2}. \tag{A3}$$

Since Eq. (A3) does not contain terms linear in v, calculation of the current does not give rise to any additional terms different from those discussed earlier. Therefore, the results obtained for the soliton current and charge are retained.

[1)]A different set of boundary conditions corresponding to a closed chain with an odd number of atoms is discussed in the Appendix.

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Translated by A. Tybulewicz