Quantum theory of topological solitons in a one-dimensional Peierls insulator

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A quantum theory is constructed for the neutral topological order-parameter soliton in a one-dimensional Peierls insulator of the *trans*-$(CH)_x$ type. A study is made of the analytical properties of the Green functions of the electrons in the field of the soliton. With the aid of these Green functions an integral dispersion equation is derived for small oscillations of the order parameter ("optical phonons") in an inhomogeneous Peierls insulator. It is shown that allowance for fluctuations of the phonons lowers the energy of the static soliton in comparison with its quasiclassical value. A mechanism is considered which brakes the moving soliton through the generation of "optical phonons." A nonlinear velocity dependence is found for the soliton kinetic energy.

INTRODUCTION

A large number of papers have appeared recently on the subject of the linear polymer polyacetylene $(CH)_x$. Experimental confirmation[1] of the spinless character of the current carriers in $(CH)_x$ permits the hypothesis that the conductivity of polyacetylene is due to topological solitons (see the review by Heeger and MacDiarmid[2]). Various measurements (electrical, magnetic, optical) confirm the presence of order-parameter solitons in $(CH)_x$. The generally accepted theoretical model[3–5] assumes that polyacetylene is a quasi-one-dimensional Peierls insulator with a doubled period of the carbon-atom lattice. There are two modifications of polyacetylene: *trans*-$(CH)_x$ and *cis*-$(CH)_x$. In the *trans* phase the gap Δ in the single-particle spectrum of the π electrons is a purely Peierls origin, while in the *cis* phase the gap has a "hard" component. The topological solitons in *trans*-$(CH)_x$ are in essence simply defects in the alternation of π bonds, and in the ideal lattice move freely along the chain.

The quasiclassical theory of these solitons was constructed in Refs. 3–5. Nakahara and Maki[6] first posed the problem of evaluating the quantum corrections to the soliton energy in the framework of the adiabatic model of the Peierls insulator. To obtain concrete answers those authors used the long-wavelength approximation in deriving the dispersion relation for phonons in the field of the soliton and employed a variational method for determining the bound-state energies and the scattering phase of the phonons. At the same time, for evaluating the quantum corrections to the soliton energy they used the exact (not the long-wavelength) phonon spectrum for a homogeneous Peierls insulator. The inconsistency of this approach casts doubt on the quantitative results of Ref. 6.

In the present paper we use the functional approach to construct a systematic quantum theory of topological solitons in a one-dimensional Peierls insulator with a doubled period. We analyze in detail the analytical structure of the Green functions of the electrons in the field of the soliton and use these Green functions to obtain an exact integral dispersion equation for phonons in an inhomogeneous Peierls insulator. Using the trace formulas and Levinson's theorem, we estimate the quantum correction ΔE_q to the quasiclassical energy E_s of the order-parameter soliton. This correction turns out to be negative, and for the actual parameters[2] of $(CH)_x$ we have $|\Delta E_q| \lesssim 0.5\, E_s$. We find the velocity dependence of the soliton kinetic energy with quantum effects taken into account. We show that at soliton velocities which are comparable to the characteristic phonon velocities of the Peierls lattice, there is a substantial renormalization of the effective soliton mass. All the calculations are carried out in the low-temperature limit.

FORMULATION OF THE MODEL

In the continuum approximation the Lagrangian density of a one-dimensional Peierls insulator is of the form $(\hbar = v_F = 1)^{4,5}$

$$\mathscr{L}=-\frac{\Delta^2}{g^2}+\bar{\Psi}_\sigma\left\{i\sigma_1\frac{\partial}{\partial t}-\sigma_3\frac{\partial}{\partial x}-\Delta\right\}\Psi_\sigma\frac{\Delta^2}{g^2\omega_0{}^2}. \qquad (1)$$

Here $\bar{\Psi}_\sigma = \Psi_\sigma{}^+\sigma_1$, where the Ψ_σ are spinor wave functions of the electron-hole field, σ is the spin-projection index, $\Delta(x,t)$ is the coordinate- and time-dependent order parameter, g is the electron-phonon coupling constant, ω_0 is the frequency of bare phonons with momentum $2k_F$ (k_F is the Fermi momentum), and $\sigma_{1,3}$ are Pauli matrices. Lagrangian (1) describes the interaction of a spinor field Ψ and a scalar field Δ. If we exclude the last term, which gives the kinetic energy of the lattice, Lagrangian (1) is the same as the familiar Gross-Neveu Lagrangian[7] from field theory. The applicability of mean field theory to the description of Peierls insulator (1) guarantees that the parameter $\alpha^2 = g^2\omega_0^2/\Delta_0^2$ is small ($\alpha^2 \ll 1$), where δ_0 is the equilibrium homogeneous order parameter. The physical meaning of the inequality $\alpha \ll 1$ is clear: Initially, within times $t_0 \sim \Delta_0{}^{-1}$, the single-particle spectrum of the Peierls insulator is formed at a fixed configuration of the lattice, and the scale of the lattice fluctuations is determined by the time $t_L \sim (g\omega_0)^{-1}$. Therefore, the temporal evolution of the order parameter $\Delta(t)$ is fixed by the largest time scale of the problem, t_L, and the time dependence can be neglected in all quantities of "electronic origin." The fact that α is small also permits one to develop a perturbation theory in α when constructing a quantum theory of solitons.

The topological soliton of model (1) is[7,4,5]

$$\Delta_s(x)=\Delta_0\,\mathrm{th}\,(x\Delta_0). \qquad (2)$$

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Our problem is to determine the quantum corrections to the soliton energy (2) at low temeperatures $\beta\Delta_0 \gg 1$. For this purpose let us consider the partition function Z for model (1). In the approximation of a gas of noninteracting solitons

$$Z=\int_0^\infty dv\int D\bar{\Psi}_\sigma D\Psi_\sigma D\Delta \exp\left\{\int dx\int_0^\beta d\tau \mathscr{L}_E\right\}, \qquad (3)$$

where $\mathscr{L}_E$ is Lagrangian (1) in the Euclidean space $it\to\tau$. The functional integral is quadratic in the fermion fields and can be evaluated exactly; the functional integral over Δ will be evaluated by perturbation theory:

$$\Delta(x,t)=\Delta_s(x-vt)+\delta(x,t), \qquad (4)$$

where $\delta(x,t)$ are fluctuations of the order parameter, v is the soliton velocity (in units of v_F), with $v\lesssim\alpha\ll 1$. Doing the integral over $\bar{\Psi}$ and Ψ, we get

$$Z=\int_0^\infty dvZ^{(0)}(v)\int D\delta\exp\left\{\int dx\int_0^\beta d\tau\mathscr{L}_L+{}^1/_2\,\mathrm{Sp}\ln(\hat{K}_0+\hat{K}_1)\right.$$
$$\left.-{}^1/_2\mathrm{Sp}\ln\hat{K}_0\right\}, \qquad (5)$$

where

$$Z^{(0)}(v)=\exp\left\{\frac{1}{2}\mathrm{Sp}\ln\hat{K}_0-\int dx\int_0^\beta d\tau\frac{\Delta_s^2}{g^2}\right\}. \qquad (6)$$

The symbol Sp is taken to mean

$$\mathrm{Sp}\,\hat{M}=\sum_\sigma \mathrm{tr}\int_{-\infty}^{\infty}dx\int_0^\beta d\tau\langle x\tau|\hat{M}|x\tau\rangle, \qquad (7)$$

where tr denotes summation over the matrix indices of the operator $\hat{M}$. The operators $\hat{K}_0$ and $\hat{K}_1$ are

$$\hat{K}_0=-\partial_\tau^2-\partial_x^2+\Delta_s^2+\sigma_3\Delta'+\sigma_1\dot{\Delta}_s, \qquad (8)$$

$$\hat{K}_1=\sigma_1\dot{\delta}+\sigma_3\delta'+2\Delta_s\delta+\delta^2. \qquad (9)$$

The lattice part $\mathscr{L}_L$ of the Lagrangian is of the form

$$\mathscr{L}_L=-\frac{1}{(g\omega_0)^2}\{\dot{\Delta}_s^2+2\dot{\Delta}_s\dot{\delta}+\dot{\delta}^2\}-\frac{1}{g^2}(\delta^2+2\Delta_s\delta). \qquad (10)$$

In (8)–(10) all the time derivatives are taken with respect to the imaginary time τ.

As we have already mentioned, the time derivatives of Δ_s and δ in the electron operators $\hat{K}_0$ and $\hat{K}_1$ can be dropped, and then $Z^{(0)}$ can be taken outside of the integral over v.

THE QUASICLASSICAL TOPOLOGICAL SOLITON

We evaluate the spur of the elliptic operator $\hat{K}_0$ using the generalized ζ-function method (Ref. 8, see also Ref. 9). By definition

$$\zeta(s)=\sum_\alpha \lambda_\alpha^{-s}, \qquad (11)$$

λ_α is the set of eigenvalues of the operator $\hat{K}_0$, and

$$\mathrm{Sp}\ln\hat{K}_0=-\zeta'(0)-\zeta(0)\ln C_R^2, \qquad (12)$$

where C_R is a normalization constant (see below).

It is not hard to see that the complete orthonormalized set of solutions of the equation

$$\hat{K}_0\begin{pmatrix}u\\v\end{pmatrix}=\lambda_\alpha\begin{pmatrix}u\\v\end{pmatrix} \qquad (13)$$

on the interval $-L/2\leqslant x\leqslant L/2$ (L is the length of the cabin, henceforth assumed infinite) and $0\leqslant\tau\leqslant\beta$ with the necessary antiperiodicity in τ is (see also Ref. 4)

$$\begin{pmatrix}u_{sc}\\v_{sc}\end{pmatrix}=\frac{1}{(2\beta L)^{1/2}}e^{ikx-i\omega_n\tau}\begin{pmatrix}1\\(k^2+\Delta_0^2)^{-1/2}\varepsilon\Delta_0(ik/\Delta_0-\mathrm{th}\,x\Delta_0)\end{pmatrix}. \qquad (14)$$

The eigenvalues are $\lambda_{sc}=k^2+\omega_n^2+\Delta_0^2$, where $\varepsilon=\pm 1$, $\omega_n=(2n+1)\pi/\beta$, n is an integer $(-\infty<n<\infty)$ and

$$\begin{pmatrix}u_b\\v_b\end{pmatrix}=\left(\frac{\Delta_0}{4\beta}\right)^{1/2}e^{-i\omega_n\tau}\begin{pmatrix}0\\\mathrm{ch}^{-1}(x\Delta_0)\end{pmatrix} \qquad (15)$$

with $\lambda_b=\omega_n^2$. The functions Ψ_{sc} correspond to scattering states and Ψ_b to bound states of the electron to the soliton. The completeness condition in terms of the wave functions u, v is[1)]

$$2\sum_\alpha u_\alpha(x,\tau)u_\alpha^*(x',\tau')=2\sum_\alpha v_\alpha(x,\tau)v_\alpha^*(x',\tau')$$
$$=\delta(x-x')\delta(\tau-\tau'). \qquad (16)$$

If electron-electron correlations are ignored and there is no external magnetic field, allowance for the electron spin in (1) amounts to a trivial doubling of the components of the field Ψ. To simplify the notation we shall write out the wave functions for a spinless "electron" (13)–(16) and take the spin into account by multiplying by the statistical factor of 2 in the final expressions [the sum over spin projections σ in (6)].

We note that the bound-state functions (15) are normalized to one-half the fermion number [only for such a relative normalization of (14) and (15) can completeness condition (16) be satisfied]. The nontrivial normalization of the zeroth mode is of a general character for fermion systems in the presence of topological solitons (in this regard see the detailed discussion in Ref. 10). For "spinless electrons" this normalization means that topological order-parameter solitons carry a half-integer electric charge ($+|e|/2$ for an unfilled level, $-|e|/2$ for $n_0=1$; here $n_0=0$, 1 is the occupation number of the level). The presence of spin leads to a doubling of the components, wave function (15) is normalized to unity (here, of course, the maximum occupation number doubles, $n_0=0$, 1, 2, and we have a nontrivial spin-charge relation for the topological soliton ($n_0=0$, 2; $s=0$; $Q=\pm|e|$; $n_0=1$; $s=\pm 1/2$; $Q=0$).[3,4] Let us briefly remark on the connection between the spectrum of the electrons in the field of the soliton and the supersymmetry.[2)] For this purpose we rewrite Eq. (13) in the form

$$H_{ss}\Psi=\lambda\Psi,\quad H_{ss}={}^1/_2(-\partial_x^2+\Delta_s^2+\sigma_3\Delta_s'),\quad \lambda={}^1/_2(\lambda_\alpha-\omega_n^2). \qquad (13a)$$

The operator H_{ss} is the model Hamiltonian for supersymmetric quantum mechanics. As we know, one of the basic properties of supersymmetry is that the ground-state energy goes to zero. The spectrum of H_{ss} depends importantly[12] on the topology of the "potential" $\Delta_s(x)$. If $\Delta_s(x)$ has an odd number of zeros [as for the case of topological soliton (2)], the supersymmetry of model (13), (13a) is not broken and, consequently, there always exists a nondegenerate level $\lambda=0$

($\lambda_\alpha = \omega_n^2$); the zero-frequency mode. All the remaining levels are doubly degenerate, which in the present problem implies a degeneracy of the particle and hole energies.

If $\Delta_s(x)$ has an even number of zeros or no zeros at all (in particular, this is the case when the potential $\Delta_s(x)$ is the polaron of a Peierls insulator),[13] the supersymmetry is spontaneously broken and the ground-state energy level is positive: $\lambda > 0$. Therefore, the energy of the electron bound state in a lattice field of the polaron configuration is always positive.

One is readily convinced that the condition

$$\sum_\alpha (|v_\alpha|^2-|u_\alpha|^2)=0$$

implies exact compensation of the local change in the charge density of the neutral soliton $n_0 = 1$ (Refs. 3, 4).

According to (5), (6), and (12), the energy density of a Peierls insulator with a single static soliton in neglect of fluctuations is

$$\mathscr{E}=-\lim_{\beta\to\infty}\frac{1}{L\beta}\ln Z^{(0)}=\frac{\Delta_0^2}{g^2}+\frac{1}{L}\int dx\frac{\Delta_s^2(x)-\Delta_0^2}{g^2}+\frac{1}{2\beta L}\{\zeta'(0)+\zeta(0)\ln C_R^2\}. \quad (17)$$

Here the generalized ζ function is constructed from the spectrum (14), (15) with a density of states $n(k) = (L + \chi'(k))/2\pi$ which incorporates the phase of the scattering of the elementary excitations by the soliton[7]:

$$\zeta(s)=2L\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\lambda_{sc}^{-s}+2\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\chi'(k)\lambda_{sc}^{-s}+2\sum_{n=-\infty}^{\infty}\lambda_b^{-s}, \quad (18)$$

where $\chi(k) = \pi - 2\arctan(k/\Delta_0)$ is the phase of the scattering of the electron by the kink. The factor of 2 takes the electron spin into account. The renormalization constant C_R is fixed in the limit $L\to\infty$, and, according to Ref. 9, is

$$C_R=\Delta_0\exp(\pi/g^2). \quad (19)$$

Omitting the inessential details, we obtain for $\beta\Delta_0 \gg 1$

$$\mathscr{E}=-\frac{\Delta_0^2}{2\pi}+\frac{1}{L}\frac{2\Delta_0}{\pi}. \quad (20)$$

The second term in (20) is the quasiclassical energy of a soliton in a Peierls insulator and, naturally, coincides with the energy of a Gross-Neveu soliton ($N = 2$; see Ref. 7 and also Refs. 4 and 5).

For $T \neq 0$ the energy ε is replaced by the free energy F, and a calculation of (18) gives (see also Ref. 9)

$$F=F_0(T,\Delta)+\frac{1}{L}\frac{2\Delta(T)}{\pi}, \quad (21)$$

where $F_0(T)$ is the free energy density of a Peierls insulator with a homogeneous order parameter, and $\Delta(T)$ is the equilibrium value of the order parameter at the given temperature T:

$$\left.\frac{\partial F_0(\Delta,T)}{\partial\Delta}\right|_{\Delta=\Delta(T)}=0. \quad (22)$$

The formulas for $F_0(\Delta,T)$ and $\Delta(T)$ can be obtained in explicit form only in the low-temperature ($\beta\Delta \gg 1$) and high-temperature ($\beta\Delta \ll 1$) limits.[9]

The soliton motion is associated with a straining of the lattice, and so its maximum velocity is $v_m \sim \alpha v_f \ll v_F$. By virtue of the Lorentz invariance of the electronic part of Lagrangian (1) the motion correction to the quasiclassical soliton energy does not exceed α^2. Therefore, the velocity must be taken into account only in the lattice terms, since the soliton mass is $M_s \sim \Delta_0/\alpha^2$ and is much larger than the mass of a free fermion.[4]

COLLECTIVE VIBRATIONS IN A PEIERLS INSULATOR. QUANTUM CORRECTIONS TO THE ENERGY

The quantum corrections to Z are contained in the factor $Z/Z^{(0)}$. Let us expand the last two terms in (5) to second order in δ and δ':

$$\tfrac{1}{2}\,\mathrm{Sp}\ln(\hat{K}_0+\hat{K}_1)-\tfrac{1}{2}\,\mathrm{Sp}\ln\hat{K}_0\approx\tfrac{1}{2}\,\mathrm{Sp}(\hat{K}_0^{-1}\hat{K}_1)-\tfrac{1}{4}\,\mathrm{Sp}(\hat{K}_0^{-1}\hat{K}_1\hat{K}_0^{-1}\hat{K}_1). \quad (23)$$

For the operator $\hat{K}_0$ the resolvent, defined by the equation

$$\hat{K}_0\hat{G}_0=\hat{I}_2\delta(x-x')\delta(\tau-\tau'),$$

is

$$\hat{G}_0(x\tau|x'\tau')=\langle x\tau|\hat{K}_0^{-1}|x'\tau'\rangle=\sum_{\substack{\alpha\\ \varepsilon=\pm1}}\frac{1}{\lambda_\alpha}\times\begin{pmatrix}u_\alpha(x,\tau)\\ \varepsilon v_\alpha(x,\tau)\end{pmatrix}(u_\alpha^*(x',\tau'),\varepsilon v_\alpha^*(x',\tau'))=\sum_\alpha\frac{1}{\lambda_\alpha}\begin{pmatrix}2u_\alpha u_\alpha^* & 0\\ 0 & 2v_\alpha v_\alpha^*\end{pmatrix}=\begin{pmatrix}g_{11} & 0\\ 0 & g_{22}\end{pmatrix}. \quad (24)$$

Let us first consider the first term on the right-hand side of (23)

$$\tfrac{1}{2}\,\mathrm{Sp}\,\hat{K}_0^{-1}\hat{K}_1=\tfrac{1}{2}\sum_\sigma \mathrm{tr}\int dx\int_0^\beta d\tau\,\hat{G}_0(x\tau|x\tau)\hat{K}_1(x\tau)=\int dx\int_0^\beta d\tau\{\delta'(g_{11}-g_{22})+(2\Delta_s\delta+\delta^2)(g_{11}+g_{22})\}. \quad (25)$$

The explicit form of the functions $g_{11}(x\tau|x'\tau')$ and $g_{22}(x\tau|x'\tau')$ for $\beta\Delta_0 \gg 1$ is

$$g_{11}(x\tau|x'\tau')=\frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty}dk\,d\omega\frac{\exp[ik(x-x')-i\omega(\tau-\tau')]}{k^2+\omega^2+\Delta_0^2}, \quad (26)$$

$$g_{22}(x\tau|x'\tau')=g_{11}(x\tau|x'\tau')-\frac{\Delta_0}{(2\pi)^2}\iint\frac{dk\,d\omega}{\omega^2}\times\frac{\exp[ik(x-x')-i\omega(\tau-\tau')]}{k^2+\omega^2+\Delta_0^2}\{\Delta_0(\mathrm{th}\,x\Delta_0\,\mathrm{th}\,x'\Delta_0-1)+ik(\mathrm{th}\,x\Delta_0-\mathrm{th}\,x'\Delta_0)\}. \quad (27)$$

Equation (27) contains a singular integral, and we must give a prescription for its evaluation. As we know, upon the analytical continuation $\omega\to i\omega$ the Matsubara Green function is the same as the retarded. Denoting the second term in (27) as $g_s(x\tau|x'\tau')$, we have the important relation

$$\int_{-\infty} d\omega^2 g_s(x,x'|i\omega)=0, \quad (28)$$

[equivalent to $\mathrm{Im} g_s(x,x'|i\omega)$], which expresses the law of conservation of particle number in the presence of the soliton.

It is clear from (28) that the regularization of the singular integral (27) amounts to taking into account only its principal value. The question of circumventing the zero-frequency mode in constructing the Green functions in quantum field theory has been discussed only for scalar models of the sine-Gordon and φ_2^4 types.[14] Reasoning that the zero-frequency mode in this case corresponds to the collective coordinate of the isoenergetic motion of the soliton and therefore cannot contribute to the imaginary part of the polarization operator, Abbott[14] concluded that the rule for circumventing the zero-frequency mode amounts to taking just the principal value of the integral. Our analysis shows that an analogous rule (the singular integrals for the Green functions should be evaluated by the Sokhotskiĭ formulas, and for the zero-frequency mode only the real part is retained) also applies in the fermion theories, although the physical justification for such a regularization procedure is a completely different. The coincidence of the rules for bypassing the zero-frequency mode is of course, dictated by the analytical structure of the integrals, and can evidently be explained by a hidden supersymmetry of the theory, since the zero-frequency modes in the boson and fermion sectors are related by a supersymmetry transformation.

Finally, for the inhomogeneous part g_s of the Green function we find

$$g_s(x\tau|x'\tau')=-\frac{\Delta_0^2}{(2\pi)^2}\iint dk\,d\omega\frac{e^{-i\omega(\tau-\tau')}-1}{\omega^2(k^2+\Delta_0^2+\omega^2)}$$
$$\times e^{ik(x-x')}\left\{\mathrm{th}\,x\Delta_0\,\mathrm{th}\,x'\Delta_0-1+i\frac{k}{\Delta_0}(\mathrm{th}\,x\Delta_0-\mathrm{th}\,x'\Delta_0)\right\}. \quad (29)$$

It is easy to see that $g_s(x\tau|x'\tau)=0$. Together with the self-consistency condition

$$\frac{\delta}{\delta\Delta(x)}\left\{\iint dx\,d\tau\frac{\Delta_s^2}{g^2}-\frac{1}{2}\mathrm{Sp}\ln\hat{K}_0\right\}=0, \quad (30)$$

or

$$g^{-2}=\mathrm{Sp}\,\hat{G}_0(x\tau|x\tau), \quad (31)$$

this gives the correction $\Delta_0=\Delta_0(L\to\infty)+O(1/L)$ solely in terms of the change in the density of scattering states.

With allowance for the self-consistency equation $g^{-2}=2g_{11}(x\tau|x\tau)$ we have

$$\iint dx\,d\tau\,\mathscr{L}_L+\frac{1}{2}\mathrm{Sp}\,\hat{K}_0^{-1}\hat{K}_1$$
$$=\frac{1}{(g\omega_0)^2}\iint dx\,d\tau\{-\dot{\delta}^2-\dot{\Delta}_s^2+2\delta\ddot{\Delta}_s\}. \quad (32)$$

Let us analyze the last term in (23):

$$\tfrac{1}{4}\mathrm{Sp}(\hat{K}_0^{-1}\hat{K}_1\hat{K}_0^{-1}\hat{K}_1)=\iint dx\,d\tau\,dx'\,d\tau'\{(\delta'\tilde{\delta}'+4\Delta_s\tilde{\Delta}_s\delta\tilde{\delta})$$
$$\times|g_{11}|^2-\tfrac{1}{2}\delta\tilde{\delta}D_xD_{x'}(|g_{11}|^2-|g_{22}|^2)\}\equiv\iint dx\,d\tau J(x,\tau). \quad (33)$$

Here

$$D_y=d/dy+2\Delta_s(y),\quad g_{11}=g_{11}(x\tau|x'\tau'),\quad g_{22}=g_{22}(x\tau|x'\tau'),$$

and the tilde denotes a dependence on the arguments (x',τ'). In (33) we have retained terms which are quadratic in the fluctuations.

First, using (32) and (33), we obtain the spectrum of small oscillations of the order parameter of a homogeneous Peierls insulator. In $J(x,\tau)$ it is natural to separate the terms due to homogeneous-vacuum fluctuations Δ_0 from the soliton-governed terms. The first group of terms, which we denote J_0, is

$$J_0=\iint dx'\,d\tau'\{\delta'(x,\tau)\delta'(x',\tau')$$
$$+4\Delta_0^2\delta(x,\tau)\delta(x',\tau')\}|G_0(x\tau|x'\tau')|^2, \quad (34)$$

where

$$G_0(x\tau|x'\tau')=\frac{1}{2\pi\beta}\sum_n\int dk\frac{\exp[ik(x-x')-i\omega_n(\tau-\tau')]}{k^2+\omega_n^2+\Delta_0^2}. \quad (35)$$

The inequality $\alpha\ll1$ permits making J_0 local in τ.

Characteristically, in fact, $\tau\sim(g\omega_0)^{-1}$, while in the kernel G_0 we have for the scale of the difference $\tau-\tau'\Delta_0^{-1}$. Therefore, in the curly brackets in (34) we can make the replacement $\delta(x',\tau')\to\delta(x',\tau)$.

The equation of motion for fluctuations in the homogeneous case is

$$\delta S_0^{(\delta)}=0,\quad S_0=\iint dx\,d\tau\,\mathscr{L}_0^{(\delta)}, \quad (36)$$

where

$$\mathscr{L}_0^{(\delta)}=-\frac{\dot{\delta}^2}{(g\omega_0)^2}-\iint dx'\,d\tau'\{\delta'(x,\tau)\delta'(x',\tau)$$
$$+4\Delta_0^2\delta(x,\tau)\delta(x',\tau)\}|G_0(x\tau|x'\tau')|^2. \quad (37)$$

Substituting $\delta\propto\exp(ikx-i\omega\tau)$ in (37), we obtain, after analytical continuation to the real-frequency axis,[6]

$$\omega^2(k)=\frac{(g\omega_0)^2}{\pi}\frac{(1+\zeta^2)^{1/2}}{\zeta}\mathrm{Arsh}\,\zeta,\quad \zeta=k/2\Delta_0. \quad (38)$$

In the long-wavelength limit $k\ll\Delta_0$ spectrum (38) has the form[15]

$$\omega^2(k)\approx\frac{(g\omega_0)^2}{\pi}\left[1+\frac{k^2}{12\Delta_0^2}\right]. \quad (39)$$

Let us find the phonon spectrum in a Peierls insulator in the presence of a topological order-parameter soliton. The corresponding integral dispersion equation, according to (32) and (33) for $\delta(x,\tau)=\delta(x)e^{i\omega\tau}$, is

$$\omega_\alpha^2(g\omega_0)^{-2}\delta_\alpha(x)-\int dx'\delta_\alpha(x')R(x,x')=0, \quad (40)$$

where the kernel is

$$R(x,x')=\int d\tau' e^{i\omega(\tau-\tau')}\left\{\frac{d^2}{dx\,dx'}|g_{11}|^2+4\Delta_s\tilde{\Delta}_s|g_{11}|^2\right.$$
$$\left.-\frac{1}{2}D_xD_{x'}(|g_{11}|^2-|g_{22}|^2)\right\}. \quad (41)$$

The first two terms in (41) do not contain the inhomogeneous part g_s of the Green function, and their analysis presents no difficulty. The last term in the polarization operator (41) contains both linear and quadratic (in g_s) contributions. The linear terms in the leading approximation for $\alpha \ll 1$ can be written in the form

$$\int_{-\infty}^{\infty} d(\tau'-\tau)\, e^{-i\omega(\tau'-\tau)} \left\{ g_{11}(x\tau|x'\tau')\, g_s(x'\tau'|x\tau) + \begin{pmatrix} x \leftrightarrow x' \\ \tau \leftrightarrow \tau' \end{pmatrix} \right\}$$

$$\approx -\frac{\Delta_0^2}{4\pi^3} \iiint dk\,dq\,d\Omega \cdot \frac{\exp[i(k-q)(x-x')]}{(k^2+\Delta_0^2)(k^2+\Omega^2+\Delta_0^2)(q^2+\Omega^2+\Delta_0^2)}$$

$$\times \frac{\operatorname{ch}(x-x')\Delta_0 + i(q/\Delta_0)\operatorname{sh}(x-x')\Delta_0}{\operatorname{ch} x\Delta_0 \operatorname{ch} x'\Delta_0}. \qquad (42)$$

Upon integration of the term $g_s(x\tau|x'\tau')g_s(x'\tau'|x\tau)$ over $\tau-\tau'$ it turns out that the main contribution to the integral is from the soliton level with energy equal to zero (the zero-frequency mode), and therefore the function g_s can be replaced by an averaged value which does not take into account the contribution of the scattering states, i.e.,

$$g_s(x\tau|x'\tau') \approx -{}^1/_4\Delta_0|\tau-\tau'|\operatorname{ch}^{-1}(x\Delta_0)\operatorname{ch}^{-1}(x'\Delta_0), \qquad (43)$$

which has a time average of zero. It is scarcely possible to give an exact analysis of the structure of $R(x,x')$, but it can be inferred that, at least at large distances $|x-x'| \gg \Delta_0^{-1}$, the soliton acts as a potential well for phonons.

The kernel $R(x,x') = R(x',x)$ is symmetric, and so one can use the trace formula (see, e.g., Ref. 16)

$$\sum_\alpha \omega_\alpha^2 = (g\omega_0)^2 \int dx R(x,x). \qquad (44)$$

Since we are interested in soliton effects, we subtract from (44) the homogeneous-vacuum contribution

$$\sum_\alpha \omega_\alpha^2 - \frac{L}{2\pi}\int dk\omega^2(k) = (g\omega_0)^2 \int dx \left\{ -\frac{4}{\operatorname{ch}^2 x\Delta_0}\overline{|g_{11}|^2} - \frac{1}{2} D_x D_{x'} \overline{(|g_{11}|^2 - |g_{22}|^2)} \right\}_{x'=x}. \qquad (45)$$

Here the superior bar denotes an averaging of (41) over $(\tau-\tau')$. Substituting in (45) the explicit form of the Green functions, we find

$$R_s(x,x) = -\frac{\Delta_0}{2\pi}\operatorname{ch}^{-2}(x\Delta_0)\left(\pi + \ln\frac{2k_F}{\Delta_0}\right) + \frac{\Delta_0}{8}\left(1-\frac{2}{\pi}\right)\operatorname{ch}^{-4}(x\Delta_0). \qquad (46)$$

Thus

$$\sum_\alpha \omega_\alpha^2 - \frac{L}{2\pi}\int dk\omega^2(k) = (g\omega_0)^2\left\{-\frac{7}{6} - \frac{1}{18\pi} - \frac{1}{\pi}\ln\frac{2k_F}{\Delta_0}\right\}. \qquad (47)$$

On the other hand, the left side of (47) can be written as the sum of the squares of the bound-state frequencies and an integral over the energies of the scattering states. Taking into account the change of the density of continuum states in the field of the soliton (see, e.g., Ref. 17), we have

$$\sum_\alpha \omega_\alpha^2 - \frac{L}{2\pi}\int dk\omega^2(k) = \sum_{i=1}^{m} \omega_i^2 + \int_{\bar\omega}^{\omega_F} \rho(\omega)\omega^2 d\omega, \qquad (48)$$

where $\omega_i < \bar\omega$ are the frequencies of the bound states of the phonons at the soliton, m is the number of bound states,

$$\bar\omega = g\omega_0/\pi^{1/2},$$
$$\rho(\omega) = \eta'(\omega)/\pi,$$

$\eta(\omega)$ is the phonon–soliton scattering phase, $\omega^2(k)$ is given by (38), and $\omega_F = \omega(k_F)$. It follows from (47) and (48) that $\rho(\omega) < 0$, and we have

$$\sum_{i=1}^{m} \omega_i^2 - \int_{\bar\omega}^{\omega_F} d\omega|\rho(\omega)|\omega^2 = -(g\omega_0)^2\left(\frac{7}{6} + \frac{1}{18\pi} + \frac{1}{\pi}\ln\frac{2k_F}{\Delta_0}\right). \qquad (49)$$

The quantity on the right-hand side of (49) is a lower bound on the sum which determines the quantum correction ΔE_q to the soliton energy:

$$\Delta E_q = \sum_{i=1}^{m} \omega_i - \int_{\bar\omega}^{\omega_F} d\omega\omega|\rho(\omega)|. \qquad (50)$$

In fact, by virtue of the translational invariance of the problem (the continuum approximation), the spectrum of frequencies ω_α contains a mode $\omega_0 = 0$, and all the other bound-state energies satisfy the inequality $0 < \omega_i < \bar\omega$. Further, since the integral over the scattering-state frequencies is a monotonically increasing function of the upper limit, we have

$$\frac{1}{\bar\omega}\left\{\sum_{i=1}^{m}\omega_i^2 - \int_{\bar\omega}^{\omega_F} d\omega\omega^2|\rho(\omega)|\right\} \leqslant \Delta E_q \leqslant \bar\omega\left\{m - \int_{\bar\omega}^{\omega_F} d\omega|\rho(\omega)|\right\}. \qquad (51)$$

In the last integral in inequality (51) the upper limit of integration in the leading approximation for $\alpha \ll 1$ $(\omega_f \gg \omega)$ can be replaced by infinity. But then, according to Levinson's theorem (see, e.g., Ref. 18), the right-hand side of inequality (51) is equal to zero. Therefore, the quantum correction to the soliton energy is always negative, and for polyacetylene ($2k_F \approx 10$ eV, $\Delta_0 \approx 0.7$ eV) its absolute value is not more than $\approx 50\%$.

Let us finally consider the contribution of the collective mode to the kinetic energy of the moving soliton. We write

$$Z_q = \frac{Z}{Z_0} = \int_0^\infty dv \exp\left(-\iint dx\,d\tau \frac{\dot\Delta_s^2}{(g\omega_0)^2}\right)\int D\delta \times \exp\left(\iint dx\,d\tau \mathscr{L}_{eff}\right), \qquad (52)$$

where

$$\mathscr{L}_{eff} = -\dot\delta^2 + 2\delta\Delta_s(g\omega_0)^{-1} - (g\omega_0)^2 J(x,\tau). \qquad (53)$$

After an elementary integration of the quadratic (in δ) form in the argument of the exponential in (52), we have

$$Z_q = \int_0^\infty dv \exp\left\{-\frac{1}{2}\operatorname{Sp}\ln D\right\}\exp\left\{-\iint dx\,d\tau\frac{\dot\Delta_s^2}{(g\omega_0)^2} - \iint dx\,d\tau\,dx'\,d\tau' D^{-1}(x\tau|x'\tau')\ddot\Delta_s(x,\tau)\ddot\Delta_s(x',\tau')(g\omega_0)^{-2}\right\}. \qquad (54)$$

Here

$$D = -\partial_\tau^2 - \hat\delta J(x,\tau)/\hat\delta\delta(x,\tau), \qquad (55)$$

the symbol $\hat\delta$ denotes a variational derivative, and D^{-1} is the phonon Green function.

We define the soliton kinetic energy:

$$\mathscr{E}_k^{(s)}=v\frac{\partial L_{eff}^{(e)}}{\partial v}-L_{eff}^{(e)}, \tag{56}$$

where v is the velocity of the soliton, and

$$L_{eff}^{(e)}=-\lim_{\beta\to\infty}\frac{\beta^{-1}}{(g\omega_0)^2}\times\left\{\iint dx\,d\tau\dot{\Delta}_s^2+\iint dx\,d\tau\,dx'\,d\tau' D^{-1}(x\tau|x'\tau')\times\ddot{\Delta}_s(x,\tau)\ddot{\Delta}_s(x',\tau')\right\},\quad \Delta_s=\Delta_0\,\mathrm{th}(x-iv\tau). \tag{57}$$

The first term in (57) after substitution in (56) gives[4] simply $1/2\,M_s v^2$, where

$$M_s={}^8/_3\Delta_0(\Delta_0/g\omega_0)^2. \tag{58}$$

Analysis of the second term in (57) shows that in the leading approximation in the parameter $(\beta\bar{\omega})\ll 1$ the exact phonon Green function can be replaced by the function $D_0^{-1}(x\tau|x'\tau')$, which is a solution of the equation

$$-\partial_\tau^2 D_0^{-1}(x\tau|x'\tau')-\iint dy\,d\theta|G_0(x\tau|y\theta)|^2\times\{\partial_y^2 D_0^{-1}(y\theta|x'\tau')-4\Delta_0^2 D_0^{-1}(y\theta|x'\tau')\}=\delta(x-x')\delta(\tau-\tau'). \tag{59}$$

It follows from (59) that

$$D_0^{-1}(x\tau|x'\tau')=\frac{1}{(2\pi)^2}\iint dk\,d\Omega\frac{\exp\{ik(x-x')-i\Omega(\tau-\tau')\}}{\Omega^2+\omega^2(k)}. \tag{60}$$

After straightforward manipulations we have

$$\mathscr{E}_k^{(s)}=\frac{1}{2}M_s v^2-\frac{2}{\pi}\left(\frac{\Delta_0}{g\omega_0}\right)^4 v^4[3f(v^2)+2vf'(v^2)], \tag{61}$$

where

$$f(v^2)=\frac{\pi^2(g\omega_0)^2}{2\Delta_0^4}\int_0^\infty dk\frac{k^4\,\mathrm{sh}^{-2}(k\pi/2\Delta_0)}{\omega^2(k)-k^2v^2}. \tag{62}$$

In deriving (61) and (62) we have made use of the relation:

$$\lim_{\beta\to\infty}\frac{1}{2\pi\beta}\int_0^\beta d\tau\int_0^\beta d\tau'\exp[i(\Omega-kv)(\tau-\tau')]=\delta(\Omega-kv). \tag{63}$$

It is by virtue of (63) that we can replace D^{-1} by D_0^{-1} in (57). In fact, the difference $D^{-1}-D_0^{-1}$ after the substitution $x\to x-v\tau$ contains terms of the form $\varphi(x+v\tau)$ which, upon integration over τ, converge in the limit $\beta\to\infty$ and are smaller than $\delta(\Omega-kv)$ by a factor of order $(\beta\bar{\omega})^{-1}\ll 1$.

In dimensionless units

$$\mathscr{E}_k^{(s)}=\bar{v}^2\Delta_0\left\{\frac{1}{3\pi}-2\bar{v}^2[3\bar{f}(\bar{v}^2)+2\bar{v}\bar{f}'(\bar{v}^2)]\right\}, \tag{64}$$

where

$$\bar{f}=\int_0^\infty dx\frac{x^5\,\mathrm{sh}^{-2}(\pi x)}{(1+x^2)^{1/2}\,\mathrm{Arsh}x-\bar{v}^2x^3};\qquad \bar{v}=(4\pi)^{1/2}v\left(\frac{\Delta_0}{g\omega_0}\right). \tag{65}$$

The real part of f [the principal value of integral (65)] describes the renormalization of the soliton kinetic energy, while the imaginary part of f is the Landau damping due to the generation of "phonons." Numerical analysis shows that for $\bar{v}<\bar{v}_c\approx 5$ the imaginary part $\mathrm{Im}\mathscr{E}_k^{(s)}$ is exponentially small, and

$$\mathscr{E}_k^{(s)}\approx\Delta_0\bar{v}^2(1/3\pi-\bar{v}^2/5\pi). \tag{66}$$

It is seen from (66) that even at velocities $\bar{v}\ll\bar{v}_c$ the effective soliton mass is substantially renormalized, and the self-similar solution $\Delta_s=\Delta_0\mathrm{th}(\Delta_0(x-vt))$ in fact loses meaning even for $\bar{v}\leqslant(5/6)^{1/2}$.

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[1)]The correction $\sim O(L^{-1})$ in (16) is due to the change in the density of scattering states cancels with the corresponding change in normalization (14). Therefore, we immediately drop terms $\sim O(L^{-1})$ in (14).

[2)]For another aspect of the problem of the relation of the supersymmetry and the zero-frequency mode see Ref. 11.

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