PHYSICAL REVIEW B VOLUME 57, NUMBER 5 1 FEBRUARY 1998-I

Density of neutral solitons in weakly disordered Peierls chains

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(Received 8 July 1997; revised manuscript received 2 October 1997)

We study the effects of weak off-diagonal disorder on Peierls systems with a doubly degenerate ground state. We show that for these systems disorder in the electron hopping amplitudes induces a finite density of solitons in the minimal-energy lattice configuration of a single chain. These disorder-induced dimerization kinks are neutral and have spin $\frac{1}{2}$. Using a continuum model for the Peierls chain and treating the lattice classically, we analytically calculate the average free energy and density of kinks. We compare these results to numerical calculations for a discrete model and discuss the implications of the kinks for the optical and magnetic properties of the conjugated polymer *trans*-polyacetylene. [S0163-1829(98)05405-8]

I. INTRODUCTION

Recently we considered the effects of weak disorder in the electron hopping amplitudes on the lattice configuration of Peierls systems with a doubly degenerate ground state, using the conjugated polymer *trans*-polyacetylene as an example.[1] In the absence of disorder the ground state of a *trans*-polyacetylene chain is uniformly dimerized due to the interaction of the lattice with the half-filled band of π electrons propagating along the chain.[2] The ground-state energy is independent of the sign of the dimerization, i.e., it is equal for the two carbon-carbon bond alternations ...-long-short-long-short-... and ...-short-long-short-long-.... Disorder in the electron hopping amplitudes, originating, e.g., from random twists of bonds, removes this degeneracy. This can be understood from the fact that such conformational disorder reduces the overlap between the electron orbitals of neighboring carbon atoms and thus increases the chain energy. The energy increase is less for the long bonds (with relatively small hopping amplitudes) than for the stronger short bonds.

Due to the random nature of the disorder fluctuations, the preferable sign of the dimerization varies along the chain. This explains why domain walls (kinks), separating regions with positive and negative dimerization, can be stabilized by disorder.[1,3,4] While in the absence of disorder, kinks (or solitons) are topological excitations with a rather high energy (~ 0.5 eV in the case of *trans*-polyacetylene), they do appear in the minimal-energy lattice configuration of a disordered chain. This was first noted in numerical simulations of the Su-Schrieffer-Heerger (SSH) model.[3,4] The large kink energy is compensated by adjusting the sign of the chain dimerization to the disorder fluctuations in the intervals between the kinks. The weaker the disorder, the longer the distance between neighboring domain walls has to be. Simple arguments, based on an estimate of the size of the typical disorder fluctuation that stabilizes a kink-antikink pair, show that at weak disorder the average density of disorder-induced kinks in the minimal-energy lattice configuration is proportional to the strength of the disorder.[1]

The effect of off-diagonal disorder on a Peierls chain is similar to the effect of nonzero temperature. It is well known that the Z_2 symmetry in one-dimensional systems can be spontaneously broken only at $T=0$. At any nonzero temperature the symmetry is restored by thermally induced kinks. In this case the kink creation energy is compensated by its large entropy, as kinks can be located at any place in the chain. The topological nature of kinks is responsible for the destruction of the long-range order in isolated Peierls chains, both at arbitrarily small temperature and at arbitrarily weak disorder.

In this paper we put a firm basis under the results which we obtained through simple scaling arguments in Ref. 1, by giving a detailed calculation of the free energy and the density of kinks for half-filled Peierls chains with off-diagonal disorder. The continuum model describing such chains is introduced in Sec. II. In Sec. III we briefly repeat the arguments of Ref. 1, showing that the energy of a disordered chain can be decreased by creating a kink-antikink pair. This implies a special role of kinks. In Sec. IV we consider the partition function of a disordered chain, treating the lattice classically. Integrating out small lattice fluctuations, we obtain an effective free energy describing kinks. The details of this integration can be found in the Appendix. We then use the transfer-matrix approach to reduce the averaging of the chain's free energy over the disorder realizations to the averaging of the wave function that describes the relaxation of a spin 1/2 in a magnetic field with one random component. For long chains, the latter average can be calculated analytically. The derivative of the thus obtained free energy with respect to the chemical potential of kinks gives the average density of kinks, induced both thermally and by disorder (Sec. V).

As we shall see, in the continuum model with white Gaussian disorder and a classical lattice, the entropy of kinks becomes negative below a certain temperature T_0 which depends on the disorder strength. Therefore, in Sec. VI we also study the generation of kinks by disorder in a discrete model, which does not suffer from this pathology. The discrete model is the one-dimensional random-field Ising model (RFIM). It was realized long ago by Imry and Ma,[5] that kinks destroy the long-range order in this model even at zero temperature. We present results of numerical simulations of the average density of kinks in the RFIM as a function of both the disorder strength and temperature and compare to the analytical results for the continuum model. In Sec. VII we summarize and conclude. We also connect to previous work and discuss the effects of disorder-induced kinks on the optical and magnetic properties of quasi-one-dimensional Peierls systems.

II. CONTINUUM MODEL OF A DISORDERED PEIERLS CHAIN

We start by considering a tight-binding model that describes the hopping of electrons along a chain of atoms. The electron hopping amplitudes depend on the interatomic distances and the relative orientation of the electronic orbitals on neighboring atoms. Therefore, the hopping amplitudes are affected by both the lattice motion (the displacement of the atoms parallel to the chain) and conformational disorder (chain twists). Let t_0 denote the hopping amplitude between neighboring atoms in a perfect rigid chain of equidistant atoms with lattice constant a. Then, in the presence of atomic displacements and conformational disorder, the hopping amplitudes may be written

$$t_{m,m+1}=t_0+\alpha(u_m-u_{m+1})+\delta t_{m,m+1}. \tag{1}$$

Here, the second term is the SSH-type of electron-phonon interaction,[2] with the coupling constant α and u_m being the displacement of the mth atom from its uniform-lattice position. The third term is a random contribution resulting from the conformational disorder. While the lattice displacements u_m are dynamic variables, we will assume that the fluctuations $\delta t_{m,m+1}$ are frozen (‘‘quenched’’ disorder).

The Peierls order parameter is the alternating part of the hopping amplitudes

$$\Delta(2ma)=t_{2m-1,2m}-t_{2m,2m+1}, \tag{2}$$

which consists of two parts

$$\Delta(2ma)=\Delta_{\mathrm{lat}}(2ma)+\eta(2ma). \tag{3}$$

The first part is the lattice dimerization

$$\Delta_{\mathrm{lat}}(2ma)=\alpha(u_{2m-1}-2u_{2m}+u_{2m+1}), \tag{4}$$

which describes the alternating part of the hopping amplitude determined by the shifts u_m of the atoms and is the usual order parameter of the SSH model. The second term in Eq. (3) describes the disorder

$$\eta(2ma)=\delta t_{2m-1,2m}-\delta t_{2m,2m+1}. \tag{5}$$

We assume the random variations of the hopping amplitudes δt on different bonds to be independent.

For weak electron-phonon coupling and small disorder we can, in analogy to Ref. 6, use a continuum description of both electrons and lattice with the order parameter

$$\Delta(x)=\Delta_{\mathrm{lat}}(x)+\eta(x). \tag{6}$$

Here, $\Delta_{\mathrm{lat}}(x)$ is the continuum analog of Eq. (4) and $\eta(x)$ is the white noise disorder:

$$\langle\eta(x)\eta(y)\rangle=A\delta(x-y). \tag{7}$$

Note, that while the random chain twists always decrease the hopping amplitudes ($\delta t_{m,m+1}<0$), $\eta(x)$ can be both positive and negative, as it is the alternating part of the fluctuations.

The Hamiltonian of the continuum model has the form

$$H[\Delta_{\mathrm{lat}}(x),\eta(x)]=E_{\mathrm{lat}}[\Delta_{\mathrm{lat}}(x)]+H_{\mathrm{el}}[\Delta(x)]. \tag{8}$$

The first term is the harmonic lattice energy,

$$E_{\mathrm{lat}}[\Delta_{\mathrm{lat}}(x)]=\frac{1}{\pi\lambda v_F}\int dx\,\Delta_{\mathrm{lat}}(x)^2, \tag{9}$$

where $\lambda=4\alpha^2/\pi t_0K$ is the dimensionless electron-phonon coupling constant (K is the spring constant), $v_F=2at_0$ is the bare value of the Fermi velocity, and we set $\hbar=1$ (cf. Ref. 6). In this paper we treat the lattice classically, i.e., we disregard the lattice kinetic energy, which is reasonable for chains of sufficiently heavy atoms. It should be noted that for *trans*-polyacetylene, which consists of relatively light CH groups, quantum lattice effects may be rather important.[7–10]

The electrons in the continuum model are described by

$$\psi_\sigma(x)=\begin{pmatrix}\psi_{1\sigma}(x)\\ \psi_{2\sigma}(x)\end{pmatrix},$$

where the two amplitudes $\psi_{1\sigma}(x)$ and $\psi_{2\sigma}(x)$ correspond to particles moving, respectively, to the right and to the left with the (bare) Fermi velocity v_F, and σ is the spin projection.

The electron Hamiltonian has the form

$$H_{\mathrm{el}}[\Delta(x)]=\sum_{\sigma=\pm1}\int dx\,\psi_\sigma^\dagger(x)\left(\frac{v_F}{i}\sigma_3\frac{d}{dx}+\Delta(x)\sigma_1\right)\psi_\sigma(x)+H_{\text{el-el}}. \tag{10}$$

The first term describes the motion of electrons in the presence of both the chain distortion and the disorder (σ_1 and σ_3 are the Pauli matrices), while the second term describes the (Coulomb) interactions between electrons. Apart from the disorder and the electron-electron interaction term the Hamiltonian of our model is the same as the Hamiltonian of the continuum version of the SSH model.[6]

In the absence of disorder the (half-filled) chain reaches its minimal energy in either one of two uniformly dimerized configurations $\Delta_{\mathrm{lat}}(x)=\pm\Delta_0$. This Peierls instability was initially found for noninteracting electrons[11] ($H_{\text{el-el}}=0$). It also occurs, however, in the presence of electron-electron interactions like, e.g., the on-site Hubbard repulsion U, which opens a gap for charge excitations, but (in the absence of electron-phonon interaction) leaves the spectrum of spin excitations gapless.[12–14] Numerical calculations have shown that a moderately large U can even increase the value of the lattice dimerization.[15–17] As we shall shortly see, the existence of two degenerate ground states, which also implies the existence of kink solutions, is crucial for the appearance of disorder-induced kinks. The precise form of $H_{\text{el-el}}$ does not affect this basic phenomenon; it only is important to the extent that it determines the value of Δ_0 and the kink energy. Therefore, in this paper we do not specify the expression for $H_{\text{el-el}}$.

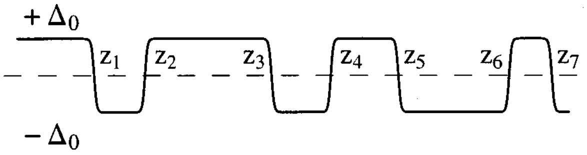

FIG. 1. Order parameter along a Peierls chain for a multikink configuration with seven kinks. $z_1, z_2, \ldots, z_7$, denote the kink positions.

An important property of the dimerized Peierls state is the existence of gaps in the spectra of spin and charge excitations. For free electrons ($H_{\text{el-el}}=0$) both gaps are equal, while in the presence of Coulomb repulsion the spin gap is smaller than the charge gap.[13,14] In what follows, we will assume the temperature to be much smaller than the spin gap, so that we can neglect electronic excitations and replace $H_{\text{el}}[\Delta(x)]$ by its ground-state expectation value (adiabatic approximation),

$$E_{\text{el}}[\Delta(x)]=\langle 0|H_{\text{el}}[\Delta(x)]|0\rangle. \tag{11}$$

III. STABILIZATION OF KINKS BY OFF-DIAGONAL DISORDER

For the sake of completeness, we briefly repeat in this section the arguments of Ref. 1, which show that the lowest-energy lattice configuration in the presence of disorder may contain kinks.

At zero temperature the lattice configuration, i.e., $\Delta_{\text{lat}}(x)$, has to be found by minimizing the total chain energy,

$$E[\Delta_{\text{lat}}(x),\eta(x)]=E_{\text{el}}[\Delta(x)]+E_{\text{lat}}[\Delta_{\text{lat}}(x)], \tag{12}$$

with respect to $\Delta_{\text{lat}}(x)$ at a given disorder realization $\eta(x)$. This makes $\Delta_{\text{lat}}(x)$ implicitly dependent on $\eta(x)$.

As noted in Sec. II, in the absence of disorder the total energy of a half-filled chain has two minima, $\Delta(x)=\pm\Delta_0$, corresponding to two uniformly dimerized configurations with the same energy. Apart from the minima, there are infinitely many lattice configurations that are nearly perfect extrema of the total energy. These are the multikink configurations, in which a sequence of solitons and antisolitons interpolate between $-\Delta_0$ and $+\Delta_0$ and vice versa (Fig. 1). A kink is locally stable, i.e., the chain energy increases, when its form is perturbed. The energy of a multikink configuration can be decreased only by changing the distances between the kinks. However, when the separation between neighboring kinks is large compared to their size (which is of the order of the correlation length $\xi_0=v_F/\Delta_0$),[2] the change of the energy caused by shifts of the kinks is exponentially small, so that the energy of the configuration with N kinks is approximately

$$E_N=E_0+N\mu. \tag{13}$$

Here, μ is the energy needed to create a single kink (about 0.5 eV for *trans*-polyacetylene) and E_0 is the chain energy in the absence of kinks. The kinks can be either charged and spinless, or neutral with spin $\frac{1}{2}$.[2] In the SSH model ($H_{\text{el-el}}=0$), both types have the same energy;[2] if the Coulomb repulsion between electrons is taken into account, the neutral soliton has lower energy.[18,19] Since the on-site Coulomb repulsion in *trans*-polyacetylene is appreciable,[20] we will assume that only neutral kinks are induced by disorder.

Next we find the change of the energy of a multikink configuration due to weak disorder. We will denote the lattice configuration containing N kinks, whose positions are described by the N-dimensional vector $\mathbf{z}=(z_1,z_2,\ldots,z_N)$, by $\Delta_N(x|\mathbf{z})$. To first order in $\eta(x)$, the correction to the energy of the configuration reads

$$\delta E_N=-\frac{2}{\pi\lambda v_F}\int dx\,\Delta_N(x|\mathbf{z})\,\eta(x), \tag{14}$$

where the extremum condition for the configuration $\Delta_N(x|\mathbf{z})$ at zero disorder was used.

For instance, the change of the energy of the uniformly dimerized configuration $[\Delta(x)=\Delta_0]$ due to disorder is

$$\delta E_0=-\frac{2\Delta_0}{\pi\lambda v_F}\int dx\,\eta(x), \tag{15}$$

while for the configuration with an antikink at z_1 and a kink at z_2, such that the whole disorder fluctuation lies between z_1 and z_2, the change of energy equals $\delta E_2=-\delta E_0$, because between z_1 and z_2 $\Delta_2(x|z_1,z_2)\approx-\Delta_0$. We thus see that in the disordered chain, the configuration obtained by the perturbation of a kink-antikink pair is energetically favorable to the perturbed uniform configuration if

$$-\int dx\,\eta(x)>\gamma_k\lambda v_F. \tag{16}$$

Here we introduced $\gamma_k=\pi\mu/(2\Delta_0)$, which for free electrons (SSH model) equals 1. Since the fluctuations in $\int_0^L dx\,\eta(x)$ grow with the chain size L, for a sufficiently long chain the inequality Eq. (16) can certainly be fulfilled, no matter how small the disorder is.

We note that in addition to multikink configurations, also nontopological lattice configurations exist that are extrema of the total chain energy. An example is the polaron.[21,22] However, since the polaron disturbs the lattice only locally, in an interval of length $l\sim\xi_0$ (where ξ_0 is the correlation length), a disorder fluctuation having large magnitude in this interval is needed to stabilize it. At weak disorder the probability density of such a fluctuation is exponentially small. On the other hand, the disorder fluctuations stabilizing kinks, i.e., those that satisfy Eq. (16), can have small magnitude compensated by a large spatial extension given by the distance between neighboring kinks. The weight of such a fluctuation grows with its length and becomes of the order unity if the length equals the average distance between the disorder-induced kinks.[1] In other words, the fluctuations that stabilize kinks are not at all suppressed. This is why in what follows we take into account only multikink configurations, disregarding all other large variations of the Peierls order parameter.

IV. FREE ENERGY OF DISORDERED CHAINS

We start by considering the partition function of a weakly disordered Peierls chain. As was mentioned above, we treat the lattice classically and assume the temperature to be sufficiently small to neglect electron excitations across the gap.

The partition function is then given by the weighted sum over all possible lattice configurations

$$Z[\eta(x)]=\int D\Delta_{\rm lat}\exp\{-\beta E[\Delta_{\rm lat}(x),\eta(x)]\},\qquad(17)$$

and is a functional of the disorder realization $\eta(x)$. In Eq. (17) we have omitted the part related to the kinetic energy of the lattice, as ultimately we will only be interested in the density of kinks in the chain.

It is, of course, impossible to perform the integration over $\Delta_{\rm lat}(x)$ in the partition function exactly, since even the dependence of the electron energy on $\Delta(x)$ is, in general, not known. However, when the temperature tends to zero, only the lattice configurations near the absolute minimum of the chain energy contribute significantly to the partition function. As we discussed in the previous section, in the presence of weak disorder the minimal energy lattice configuration is close to a certain multikink configuration. How many kinks it contains and where they are located depends on $\eta(x)$. To make sure that for any disorder realization we take all important lattice configurations into account, we perform the integration in Eq. (17) over $\Delta(x)$ close to all possible multikink configurations. Thus, we first perform the saddle-point integration near the configuration $\Delta_N(x|\mathbf{z})$ with fixed number and positions of kinks, and then we integrate over the positions $z_1<z_2<\ldots<z_N$ of the kinks and sum over their number N.

The details of the saddle-point calculation are contained in the Appendix. The resulting expression for the free energy of a chain with disorder realization $\eta(x)$ is

$$F[\eta(x)]=F_0+F_1[\eta(x)],\qquad(18)$$

where the first term is the free energy of a chain without kinks and at zero disorder, and the second term is given by

$$F_1[\eta(x)]=-\frac{1}{\beta}\ln\left[\sum_N\frac{1}{d(T)^N}\int d^Nz\exp\left\{-\beta\left(\mu N-\frac{2}{\pi\lambda v_F}\int dx\Delta_N(x|\mathbf{z})\,\eta(x)\right)\right\}\right].\qquad(19)$$

Here $d(T)$ is a variable having dimension of length defined by Eq. (A17).

We assume the size of the kinks to be much smaller than the average distance between them. In this case the kinks can be replaced by abrupt steps,

$$\Delta_N(x|\mathbf{z})\rightarrow\Delta_0 f_N(x|\mathbf{z})\equiv\Delta_0\prod_{n=1}^{N}\operatorname{sgn}(z_n-x).\qquad(20)$$

Equation (19) can then be rewritten as

$$F_1[\eta(x)]=-\frac{1}{\beta}\ln\left[\sum_N\frac{1}{d(T)^N}\int d^Nz\exp\left\{-\beta\left(\mu N-\kappa\int dx f_N(x|\mathbf{z})\,\eta(x)\right)\right\}\right],\qquad(21)$$

where we introduced

$$\kappa=\frac{2\Delta_0}{\pi\lambda v_F}.\qquad(22)$$

In the absence of disorder ($\eta(x)=0$) the integration over the kink positions in Eq. (21) is trivial and the free energy can be easily found,

$$F_1[\eta(x)=0]=-\frac{L}{d(T)\beta}e^{-\beta\mu}.\qquad(23)$$

In this case there are only thermally induced kinks and their density

$$n_{\rm therm}=\frac{1}{L}\frac{\partial F}{\partial\mu}=\frac{1}{d(T)}e^{-\beta\mu},\qquad(24)$$

is exponentially small at $T=\beta^{-1}\ll\mu$. This condition, which was already assumed to hold in writing Eq. (11), is always met for solitons in *trans*-polyacetylene ($\mu\sim0.5$ eV).

Disorder breaks the translational invariance. Nevertheless, the integration over the positions of kinks and the sum over their number can be performed immediately, by noting that Eq. (21) can be written in terms of the matrix elements of an ordered exponential

$$F_1[\eta(x)]=-\frac{1}{\beta}\ln\sum_{\nu,\nu'}\left\langle\nu'\right|\mathrm{T}\exp\left[\int_0^L dx\times[\zeta(x)\sigma_3+\rho\sigma_1]\right]\left|\nu\right\rangle,\qquad(25)$$

where $\zeta(x)=\beta\kappa\eta(x)$, $\rho=e^{-\beta\mu}/d(T)$, and $|\nu\rangle$ is an eigenvector of the Pauli matrix σ_3,

$$\sigma_3|\nu\rangle=\nu|\nu\rangle.$$

The sum in Eq. (25) over $\nu,\nu'=\pm1$ corresponds to the sum over all possible signs of the dimerization at the chain ends. We stress that this choice of boundary conditions is a matter of convenience and does not affect our final result for the density of solitons. The ordered exponential describes the evolution (in imaginary time x) of a spin 1/2 in a magnetic field, which has a constant x component and a random time-dependent z component. The corresponding time-dependent Hamiltonian is

$$H(x)=\zeta(x)\sigma_3+\rho\sigma_1.\qquad(26)$$

Kinks induced in a disordered chain correspond to spin flips and the sum over all possible numbers of kinks and the integration over their positions in Eq. (21) correspond to the expansion of the evolution operator in Eq. (25) in powers of the random magnetic field.

It is now convenient to rotate the ''coordinate'' frame by an angle $\pi/2$ around $\mathbf{e}_2$, which transforms the Hamiltonian H into

$$H'(x)=\exp\left(i\frac{\pi}{4}\sigma_2\right)H\exp\left(-i\frac{\pi}{4}\sigma_2\right)=-\zeta(x)\sigma_1+\rho\sigma_3.\qquad(27)$$

The expression for the free energy then becomes

$$F_1[\eta(x)] = -\frac{1}{\beta}\ln\left(2\left\langle + \left| \mathrm{T}\exp\left[\int_0^L dx H'(x)\right]\right| + \right\rangle\right)$$

$$= -\frac{1}{\beta}\ln(2\psi_\uparrow(L)), \tag{28}$$

where we introduced the wave function of the spin, $\psi(x) = \binom{\psi_\uparrow(x)}{\psi_\downarrow(x)}$, which satisfies the equation

$$\frac{d\psi}{dx} = H'(x)\psi, \tag{29}$$

with the initial condition $\psi(0) = \binom{1}{0}$.

We now introduce $v(x)$ and $\phi(x)$, such that

$$\psi = v\begin{pmatrix} \cosh\left(\dfrac{\phi}{2}\right) \\ \sinh\left(\dfrac{\phi}{2}\right) \end{pmatrix}. \tag{30}$$

The equation for $v(x)$,

$$\frac{1}{v}\frac{dv}{dx} = \rho\cosh(\phi), \tag{31}$$

can be easily integrated, yielding

$$\psi_\uparrow(L) = \cosh\left(\frac{\phi(L)}{2}\right)\exp\left[\rho\int_0^L dx\cosh(\phi(x))\right]. \tag{32}$$

The equation for $\phi(x)$ has the form of a Langevin equation[23]

$$\frac{d\phi}{dx} = -\frac{dU(\phi)}{d\phi} + f(x), \tag{33}$$

with the potential

$$U(\phi) = 2\rho\cosh(\phi), \tag{34}$$

and the random force

$$f(x) = -2\zeta(x) = 2\beta\kappa\eta(x). \tag{35}$$

Since the potential $U(\phi)$ grows at $\phi \to \pm\infty$, the distribution of ϕ at large x tends to the equilibrium distribution, given by the Boltzmann formula

$$P_{eq}(\phi) = e^{-U(\phi)/T_f} \bigg/ \int_{-\infty}^{+\infty} d\phi e^{-U(\phi)/T_f}. \tag{36}$$

where the effective temperature, $T_f = 2A(\beta\kappa)^2$, is determined by the correlation function of the random force

$$\langle f(x)f(y)\rangle = 4A(\beta\kappa)^2\delta(x-y) \equiv 2T_f\delta(x-y). \tag{37}$$

Assuming the chain length L to be much larger than the average distance between kinks, we can use the equilibrium distribution function Eq. (36) to average the free energy over the disorder. Using Eqs. (28) and (32) and neglecting $1/L$ terms, we obtain

$$\langle F\rangle = F_0 - \frac{L\rho}{\beta}\langle\cosh(\phi)\rangle_{\text{eq}}. \tag{38}$$

The average of $\cosh(\phi)$ over the equilibrium distribution function Eq. (36) can be expressed in terms of the modified Bessel functions,

$$\langle\cosh(\phi)\rangle_{\text{eq}} = \int_{-\infty}^{+\infty} d\phi P_{\text{eq}}(\phi)\cosh(\phi) = \frac{K_1(z)}{K_0(z)}, \tag{39}$$

with $z = 2\rho/T_f \propto \exp(-\beta\mu)$. As we assumed before already that $T \ll \mu$, we can use the approximate expressions for the modified Bessel functions at small value of the argument z. The average free energy of a disordered Peierls chain can then be written in the form

$$\langle F\rangle = F_0 - LA\left(\frac{2\Delta_0}{\pi\lambda v_F}\right)^2 \frac{1}{\mu + (3/2)T\ln(eT_0/T)}, \tag{40}$$

where the temperature T_0 is defined by

$$T_0 = \frac{1}{e\lambda v_F}\left(\frac{4A\Delta_0^2}{\pi\gamma\sqrt{cr}}\right)^{2/3}, \tag{41}$$

and $\gamma = 1.781\,072\ldots$, is the exponential of Euler's constant.

V. AVERAGE DENSITY OF KINKS

We now turn to the average density n of disorder-induced kinks, which is obtained by differentiating the free energy Eq. (40) with respect to μ [cf. Eq. (24)]. This leads to

$$n = \frac{A}{(\gamma_k\lambda v_F)^2}\frac{1}{[1 + (3T/2\mu)\ln(eT_0/T)]^2}, \tag{42}$$

which at zero temperature reduces to

$$n(T=0) = \frac{A}{(\gamma_k\lambda v_F)^2}. \tag{43}$$

This zero-temperature result was derived in Ref. 1 by using scaling arguments.

Strictly speaking, however, we cannot set $T = 0$ in our general result, because for $T < T_0$ the entropy of kinks,

$$\langle S_{\text{kink}}\rangle = -\frac{\partial\langle F\rangle}{\partial T} \propto \ln\left(\frac{T}{T_0}\right), \tag{44}$$

becomes negative and the density of kinks increases with decreasing temperature. We note that in the expression for the free energy Eq. (40), the kink energy μ is effectively replaced by

$$\mu(T) = \mu + \frac{3}{2}T\ln\left(\frac{eT_0}{T}\right). \tag{45}$$

This can be readily understood as follows. Each kink enters in the expression Eq. (18) with a weight

$$e^{-\beta\mu(T)} = \frac{l(T)}{d(T)}e^{-\beta\mu}, \tag{46}$$

where $l(T)$ is the typical size of the thermal fluctuation of the kink position. For the white noise disorder that we consider, $l(T)$ can be estimated from the condition

$$(\beta\kappa)^2 A l(T) \sim 1. \tag{47}$$

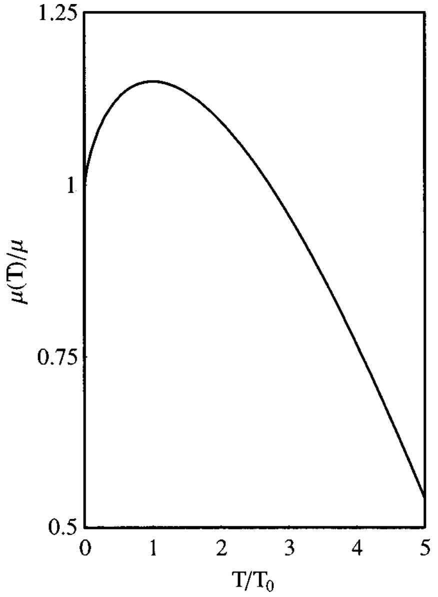

FIG. 2. Temperature dependence of the effective chemical potential of kinks according to Eq. (45) for $\mu = 10T_0$.

This derives from the criterion that shifting the kink over $l(T)$ from its optimal position should cause a fluctuation of the order of T in its interaction energy Eq. (14) with the disorder. Using Eq. (A17) we find that

$$\frac{l(T)}{d(T)} \propto T^{3/2}, \tag{48}$$

which in combination with Eq. (46) indeed gives Eq. (45) for $\mu(T)$. The temperature dependence of $\mu(T)$ is plotted in Fig. 2. Below $T = T_0$, $d\mu(T)/dT > 0$, i.e., kinks become less ''heavy'' as temperature decreases, which explains the pathological behavior of the entropy.

Keeping in mind that our description of the lattice is both classical and continuum, this pathology is hardly suprising. In practice, quantum effects will prevent the entropy from becoming negative at low temperatures. A simpler way to regularize the model lies in a discretization. From Eqs. (45) and (46), it follows that T_0 is determined by the condition $l(T) \sim d(T)$. For smaller temperatures, $l(T)$ gets smaller than $d(T)$, which plays the role of an effective lattice constant and becomes arbitrarily small at small temperatures. Clearly, however, the continuum description of the off-diagonal disorder fails when $l(T)$ drops below the lattice constant a. Moreover, the Peierls-Nabarro barrier[24] at low temperature fixes the kink position within the unit cell of the atomic lattice. These facts motivate us to consider in the next section a discrete version of Eq. (18), in which a temperature-independent lattice constant d is used and the integrations over kink positions are substituted by finite lattice sums.

It should be noted that just replacing $d(T)$ in Eq. (18) by a temperature-independent distance d does not, by itself, make the entropy positive. Retracing the steps following Eq. (18) in that case leads to

$$\langle F \rangle = F_0 - LA\left(\frac{2\Delta_0}{\pi\lambda v_F}\right)^2 \frac{1}{\mu + 2T\ln(eT_0'/T)}, \tag{49}$$

with

$$T_0' = \frac{2\Delta_0}{\pi e\lambda v_F}\left(\frac{2dA}{\gamma}\right)^{1/2}. \tag{50}$$

The density of disorder-induced kinks is then found to be

$$n = \frac{A}{(\gamma_k \lambda v_F)^2} \frac{1}{[1 + (2T/\mu)\ln(eT_0'/T)]^2}. \tag{51}$$

Obviously, this result has the same zero-temperature limit as Eq. (42) and it also shows a similar pathology below a certain temperature, which now is given by T_0'. Only if we discretize the kink positions on the lattice with constant d, will we indeed obtain a classical model that also at low temperatures gives sensible results.

VI. DISCRETE MODEL AND NUMERICAL RESULTS

As motivated in the previous section, we now consider a discrete model, in which the chain is divided into M cells of length d (independent of T) and kinks are allowed to be located only at the boundaries $x_m = md$ ($m = 1, \ldots, M$) between the cells. Then the function $f(x) = \Delta(x)/\Delta_0$ [cf. Eq. (20)] has a constant value ± 1 inside each cell. In other words, the chain configuration is described by a set of Ising variables, $\{\sigma_1, \sigma_2, \ldots, \sigma_M\}$, where σ_m is the value of $f(x)$ in the mth cell. We impose periodic boundary conditions $\sigma_{M+1} = \sigma_1$. Kinks occur between cells with opposite values of σ and the sum over all possible configurations of the Ising spins represents the sum over the number of kinks, as well as over their positions on the one-dimensional lattice. This lattice model for the statistics of disorder-induced kinks is equivalent to the one-dimensional random-field Ising model[5] (RFIM). The constant-d continuum model which led to Eq. (51) is, in fact, the continuum version of this RFIM.

The partition function of the one-dimensional RFIM reads

$$Z = \sum_{\{\sigma_m\}} e^{-\beta E\{\sigma_m\}}, \tag{52}$$

with

$$E\{\sigma_m\} = \sum_{m=1}^{M}\left[\mu\frac{(1 - \sigma_m\sigma_{m+1})}{2} - h_m\sigma_m\right]. \tag{53}$$

The first term in Eq. (53) equals μ times the number of spin flips in the chain and thus represents the total kink creation energy. The second term describes the interaction with the random ''magnetic'' field defined by

$$h_m = \kappa \int_{x_m}^{x_{m+1}} dx\, \eta(x), \tag{54}$$

i.e., the value of the field in each cell is proportional to the value of disorder in the continuum model integrated over the cell. The distribution of the random field is also Gaussian, with correlator:

$$\langle h_k h_l \rangle = D\delta_{kl}, \tag{55}$$

where $D = d\kappa^2 A$.

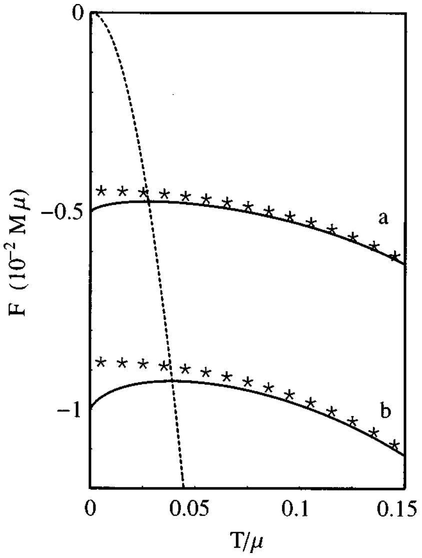

FIG. 3. The free energy of dimerization kinks in a Peierls chain as a function of temperature for two values of the disorder strength: $D=0.005\mu^2$ (a) and $D=0.01\mu^2$ (b). The solid lines give the analytical result Eq. (49), while the stars indicate the numerical results. The part of the free energy related to an ordered chain without kinks (F_0) is discarded. $M=L/d$ denotes the number of unit cells. The dashed curve intersects the solid lines at the temperature for which the analytically calculated entropy equals zero.

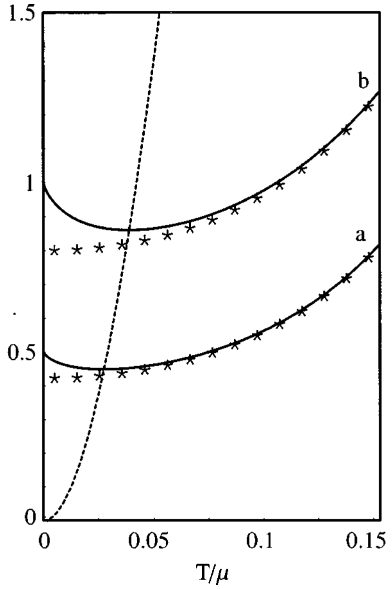

FIG. 4. The density of dimerization kinks in a Peierls chain as a function of temperature for two values of the disorder strength: $D=0.005\mu^2$ (a) and $D=0.01\mu^2$ (b). The solid lines give the analytical result Eq. (51) and the stars indicate the numerical results. Dashed curve as in Fig. 3.

It is well known that arbitrarily small disorder or temperature destroys the long-range order in the one-dimensional RFIM.[5] The density of the thermally excited domain walls in the absence of disorder is $e^{-\beta\mu}$, while at zero temperature the density of the disorder-induced kinks is proportional to the strength of the disorder. A full calculation of the average free energy and the density of kinks in the RFIM involves numerical simulations. We performed such simulations using the transfer-matrix approach, as we did in the continuum treatment. In the discrete case, the Schrödinger equation (29) for the continuum model is replaced by

$$\psi_{m+1}=\hat{T}_m\psi_m, \tag{56}$$

with the transfer matrix $\hat{T}_m$,

$$\hat{T}_m=\begin{pmatrix} \exp\{\beta h_m\} & \exp\{-\beta(\mu-h_m)\} \\ \exp\{-\beta(\mu+h_m)\} & \exp\{-\beta h_m\} \end{pmatrix}, \tag{57}$$

The free energy for a given realization $\{h_m\}$ of the random field is then given by

$$F[\{h_m\}]=-T\ln\left(\mathrm{Tr}\prod_{m=1}^{M}\hat{T}_m\right). \tag{58}$$

To obtain a smooth temperature dependence of the density of kinks, we had to average the free energy over 10^3 random-field realizations for a chain with 10^3 sites.

We now turn to the results of these simulations. In Fig. 3 the free energy is plotted as a function of temperature for two values of the disorder strength: $D=0.005\mu^2$ and $D=0.01\mu^2$. Stars indicate the numerical results for the discrete model, while the solid lines represent the continuum version of the RFIM [Eq. (49)]. The latter curves have maxima at $T=T_0'$, below which the entropy becomes negative. For convenience, we also plotted the dashed curve, which passes through the maxima of the solid lines. The continuum results become meaningless to the left of this curve. The slope of the numerically obtained free energy of the discrete model is always negative, corresponding to a positive entropy, which tends to 0 as $T\to 0$. We also observe that above T_0' the numerical (discrete) and analytical (continuum) results only differ little from each other.

In Fig. 4 we give the density of kinks as a function of temperature for the same two values of the disorder as in Fig. 3. Again, solid lines and stars represent the continuum model and the discrete model, respectively, while the dashed curve passes through the minima of the continuum results, below which the continuum model becomes meaningless. The temperature dependence of the density of kinks for $T<0.15\mu$ is very slow. At $T=0.15\mu$ the density of thermally induced kinks in a chain without disorder is about $1.3\times 10^{-3}/d$. This means that the increase of the kink density observed in Fig. 4 is mostly related to the fact that more multikink configurations become available in a disordered chain as temperature grows.

Figure 5 shows the density of kinks as a function of the disorder strength D at $T=0$. Stars give the numerical results for the discrete model (simulated at $T=0.005\mu$ in order to avoid numerical instabilities). The dashed line gives the $T=0$ continuum result, Eq. (43), which in terms of D reads $n(T=0)=D/(d\mu^2)$. As is observed from Fig. 4, for decreasing disorder these two results get in better agreement with each other. This is a consequence of the fact that T_0' then also decreases. In the limit of $D\to 0$, the agreement should become exact, as indeed appears from Fig. 5. For higher disorder, however, the nonphysical nature of the continuum model for $T<T_0'$ causes the numerical and analytical results to deviate by an increasing amount at $T=0$. An alternative

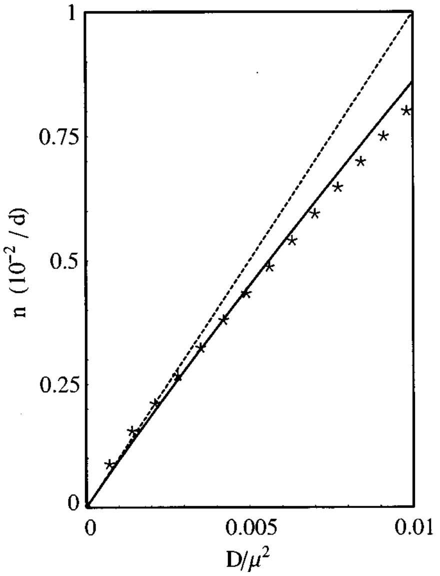

FIG. 5. Density of dimerization kinks in a Peierls chain as a function of disorder strength. The dashed line represents the analytical continuum result Eq. (51) taken at $T=0$, the solid line gives the same result at $T=T_0'$, while the stars indicate the results of numerical simulations of the discrete model at $T=0.005\mu$ (which for all practical purposes may be considered zero temperature).

approach to obtain an analytical zero-temperature result, is to use the continuum result Eq. (51) at the lowest possible value where the result is still physical, i.e., at $T=T_0'$. The thus obtained value of the density of kinks as a function of the disorder is also plotted in Fig. 5 (solid line) and is indeed seen to be in much better agreement with the numerical $T=0$ results over a large interval of the disorder. This shows the importance of the corrections to the linear D dependence, expected on the basis of scaling arguments,[5] of the density of domain walls in the RFIM.

VII. SUMMARY AND DISCUSSION

In this paper we studied a continuum model describing Peierls chains with a doubly degenerate ground state in the presence of weak off-diagonal disorder. In such chains, thermally and disorder-induced neutral solitons (dimerization kinks) occur. By integrating out all irrelevant lattice degrees of freedom, we obtained the free energy of these kinks. This free energy was then averaged over the disorder realizations leading to an analytical expression Eq. (42) for the average density of kinks.

In the continuum model, the entropy of the kinks was found to become negative below a certain temperature T_0. At this temperature the thermal fluctuation of the kink positions $l(T)$ becomes of the order of the effective ''lattice constant'' $d(T)$. It was then argued that below this temperature one should either take the effects of the lattice discreteness into account, or consider the lattice quantum mechanically. We noted that the discrete version of the model that describes the thermal or disorder-induced kinks is the one-dimensional RFIM. The free energy and the density of kinks in the latter model were found numerically and the results were compared with the continuum model. It was found that for $T>T_0$, both models are in good agreement.

To obtain the free energy of the kinks (Appendix), we used a technique developed for the semiclassical solution of quantum problems.[25] This is not accidental, because a Peierls chain with a doubly degenerate ground state in the presence of weak disorder or at a small temperature behaves similarly to a quantum particle in a double well. If the wells are very deep, the small quantum fluctuations around the two classical vacua may be relatively insignificant. A more important effect, however, is that the quantum particle can tunnel between the two minima. The tunneling probability is described by instantons, which are the imaginary-time classical trajectories leading from one minimum of the potential to the other. In fact, an exact mapping exists between the instanton gas for a double-well potential and the gas of thermally induced kinks.[26] The disorder-induced kinks are somewhat different: their positions, unlike the instanton positions, are not arbitrary. These kinks are, to some extent, pinned by the disorder which induces them.

The main assumption of our calculation is the validity of the expansion of the free energy in powers of the disorder. As was already discussed in Ref. 1, this translates into the condition

$$n\xi_0 \ll 1, \tag{59}$$

meaning that the average distance between kinks should be much larger than their size. For stronger disorder the lattice distortions would be random over the length scale of the order of ξ_0, and the notion of multikink configurations would lose sense.

Effects of disorder on the properties of Peierls chains have been studied before by a number of authors. Many of these studies were devoted to charged solitons induced by random doping[27] and the effects of localized bond and site impurities on the electronic states.[28] The minimal-energy lattice configuration in the presence of a finite density of bond impurities was studied numerically in Refs. 3,4. There it was found that for some disorder realizations the configuration contained kinks. As these calculations were performed within the SSH model (in which electron-electron interactions are not included), the obtained disorder-induced kinks did not have a definite charge or spin. Also, no attempt was made in these papers to obtain (numerically or analytically) the density of solitons as a function of the disorder strength.

Another large body of work on disordered Peierls systems deals with the fluctuating gap model (FGM).[29] This work not only addresses the study of disorder *per se*,[30,31] but also includes studies of quantum lattice fluctuations modeled by static disorder.[32–34] In the FGM, one assumes that the lattice part $\Delta_{\rm lat}$ of the order parameter is a constant throughout the chain and does not respond to the local disorder. This immediately eliminates the possibility of disorder-induced solitons. Nevertheless, solitons play an important role in the FGM: we recently showed that the optimal fluctuation that determines the density of states inside the pseudogap in this model has the form of a soliton-antisoliton pair.[35]

We finally mention that, while we considered weak off-diagonal disorder, one may also consider a type of disorder where the electron conjugation over certain bonds is broken completely ($t_{n,n+1}=0$). This model leads to a distribution of chain sizes.[36] If the conjugation breaks occur randomly, chains with an odd number of carbon atoms will occur, which necessarily contain a kink.[37] Thus, the density of kinks is proportional to the disorder strength (i.e., the density of chain breaks), as it is in our model [see Eq. (43)].

As was already discussed in our previous paper,[1] the electron state in the presence of neutral solitons is different from that of a perfectly dimerized chain. This gives the possibility to detect the disorder-induced kinks. First, the kinks should give rise to a peak in the optical-absorption spectrum that occurs inside the gap of the perfectly dimerized chain. Second, having spin 1/2, the neutral kinks contribute to the Curie susceptibility. As we noted in Ref. 1, experiments on undoped *trans*-polyacetylene do not seem to agree with the large density of free solitons that one would expect on the basis of the small average electron conjugation length (several tens of carbon atoms[36]) in this material. In particular, experiments indicate that only 1 free spin occurs per 3000 carbon atoms.[38] It should be noted, however, that a meaningful comparison between theory and experiment can only be made if one accounts for interchain interactions, which suppress the generation of isolated kinks.[39] A study of the interplay between the disorder-induced kinks, destroying the long-range coherence, and the interchain interactions, binding kinks into pairs, will be reported elsewhere. It should be noted that this interplay seems to be very important to describe the Peierls phase transition.[40]

We finally note that another important issue is the quantum treatment of the lattice dynamics coupled to the spin dynamics of the kinks. The interaction between neighboring kinks may bind their spins into a singlet ground state, thus explaining why the density of free spins observed in undoped *trans*-polyacetylene is so low. We plan to address this problem in the future.

ACKNOWLEDGMENTS

This work is supported by the Stichting Scheikundig Onderzoek in Nederland (SON) and the Stichting voor Fundamenteel Onderzoek der Materie (FOM).

APPENDIX

In this appendix we obtain the effective free energy of kinks by integrating out all irrelevant lattice degrees of freedom in the partition function of the disordered chain Eq. (17).

It is convenient to replace the integration over lattice configurations Δ_{lat} by the integration over $\Delta(x)$, which also includes the disorder [cf. Eq. (6)] . The chain energy can be written as

$$E[\Delta_{\text{lat}}(x),\eta(x)]=E_{\text{el}}[\Delta(x)]+E_{\text{lat}}[\Delta(x)-\eta(x)]. \tag{A1}$$

Since the lattice energy is quadratic in $\Delta_{\text{lat}}=\Delta(x)-\eta(x)$, we obtain

$$E[\Delta_{\text{lat}}(x),\eta(x)]=E[\Delta(x),0]-\frac{2}{\pi\lambda v_F}\int_0^L dx\Delta(x)\eta(x)+\frac{1}{\pi\lambda v_F}\int_0^L dx\,\eta(x)^2, \tag{A2}$$

where the first term is the chain energy at zero disorder and L is the chain length.

For $\Delta(x)$ close to the multikink configuration $\Delta_N(x|\mathbf{z})$ we can expand the chain energy $E[\Delta(x),0]$ in powers of $\xi(x)$ defined by

$$\xi(x)=\Delta(x)-\Delta_N(x|\mathbf{z}). \tag{A3}$$

Retaining terms up to second order in $\xi(x)$, we have

$$E[\Delta,0]=E_0+N\mu+\frac{1}{\pi\lambda v_F}\int_0^L dx\,\xi(x)\hat{D}_N(\mathbf{z})\xi(x). \tag{A4}$$

Here, we assumed the distances between kinks to be much larger than the correlation length ξ_0. As we discussed in Sec. III, in the absence of disorder the multikink configuration is then an almost exact extremum of the chain energy, which is why Eq. (A4) does not contain a first-order term. The operator $\hat{D}_N(\mathbf{z})$ is defined through

$$\hat{D}_N(\mathbf{z})\xi(x)=\int dy D_N(x,y|\mathbf{z})\xi(y), \tag{A5}$$

with the kernel $D_N(x,y|\mathbf{z})$ related to the second variational derivative of the total chain energy

$$\frac{1}{\pi\lambda v_F}D_N(x_1,x_2|\mathbf{z})=\frac{1}{2}\left.\frac{\delta^2E[\Delta,0]}{\delta\Delta(x_1)\delta\Delta(x_2)}\right|_{\Delta=\Delta_N(x|\mathbf{z})}. \tag{A6}$$

Let $\Omega=\sqrt{4K/M}$ denote the bare optical phonon frequency. Then, the eigenfunctions $\phi_\alpha(x|\mathbf{z})$ of $\hat{D}_N(\mathbf{z})$ obeying

$$\hat{D}_N(\mathbf{z})\phi_\alpha(x|\mathbf{z})=\left(\frac{\omega_\alpha(\mathbf{z})}{\Omega}\right)^2\phi_\alpha(x|\mathbf{z}), \tag{A7}$$

are (optical) phonon modes in the presence of N kinks with frequencies $\omega_\alpha(\mathbf{z})$.

When the kinks are far apart, the N lowest phonon frequencies ($\alpha=1,\ldots,N$) are very small, since these normal modes correspond to shifts of the kinks, which leave the chain energy practically unchanged. (The frequency of one mode is exactly zero, as it corresponds to the translation of the multikink configuration as a whole). To avoid double counting, the integration over the first N modes is replaced by the integration over the N kink positions, which is the standard approach in the instanton calculus.[25] Then the measure of the functional integration in the vicinity of the multikink configuration becomes

$$D\xi(x)=J_N d^N z\prod_{\alpha>N}d\xi_\alpha, \tag{A8}$$

where ξ_α are the amplitudes of the normal modes,

$$\xi(x)=\sum_\alpha \xi_\alpha\phi_\alpha(x|\mathbf{z}), \tag{A9}$$

and J_N is the Jacobian of the substitution of the integration over the N (almost) zero modes by the integration over the kink positions. We have

$$J_N=(J_1)^N\equiv c^{N/2}, \tag{A10}$$

with J_1 the Jacobian for the single-kink configuration $\Delta_1(x)$, leading to

$$c=\int dx\left(\frac{d\Delta_1(x)}{dx}\right)^2\sim\frac{\Delta_0^2}{\xi_0}. \tag{A11}$$

The constant c can be expressed as $c=\pi\lambda v_F\Omega^2M_k/2$, with M_k the soliton mass, which in the SSH model is about $6m_e$.[2]

The Gaussian integration over the amplitudes of the nonzero modes now reduces the partition function to

$$Z=Z_0\sum_N\left(\frac{4\beta c}{\pi^2\lambda v_F}\right)^{N/2}\int d^NzR_N(\mathbf{z})\exp\{-\beta W_N(\mathbf{z})\}. \tag{A12}$$

Here

$$W_N(\mathbf{z})=N\mu-\frac{2}{\pi\lambda v_F}\int_0^L dx\Delta_N(x|\mathbf{z})\,\eta(x)+\frac{1}{\pi\lambda v_F}\left(\int_0^L dx\,\eta(x)^2-\sum_{\alpha>N}\frac{\Omega^2}{\omega_\alpha^2(\mathbf{z})}\,\eta_\alpha^2\right), \tag{A13}$$

with η_α the expansion coefficients of $\eta(x)$ over the orthonormal basis $\phi_\alpha(x|\mathbf{z})$ [cf. Eq. (A9)]. Z_0 is the partition function of the chain in the absence of kinks and disorder:

$$Z_0=e^{-\beta E_0}\prod_\alpha\left(\pi\sqrt{\frac{\lambda v_F}{\beta}}\frac{\Omega}{\omega_\alpha(0)}\right), \tag{A14}$$

where $\omega_\alpha(0)$ denote the phonon frequencies in the absence of kinks and disorder. Finally, the factor $R_N(\mathbf{z})$ in Eq. (A12) is the product of nonzero phonon frequencies for the lattice configuration containing no kinks divided by the same product for the configuration with N kinks,

$$R_N(\mathbf{z})=\left(\prod_\alpha\frac{\omega_\alpha(0)}{\Omega}\right)\left(\prod_{\alpha>N}\frac{\omega_\alpha(\mathbf{z})}{\Omega}\right)^{-1}. \tag{A15}$$

Similarly to Eq. (A10), for widely separated kinks, $R_N(\mathbf{z})$ equals the Nth power of the regularized product of nonzero phonon frequencies for a configuration with one kink,[25]

$$R_N(\mathbf{z})=(R_1(z_1))^N\equiv r^{N/2}, \tag{A16}$$

where r is a number of the order unity.

Finally, for weak disorder we can neglect the third term in Eq. (A13), as it is of second order in $\eta(x)$. From Eqs. (A12), (A13), and (A16) we then obtain the expressions Eqs. (18) and (19) for the free energy of a chain with disorder realization $\eta(x)$, where $d(T)$ is given by

$$d(T)=\frac{\pi}{2}\sqrt{\frac{\lambda v_FT}{cr}}\ \sim\ \xi_0\sqrt{\lambda\frac{T}{\Delta_0}}. \tag{A17}$$

In this calculation we neglected electron excitations, assuming the temperature to be sufficiently low. However, the electron ground state for the lattice configuration containing N neutral kinks, separated by distances much larger than the correlation length, is 2^N-fold degenerate, due to the fact that the spin projection of each kink can be arbitrary. Because of this degeneracy, the weight factor of each kink acquires an extra factor of 2, which was taken into account in Eq. (A12). The degeneracy is not exact: excitations of this spin system have a typical energy of the order of the exchange constant for the spins of two neighboring kinks. Thus, our assumption requires that the temperature is much larger than this energy $[\Delta_0\exp(-1/(n\xi_0))]$, yet much smaller than the Peierls gap $[\Delta_0]$.

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