5 Magnetic Susceptibility in Interacting Polymer Chains Due to Disorder-Induced Neutral Solitons

In this chapter we account for interchain interactions in disordered Peierls systems, which, if sufficiently strong, result in a bond-ordered phase, in which the neutral solitons are bound into pairs. We analytically calculate the corresponding pair size distribution and study the magnetic response due to the spins of neutral solitons induced by disorder in trans-polyacetylene. As the spins of the solitons have a distance-dependent antiferromagnetic coupling, knowledge of the pair size distribution allows us to calculate the magnetic susceptibility in the ordered phase. At low temperatures, the result deviates from the usual Curie behavior in a way that depends on the relative strength of the disorder and the interchain interactions. We compare our results to the observed magnetic susceptibility of trans-polyacetylene and we suggest new experiments extending towards lower temperatures.

Sections 5.4 and 5.5 may be skipped in a first reading of this chapter.

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5.1 Introduction

In Chapter 3 we have studied the effect of off-diagonal disorder on the lattice configuration of a half-filled Peierls-Hubbard chain with a doubly degenerate ground state. An example is the $\pi$-conjugated polymer trans-polyacetylene, which in the absence of disorder has a uniformly dimerized ground state. As the energy does not depend on the sign of the lattice dimerization (which determines whether even or odd bonds are short), this ground state is doubly degenerate. For a single Peierls-Hubbard chain we showed that arbitrarily weak off-diagonal disorder induces neutral solitons (kinks) in the lattice dimerization, which interpolate between the two degenerate bond alternations. Even though the creation energy of a neutral soliton is rather large (of the order of half the gap in trans-polyacetylene), the energy loss is compensated by allowing the sign of the dimerization to adjust to the electronic disorder fluctuations. Off-diagonal disorder in conjugated polymers (i.e., disorder in the hopping amplitudes of the $\pi$-electrons) may originate from random chain twists, which decrease the overlap between the $\pi$-orbitals of neighboring carbon atoms. The density of disorder-induced neutral solitons in a single chain is proportional to the disorder strength. In trans-polyacetylene the disorder strength is presumably rather large, as the average conjugation length in this material is of the order of several tens of carbon atoms only [1]. One would then expect the neutral solitons to contribute significantly to the polymer's magnetic and optical properties, as they carry spin $\frac{1}{2}$ and result in the appearance of electronic states inside the Peierls gap.

There is, however, no direct evidence for the existence of a high density of solitons in undoped trans-polyacetylene. Electron spin resonance (ESR) experiments report only about
one free spin per 3000 carbon atoms [2, 3, 4, 5]. Moreover, it appears difficult to observe neutral solitons in optical absorption experiments, as, contrary to what is expected from the Su-Schrieffer-Heeger (SSH) model [6], they seem not to give rise to a clear midgap absorption peak [7]. This may be explained by assuming that the on-site Coulomb repulsion U is strong enough to shift the midgap peak towards the absorption edge resulting from interband transitions [8, 9]. Since both the peak and the absorption edge are significantly broadened by the quantum lattice motion [10], there may be no clear distinction between them.

X-ray scattering data do yield some indirect evidence for disorder-induced kinks. There still is considerable disagreement whether neighboring carbon chains are dimerized in phase (P2$_1$/α space group) or in anti-phase (P2$_1$/n space group) [11, 12]. While this may originate from different preparation methods leading to different space groups, it has also been pointed out that the disagreement may result from a high density (of the order of several percent) of kinks that locally change the relative sign of the dimerization in neighboring chains [13, 14]. Yet, it is not clear how such random changes would lead to sharp peaks in the x-ray spectra.

From the above it appears that a clear signature of the effect of disorder-induced solitons is still to be found. This has motivated us to study the magnetic response of disorder-induced solitons in more detail. A proper modeling of the magnetic susceptibility involves more than a calculation of the density of solitons in an isolated chain. As we noted already in Chapter 3, the actual density of neutral solitons (and thus of spins) is determined by the competition between disorder and interchain interactions, as the latter lead to the confinement of soliton-antisoliton pairs and may restore the long-range bond order. Moreover, at low temperature, the exchange between the spins of neighboring solitons on a single chain tends to bind them into a singlet state [15], which has no magnetic response. Thus, the magnetic susceptibility and, in particular, its temperature dependence should be expected to depend strongly on the interplay between disorder and interchain interactions.

In this chapter, we focus on the magnetic susceptibility of disorder-induced solitons in the phase with long-range bond order. In this case, solitons occur in isolated pairs of random size dictated by the disorder realization. We study the statistics of these pairs by mapping the problem on the anisotropic random-field Ising model, which has been studied in Chapter 4 within the chain mean-field approximation. This mapping is analogous to what we did in Chapter 3 for isolated chains. We discuss the phase diagram of this model in Section 5.2. In Section 5.3, we express the magnetic susceptibility of an ensemble of soliton-antisoliton pairs in terms of the, as yet unknown, distribution of exchange interactions. In Section 5.4, we calculate the distribution of soliton-pair sizes using the saddle-point method. From the pair size distribution we derive in Section 5.5 the distribution of exchange constants. The latter is used in Section 5.6 to calculate the magnetic susceptibility of trans-polyacetylene. We find that the low-temperature behavior of this susceptibility deviates from the Curie law and we fit our results to the experimental data obtained in Ref. [5]. In Section 5.7, we summarize and conclude.

5.2 Solitons in interacting disordered Peierls chains

In Section 3.5, we have shown that the statistics of neutral solitons in isolated weakly disordered Peierls chains can be studied using the one-dimensional random-field Ising model (RFIM). In this mapping, Ising variables $\sigma_m = \pm 1$ (with $m = 1, \ldots, M$) are defined on the sites of a
lattice with lattice constant $d$. These variables play the role of the sign of the dimerization in the Peierls chain, while the random "magnetic" field $h_m$ at site $m$ represents the off-diagonal disorder, which locally lifts the degeneracy between the two dimerization phases in the Peierls chain. Two neighboring sites on the lattice having different Ising variables, correspond to the occurrence of a soliton in the Peierls chain. Therefore, the creation energy $\mu$ of a soliton in the Peierls chain is equivalent to the exchange interaction between neighboring Ising spins. In the SSH model of trans-polyacetylene $\mu = 2\Delta_0/\pi \simeq 0.5$ eV ($\Delta_0$ is the dimerization). We emphasize, however, that this mapping is not limited to the SSH model, but also holds in the presence of electron-electron interactions, in which case the value of $\mu$ is smaller [16, 17].

Our approach may easily be extended to account for three-dimensional effects that have already been discussed in Section 2.4.2: interchain interactions (electron hopping, elastic forces, or Coulomb interactions) tend to favor a coherence of the dimerization pattern on neighboring chains, which in Ising language translates into an interaction, $2W$, between spins on neighboring chains. The strength of the interchain interaction is proportional to the confinement energy Eq. (2.107), $W = \tilde{W}d \propto e_c$, and as for quasi-one-dimensional materials, like conjugated polymers, $W \ll \mu$, we are thus dealing with a strongly anisotropic random-field Ising model. The anisotropy allows one to treat the interchain interactions in a mean-field way, an approach known as the chain mean-field approximation. The energy of the resulting Ising model, which we sketch in Figure 5-1, is given by:

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

(5.1)

and was already introduced in Section 3.5 with $B = 0$. We briefly recall, that the first term describes the energy cost for creating $\frac{1}{2} \sum_{m=1}^{M} (1 - \sigma_m \sigma_{m+1})$ kinks and the second term describes the interaction energy with the random magnetic field. The latter is assumed to have a Gaussian distribution with zero mean ($\langle h_m \rangle = 0$) and correlator

$$\langle h_m h_n \rangle = D \delta_{m,n},$$

(5.2)

where $D = dk^2A$ is the disorder strength as defined in Section 3.5. We consider the case of weak disorder: $D \ll \mu^2$. Finally, the third term in Eq. (5.1) describes the interchain interactions in the mean-field approximation, where the homogeneous "magnetic" field $B$ is proportional to the average order parameter,

$$B = W \langle \langle \sigma \rangle \rangle,$$

(5.3)

and the double brackets denote both the thermal and the random-field average. In Figure 5-1 the effect of interchain interactions on disorder-induced neutral solitons is sketched.

To end the explanation of our model, a few remarks are in place. First, by replacing the dimerization by a discrete Ising variable, we have neglected the true dimerization profile associated with a soliton. As the extent of this profile is given by the correlation length $\xi_0$, our "sudden-kink approximation" is valid as long as the soliton density is small compared to $1/\xi_0$, as is the case for weak disorder. Taking into account the true dimerization profile results in an effective increase of the kink creation energy of the order $\sqrt{D \xi_0/a}$ (with $a$ the average carbon-carbon distance in trans-polyacetylene) and, thus, in a small reduction of the soliton
Figure 5-1: (a) The RFIM Eq. (5.1) in the absence of the homogeneous B-field \(B = 0\). The Ising spins \(\sigma_m = \pm 1\) tend to follow the local sign of the random field \(h_m\) resulting in spin-flips along the chain segment that correspond to disorder-induced neutral solitons in the dimerization of a polymer chain. (b) The RFIM for the same disorder fluctuation \(h_m\) as in (a) but with nonzero homogeneous field \(B > 0\) that represents interchain interactions between polymer chains. In the presence of \(B\), one sign of the dimerization is favored resulting in a decreased number of solitons.

density. This has recently been confirmed explicitly in numerical simulations which do account for the true profile [18]. Second, it should be kept in mind that the RFIM Eq. (5.1) is an effective model, obtained by integrating out small lattice fluctuations. As a result, the kink creation energy \(\mu\) weakly depends on the temperature (see Eq. (3.58) in Section 3.4). Third, above we have not specified the value of the Ising lattice constant \(d\) (which should not be confused with the lattice constant \(a\) of the polymer chain). It should be noted that both the disorder strength \(D\) and the interchain interaction energy \(W\) scale proportional to \(d\). In Section 5.5 we show that all physical observables are \(d\)-independent in the limit \(d \to 0\).

The temperature versus disorder strength phase diagram of the model Eq. (5.1) contains two phases: the ordered phase characterized by a nonzero value of the average dimerization, \(\langle \langle \sigma \rangle \rangle \Delta_0\), and the disordered phase, in which the long-range bond order (LRBO) is destroyed by thermal and disorder-induced kinks. The two phases are separated by a second-order transition. Figure 5-2 shows the phase diagram calculated for \(W/\mu = 0.008\), a typical value for trans-polyacetylene if the interchain interactions are dominated by interchain electron hopping [19]. The stars in Figure 5-2 denote the phase boundary which we obtained by numerical simulation of the model Eq. (5.1) using an algorithm based on the transfer-matrix approach that has
5.2 Solitons in interacting disordered Peierls chains

![Diagram showing the phase diagram of the anisotropic RFIM Eq. (5.1) with a curve and markers indicating LRBO and NO phases.]

**Figure 5-2:** The phase diagram of the anisotropic RFIM Eq. (5.1) captures the essential physics of weakly disordered Peierls systems and is shown as a function of the disorder strength $D/\mu^2$ and the temperature $T/\mu$. The long-range bond order (LRBO) phase corresponds to an average dimerization $\langle \langle \sigma \rangle \rangle_{\Delta_0} \neq 0$. The numerical calculation of the critical curve (stars) agrees well with the analytical result (solid curve) obtained in Chapter 4. The dashed curve indicates the breakdown of the continuum approximation in the analytical calculation below $T = T_0$.

been discussed in Section 3.5. The order parameter $\langle \langle \sigma \rangle \rangle$ was found from a self-consistent calculation of the mean field $B$ and the critical curve was then obtained by requiring that $\langle \langle \sigma \rangle \rangle \rightarrow 0$. The smooth temperature dependence of the phase boundary was obtained by averaging the free energy over $10^4$ random-field realizations for a chain with $10^3$ sites. The solid curve in Figure 5-2 indicates the phase boundary which was calculated in Chapter 4 from the analytical expression for the average free energy (see Eq. (4.43)) of the continuum version of the model Eq. (5.1). With the exception of the small temperature region, $T < T_0$ (for details see Section 4.4.2), the results of the continuum model and the numerical simulation of the discrete model agree well.

At low temperatures the phase transition results from a competition between the disorder and the interchain interactions as becomes clear from Figure 5-1. We found in Section 4.4.2 that the critical disorder strength which separates the phases with and without LRBO at zero temperature reads

$$D_c \approx \frac{2}{3} W \mu.$$  \hspace{1cm} (5.4)

In the disordered phase, $\langle \langle \sigma \rangle \rangle = 0$, the density of disorder-induced neutral solitons (spin-flips) is according to Eq. (4.68) to lowest order in $D$ given by

$$n_s = \frac{1}{d} \frac{D}{d \mu^2},$$ \hspace{1cm} (5.5)

as is the case for a single disordered chain ($W = 0$) [20]. On the other hand, for $D < D_c$ the order parameter $\langle \langle \sigma \rangle \rangle$ is observed to increase rapidly (see Figure 4-3) with a slope that
is proportional to the ratio $\mu/W \gg 1$. Thus, in the overwhelming part of the ordered phase the system is nearly perfectly ordered with an order parameter close to unity, $\langle \langle \sigma \rangle \rangle \approx 1$, and the solitons are bound into pairs by the interchain interactions (see Figure 5-1). Well within the ordered phase ($D \ll D_c$) their density is exponentially suppressed. The distance between the soliton-antisoliton pairs is much larger than the typical pair size and from Eq. (4.70) the number of soliton-antisoliton pairs per unit length is obtained to be

$$n_p = \frac{1}{d} \frac{2W^2}{D} \exp \left( -2 \frac{W\mu}{D} \right)$$  \hspace{1cm} (5.6)$$

(for $W^2 \ll D \ll D_c$).

In the following we will focus on the LRBO phase and calculate the magnetic susceptibility due to the spins of the bound pairs of neutral solitons.

### 5.3 Magnetic susceptibility in the ordered phase

Apart from the interchain interaction discussed in the previous section, there is also an intrachain interaction between kinks. The latter interaction is strong only when the distance between kinks is of the order of their size, $\xi_0$. Thus, for weak disorder, when the density of kinks is small, it has little effect on the statistics of the kinks. It may, however, be important for the magnetic properties of disordered Peierls systems, as it results in an antiferromagnetic exchange between the spins $1/2$ of neutral kinks [15]. This exchange can bind the spins of neighboring kinks into nonmagnetic singlets, thus reducing the magnetic susceptibility of the system. We note that the spins $1/2$ of the neutral kinks should not be confused with the Ising spins which represent the sign of the lattice dimerization.

As argued in the previous section, for a nearly perfectly ordered system the typical distance between disorder-induced soliton-antisoliton pairs is much larger than the typical pair size. We may then neglect the spin exchange between kinks from different pairs. This situation is sketched in Figure 5-3 and the Hamiltonian that describes the interactions of soliton and antisoliton spins, $\vec{S}_1$ and $\vec{S}_2$, within one pair reads

$$\hat{H}_{\text{pair}} = J \left[ (\vec{S}_1 \cdot \vec{S}_2 - \frac{1}{4}) - g\mu_B H (S_1^z + S_2^z) \right],$$  \hspace{1cm} (5.7)$$

where $J$ is the exchange constant in the pair and $H$ is the external magnetic field. The pair free energy is given by

$$f(J, H) = -J - \frac{1}{\beta} \ln \left[ 1 + e^{-\beta J} (1 + 2 \cosh(\beta g\mu_B H)) \right]$$  \hspace{1cm} (5.8)$$

and the zero-field magnetic susceptibility of the pair is

$$\chi(T, J) = \left. \frac{\partial^2 f(J, H)}{\partial H^2} \right|_{H=0} = 2g^2\mu_B^2 \beta \frac{e^{-\beta J}}{1 + 3e^{-\beta J}}.$$  \hspace{1cm} (5.9)$$

The coupling $J$ decreases with the soliton-antisoliton separation $R$. Quite generally, the large-$R$ behavior is

$$J = J_0 \exp \left( -\frac{R}{\rho} \right),$$  \hspace{1cm} (5.10)$$
5.3 Magnetic susceptibility in the ordered phase

\[ + \Delta_0 \]
\[ - \Delta_0 \]
\[ \begin{array}{c}
  + g \mu_B H \\
  - g \mu_B H \\
\end{array} \]
\[ S = 1 \]
\[ S = 0 \]
\[ \begin{array}{cc}
  S_1^z & S_2^z \\
  -1/2 & -1/2 \\
  0 & 0 \\
  +1/2 & +1/2 \\
\end{array} \]

Figure 5-3: (a) Order parameter along a Peierls chain in the LRBO phase. \( z_1, z_2 \) and \( z_3, z_4 \) denote the positions of two soliton-antisoliton pairs. The dashed line represents the spin exchange between the two spins 1/2 of a soliton-antisoliton pair. The exchange interaction between spins of neighboring soliton-antisoliton pairs is neglected as the distance between two pairs in the LRBO phase is large compared to the size of a pair. (b) Energy of the singlet and triplet state for an exchange-coupled spin pair with \( S = S_1 + S_2 \) as described by the Hamiltonian Eq. (5.7).

where \( \rho = \xi_0 / d \) (\( R \) is measured in units of \( d \)) and \( J_0 \) is of the order of the spin gap. For the SSH model, in which Coulomb interactions are neglected and the spin gap equals the charge gap, \( J_0 = 4 \Delta_0 \) [15].

As \( R \) is a random quantity that is imposed by the disorder realization, also \( J \) is random. If we know the pair size distribution, \( p(R) \), the distribution of exchange values, \( w(J) \), can be obtained using Eq. (5.10). We normalize the latter to the total density of spin-pairs

\[ n_p = \int_0^\infty dJ w(J) . \]  \hspace{1cm} (5.11)

The system’s magnetic susceptibility is then given by

\[ \chi(T) = \int_0^\infty dJ w(J) \chi(T,J) , \]  \hspace{1cm} (5.12)

with \( \chi(T,J) \) as in Eq. (5.9).

Clearly, the temperature dependence of the magnetic susceptibility is determined by the pair size distribution. As we will show in detail in Sections 5.4 and 5.5, in the LRBO phase,
\( p(R) \) is sharply peaked at some \( R^* \), while for \( R \gg R^* \)

\[
p(R \gg R^*) \propto \exp \left( -\alpha \frac{R}{\rho} \right)
\]  

(5.13)

with \( \alpha \) a constant determined by the strength of the disorder and interchain interactions. Equation (5.13) in a straightforward way yields a power-law exchange distribution

\[
w(J) \propto \left( \frac{J_0}{J} \right)^{1-\alpha}
\]  

(5.14)

for \( J \ll J(R^*) \). This part of \( w(J) \) dictates the behavior of the magnetic susceptibility at low temperature, \( T \ll J(R^*) \). Pairs with \( J \gg J(R^*) \) (or: \( R \ll R^* \)) are in the nonmagnetic singlet state at these low temperatures. We thus find

\[
\chi(T \ll J(R^*)) \propto \left( \frac{J_0}{T} \right)^{1-\alpha},
\]

(5.15)

which deviates from the high temperature Curie behaviour.

We note that, in order to describe the anomalous temperature dependence of the magnetic susceptibility of charge transfer salts, Clark et al. [21] also introduced pairs of spins with a random antiferromagnetic coupling. These pairs, however, were introduced in a purely phenomenological way, whereas in our model they naturally emerge as disorder-induced soliton-antisoliton pairs with a distribution of exchange constants that follows from the pair size distribution.

### 5.4 Calculation of the pair size distribution

The pair size distribution \( p(R) \) is defined as the number of soliton-antisoliton pairs of size \( R \) per site of the Ising chain. For a given disorder realization \( \{h_m\} \) one finds from Eq. (5.1) that the energy of a configuration \( \{m_1, m_2\} \), with the soliton located between \( m_1 \) and \( m_1 + 1 \) and the antisoliton between \( m_2 \) and \( m_2 + 1 \), reads:

\[
E[m_1, m_2] = E_0 - \Delta E[m_1, m_2],
\]

(5.16)

where \( E_0 \) denotes the energy for a configuration without solitons and

\[
\Delta E[m_1, m_2] = -2\mu - 2 \sum_{m=m_1+1}^{m_2} \left( B + h_m \right)
\]

(5.17)

is the energy change due to the creation of the soliton-antisoliton pair. As we restrict ourselves to isolated soliton-antisoliton pairs, it is sufficient to consider a segment of the chain which contains one such pair located far away from its end points. Furthermore, because the sequence of solitons and antisolitons along the chain is determined by fixed boundary conditions for the lattice dimerization, we may, without loss of generality, assume that \( m_2 > m_1 \). Then, the pair size \( R \) (in units of the Ising lattice constant \( d \)) is given by

\[
R = m_2 - m_1.
\]

(5.18)
The soliton-antisoliton pair configuration \((m_1, m_2)\) is only energetically favorable if

\[
\Delta E[m_1, m_2] \geq 0.
\] (5.19)

This is, however, not sufficient to calculate the pair size distribution \(p(R)\), as we also have to impose the condition that this pair configuration has lower energy than any other pair in the considered chain segment. Thus, simultaneously, the energy of the pair configuration has to satisfy the inequalities

\[
\Delta E[m_1, m_2] \geq \Delta E[m_1', m_2'],
\] (5.20)

for all other possible pair configurations \((m_1', m_2')\). Therefore, the desired pair size distribution takes the form:

\[
p(R) = \left\langle \Theta(\Delta E[m_1, m_2]) \prod_{(m_1', m_2')} \Theta(\Delta E[m_1, m_2] - \Delta E[m_1', m_2']) \right\rangle,
\] (5.21)

where \(\Theta(x)\) is the step function:

\[
\Theta(x) = \begin{cases} 
1 & \text{for } x \geq 0 \\
0 & \text{for } x < 0
\end{cases}
\]

and the brackets, \(\langle \ldots \rangle\), denote the Gaussian average over disorder realizations \([h_m]\). The definition Eq. (5.21) ensures that, in accordance with Eq. (5.11), \(p(R)/d\) is normalized to the density of soliton-antisoliton pairs:

\[
n_p = \frac{1}{d} \int_0^\infty dR p(R).
\] (5.22)

It is easy to see that \(p(R)\) factorizes into two independent parts, \(p_{\text{out}}\) and \(p_{\text{in}}\), that account for the soliton-antisoliton pairs with a size that is, respectively, larger and smaller than \(R\):

\[
p(R) = p_{\text{out}} p_{\text{in}},
\] (5.23)

with

\[
p_{\text{out}} = \left\langle \Theta(z + s_{m_1}) \Theta(2z + s_{m_1} + s_{m_1-1}) \Theta(3z + s_{m_1} + s_{m_1-1} + s_{m_1-2}) \ldots \right\rangle \times \left\langle \Theta(z + s_{m_2+1}) \Theta(2z + s_{m_2+1} + s_{m_2+2}) \Theta(3z + s_{m_2+1} + s_{m_2+2} + s_{m_2+3}) \ldots \right\rangle
\]

and

\[
p_{\text{in}} = \left\langle \Theta(-I - Rz - \sum_{m=m_1+1}^{m_2} s_m) \prod_{L} \prod_{R} \right\rangle.
\] (5.25)

Here, we have defined the dimensionless variables \(s_m = h_m/\sqrt{D}, z = B/\sqrt{D}, I = \mu/\sqrt{D}\), while

\[
\prod_L \equiv \left\langle \Theta(-z - s_{m_1+1}) \Theta(-2z - s_{m_1+1} - s_{m_1+2}) \ldots \Theta(-Rz - s_{m_1+1} - \ldots - s_{m_2}) \right\rangle
\] (5.26)

...
and
\[
\Pi_R \equiv \\
\equiv \Theta(-z - s_{m_2}) \Theta(-2z - s_{m_2} - s_{m_2-1}) \cdots \Theta(-Rz - s_{m_2} - \ldots - s_{m_1+1}) .
\]

The reason for the factorization of Eq. (5.21) into \( p_{\text{out}} \) and \( p_{\text{in}} \) is, that a pair configuration \((m_1, m_2)\) which is energetically favorable compared to the configurations \((m_1 + n_1, m_2)\) and \((m_1, m_2 + n_2)\) with one soliton position fixed, is also favorable compared to the configuration \((m_1 + n_1, m_2 + n_2)\) with both soliton positions changed. Note that \( p_{\text{out}} \) itself also consists of two independent factors: the first factor excludes the pairs with the soliton located to the left of \( m_1 \), while the second one excludes antisoliton positions larger than \( m_2 + 1 \). Both these factors can be written in the form:
\[
Y(z) = \prod_{m=1}^{\infty} \left[ \int_{-\infty}^{+\infty} ds_m f(s_m) \Theta\left( \sum_{k=1}^{m} [z + s_k] \right) \right],
\]
where
\[
f(s) = \frac{\exp\left(-\frac{1}{2}s^2\right)}{\sqrt{2\pi}}
\]
is the Gaussian weight. As a result, for the outer factor we obtain:
\[
p_{\text{out}} = |Y(z)|^2 .
\]

The function \( Y(z) \) will be calculated later in this section.

The calculation of the inner factor is complicated by the presence of the extra \( \Theta \)-function in Eq. (5.25), which precludes the factorization of \( p_{\text{in}} \) in two independent averages. However, considerable simplification is possible, because we focus on the bond-ordered phase where \( \langle \langle \sigma \rangle \rangle \approx 1 \). Then the density of disorder-induced soliton-antisoliton pairs is small, and the main suppression factor in \( p(R) \) is the probability of the disorder realization necessary to create a pair [22, 23]. In other words, the most important contribution to \( p_{\text{in}} \) (and \( p(R) \)) comes from averaging the first \( \Theta \)-function in Eq. (5.25):
\[
\left\langle \Theta(-1 - \sum_{m=m_{1}+1}^{m_{2}} (z + s_{m})) \right\rangle = \frac{1}{2} \text{erfc}(g(R)) \approx \frac{\exp(-g(R)^2)}{\sqrt{4\pi} g(R)} ,
\]
where
\[
g(R) \equiv \frac{I + Rz}{\sqrt{2R}} .
\]
Here, the asymptotic expression for the complementary error function \( \text{erfc}(g(R)) \) was used because the minimal value for its argument is easily shown to be \( g_{\text{min}} = \sqrt{3Dc/\bar{D}} \), so that for \( D \leq Dc/2 \) the relative error becomes already less than several percent.

The interpretation of this result is that the optimal disorder fluctuation (i.e., the disorder realization with the largest weight) that can induce a soliton-antisoliton pair of size \( R \) has a
constant value $-h_R$ in the interval of length $R$ and is zero outside the interval. The amplitude $h_R$ is determined by the energy balance (see Eqs. (5.17) and (5.19)):  

$$h_R R = \mu + WR.$$  

(5.33)

The weight of the optimal fluctuation, $w = \exp \left( -Rh_R^2/(2D) \right)$, is precisely the exponential factor appearing in Eq. (5.31). At  

$$R^* = \frac{1}{z} = \frac{\mu}{W} \gg 1$$  

(5.34)

the weight reaches its maximal value, $\exp(-2W\mu/D)$. For $D \ll D_c$, the maximal weight is small (as was also found in Eqs. (5.31) and (5.32)) and the soliton-antisoliton pairs are suppressed. In that case, all disorder realizations that contribute significantly to $p(R)$ are close to the optimal fluctuation.

Bearing this in mind, we now calculate the inner factor Eq. (5.25). First, we can rewrite Eq. (5.25) in the form:

$$p_{in} = \int_{z_{R+1}}^{\infty} dz \int_{-i\infty}^{+i\infty} \frac{d\lambda}{2\pi i} e^{-\lambda S} \prod_{m=m_1+1}^{m_2} \int_{-\infty}^{+\infty} ds_m e^{-\lambda s_m} f(s_m) \Pi_L \Pi_R,$$  

(5.35)

where the integration over $\lambda$ ensures that  

$$S = - \sum_{m=m_1+1}^{m_2} s_m$$  

(5.36)

and the limits of the integration over $S$ follow from the first $\Theta$-function in Eq. (5.25).

Since the typical pair size $R^* \gg 1$ (see Eq. (5.34)), we can use the canonical formalism, in which Eq. (5.36) for the sum of $R$ random variables is satisfied only in average. We do this by “shifting” the argument of the random-field distribution on each site by $\lambda$:

$$f(s) \rightarrow f(s + \lambda) = e^{-\frac{1}{2} \lambda^2 - \lambda s} f(s),$$  

(5.37)

so that the average value now becomes $s = -\lambda$ and Eq. (5.35) reads:

$$p_{in} = \int_{z_{R+1}}^{\infty} dz \int_{-i\infty}^{+i\infty} \frac{d\lambda}{2\pi i} e^{-\lambda S + \frac{1}{2} R \lambda^2} \prod_{m=m_1+1}^{m_2} \int_{-\infty}^{+\infty} ds_m e^{-\lambda s_m} f(s_m + \lambda) \Pi_L \Pi_R.$$  

(5.38)

The integral over $\lambda$ comes from the small vicinity ($\sim 1/\sqrt{R}$) of $\lambda_0 = S/R$, where the exponential in Eq. (5.38) has its maximum. Saddle-point integration over $\lambda$ then gives:

$$p_{in} = \int_{z_{R+1}}^{\infty} \frac{ds}{\sqrt{2\pi R}} e^{-\frac{1}{2} \frac{s^2}{R}} \prod_{m=m_1+1}^{m_2} \int_{-\infty}^{+\infty} ds_m f \left( s_m + \frac{S}{R} \right) \Pi_L \Pi_R.$$  

(5.39)

Next we note that if the condition imposed by the first $\Theta$-function in Eq. (5.25) is satisfied, the arguments of the last $\Theta$-functions in $\Pi_L$ and $\Pi_R$ also almost certainly are positive. In other words, because the relevant disorder realizations are close to the optimal fluctuations, only the
first few $\Theta$-functions in $\Pi_L$ and $\Pi_R$ are really restrictive. This implies that the disorder averages of $\Pi_L$ and $\Pi_R$ in Eq. (5.39) are decoupled. Furthermore, it is easily seen from Eq. (5.28) that then $\langle \Pi_L \rangle = \langle \Pi_R \rangle = Y(s_R - z)$, so that Eq. (5.39) becomes:

$$p_{in} = \int_{z_{R+1}}^{\infty} \frac{dS}{\sqrt{2\pi s}} e^{-\frac{1}{2}s^2} \left[ Y \left( \frac{s_R}{R} - z \right) \right]^2.$$  \hspace{1cm} (5.40)

The integral over $S$ comes from the vicinity of the lower limit, $S = zR + l$ [cf. Eq. (5.33) for the optimal fluctuation]. The result of the integration is:

$$p_{in} = \sqrt{\frac{R}{2\pi}} \exp \left[ -\frac{(l + Rz)^2}{2R} \right] \left[ Y \left( \frac{l}{R} \right) \right]^2,$$  \hspace{1cm} (5.41)

where for $S$ in the argument of $Y$ we took its value at the lower limit of the integration.

From Eqs. (5.23), (5.30), and (5.41) we finally obtain for the pair size distribution:

$$p(R) = \frac{\exp(-g(R)^2)}{\sqrt{4\pi g(R)}} \left[ Y \left( \frac{1}{R} \right) \right]^2 \left| Y(z) \right|^2,$$  \hspace{1cm} (5.42)

where the function $g(R)$ is defined by Eq. (5.32).

What is left now, is the calculation of the function $Y(v)$. To this end we introduce the function $Y(s|v)$, satisfying the integral equation:

$$Y(s|v) = \int_{0}^{\infty} ds' f(s + v - s') Y(s'|v).$$  \hspace{1cm} (5.43)

Comparing the iterative solution of this equation to Eq. (5.28), one finds:

$$Y(v) = Y(0|v).$$  \hspace{1cm} (5.44)
The integral equation (5.43) can be easily solved numerically. The result is shown as stars in Figure 5-4. The solid line represents the best fit to these points by a function of the form:

\[ Y(v) = \tanh(c v) . \]  

(5.45)

The fit yields \( c \approx 1.14 \). For small \( v \), the best linear fit \( Y(v) = c' v \) yields \( c' \approx \sqrt{2} \), with a precision of several percent.

We conclude this section by a brief analysis of the pair size distribution Eq. (5.42). In Figure 5-5 we plot \( p(R) \) for four different parameter sets. It is clearly seen that \( p(R) \) reaches a maximal value at a typical pair size \( R^* \) and falls off exponentially for smaller or larger values of \( R \). Integrating \( p(R)/d \) over \( R \) gives the density of soliton-antisoliton pairs (cf. Eq. (5.22)). For \( D \ll D_c \), the exponential factor in Eq. (5.42) has a sharp peak at \( R^* \) given by Eq. (5.34). Using \( B \approx W \), the saddle-point integration around the peak gives:

\[ n_p \approx \frac{1}{d} \frac{D}{2 W^2} \left[ Y \left( \frac{W}{\sqrt{D}} \right) \right]^4 \exp \left( -2 \frac{W \mu}{D} \right) . \]  

(5.46)

Furthermore, we note that knowledge of the pair size distribution Eq. (5.42) allows us to derive the long- and short-range bond order parameter of the RIM Eq. (5.1). For a dilute gas of soliton-antisoliton pairs it is sufficient to consider a chain segment of \( N + 1 \) sites containing a single pair of size \( R \):

\[ \sigma(m) = 1 - 2 \Theta(m - m_1) \Theta(m_2 - m) , \]  

(5.47)

where \( m_1 \) and \( m_2 = m_1 + R \) denote the positions of, respectively, the soliton and the antisoliton. Replacing summations by integrations, the LRBO parameter averaged over all possible pair sizes
is easily calculated:

\[
\langle \langle \sigma \rangle \rangle = \int_0^\infty dR p(R) \int_{-\infty}^{+\infty} dm \sigma(m) = 1 - 2 \int_0^\infty dR p(R) R .
\] (5.48)

For a nearly perfectly ordered system, \( \langle \langle \sigma \rangle \rangle \simeq 1 \), we thus find from Eq. (5.48) the condition that the typical pair size \( R^* \) is much smaller than the typical number of sites \( 1/|d\sigma|_p \) between soliton-antisoliton pairs. Similarly, we calculate the correlation function

\[
\langle \langle \sigma(0)\sigma(1) \rangle \rangle = \langle \langle \sigma \rangle \rangle^2 + \langle \langle \sigma(0)\sigma(1) \rangle \rangle_c ,
\] (5.49)

where the square of the LRBO parameter is obtained from Eq. (5.48),

\[
\langle \langle \sigma \rangle \rangle^2 \simeq 1 - 4 \int_0^\infty dR p(R) R ,
\] (5.50)

and the connected correlator is found to be

\[
\langle \langle \sigma(0)\sigma(1) \rangle \rangle_c = 4 \int_0^\infty dR p(R + |l|) R .
\] (5.51)

The scale for the decay of short-range correlations is obviously set by the typical pair size \( R^* \), as \( \langle \langle \sigma(0)\sigma(1) \rangle \rangle_c \to 0 \) for \( |l| \gg R^* \).

### 5.5 The exchange distribution in the continuum limit

In the previous sections we described disordered Peierls systems using the effective RFIM Eq. (5.1). The values of the interchain interaction \( W \) and the disorder strength \( D \) in this model are proportional to the length \( d \) which we choose for the unit cell of the Ising chain and which plays the role of a short-distance cut off. On the other hand physical observables, such as the density of soliton-antisoliton pairs and the magnetic susceptibility, should not depend on \( d \). Thus, before comparing our results to the experimental data on trans-polyacetylene, we show that \( d \) drops out from the expressions for the observables in the limit \( d \to 0 \).

To this end, we re-introduce as physically meaningful quantities the disorder strength \( \bar{D} = \kappa^2 \mathcal{A} \) and the interchain interaction \( \bar{W} \) per unit length:

\[
D = d \bar{D} ,
\] (5.52)

and

\[
W = d \bar{W} .
\] (5.53)

Furthermore, from now on we will work with the physical pair size \( r = R d \). In terms of these new variables, the arguments of both \( Y \)-functions in Eq. (5.42) for the pair size distribution are \( \propto \sqrt{d} \). Therefore, for \( d \to 0 \), the arguments are small and we can use \( Y(\nu) \simeq \sqrt{2} \nu \) (see below Eq. (5.45)), giving the pair size distribution

\[
p(r) = 4 \frac{\mu^2 \bar{W}^2}{D^2 r^2} \frac{\exp \left( -g(\bar{V})^2 \right)}{\sqrt{4\pi g(\bar{V})}} ,
\] (5.54)
Table 5-1: The four sets of parameters used in the numerical calculations for a fixed density of spin pairs, $n_p = 1/6000 \alpha^{-1}$. The value for $\alpha$ as defined in Eq. (5.59) is obtained using the SSH-parameter $\xi_0 = 7\alpha$ for the correlation length.

<table>
<thead>
<tr>
<th>$\tilde{W}$ ($\mu/\alpha$)</th>
<th>$\tilde{D}$ ($\mu^2/\alpha$)</th>
<th>$J_0$ (K)</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.038</td>
<td>0.010</td>
<td>400</td>
<td>0.5</td>
</tr>
<tr>
<td>0.055</td>
<td>0.014</td>
<td>130</td>
<td>0.75</td>
</tr>
<tr>
<td>0.070</td>
<td>0.017</td>
<td>72</td>
<td>1.0</td>
</tr>
<tr>
<td>0.100</td>
<td>0.023</td>
<td>39</td>
<td>1.5</td>
</tr>
</tbody>
</table>

where

$$g(r) = \frac{\mu + \tilde{W}r}{\sqrt{2D}r}.$$  \hspace{1cm} (5.55)$$

Similarly, from Eq. (5.46), the total density of neutral soliton-antisoliton pairs in the limit $d \to 0$ is found to be:

$$n_p \approx \frac{2\tilde{W}^2}{D} \exp\left(-2\tilde{W}\mu/D\right),$$ \hspace{1cm} (5.56)$$

which coincides with Eq. (5.6) obtained in Section 4.4.2 within the continuum approximation for the RFIM Eq. (5.1).

Furthermore, in terms of continuum variables, the exchange coupling Eq. (5.10) reads:

$$J(r) = J_0 \exp\left(-\frac{r}{\xi_0}\right).$$ \hspace{1cm} (5.57)$$

Thus, in the continuum limit the distribution of exchange constants becomes:

$$w(J) = \int_0^\infty dr \tilde{p}(r) \delta(J - J(r)) = \frac{1}{2} \frac{1}{\xi_0} \frac{\mu^2 \tilde{W}^2}{D^2 \ln|J/J_0|/2} \frac{\exp\left(-g(J)^2\right)}{\sqrt{4\pi g(J)}},$$ \hspace{1cm} (5.58)$$

with $g(J) \equiv g(r = \xi_0 \ln(J_0/J))$ (cf. Eq. (5.55)).

In Figure 5-6 we plot the distribution $w(J)$ for four different parameter sets $\{\tilde{D}, \tilde{W}, J_0\}$ chosen such that the density of soliton-antisoliton pairs is fixed at $n_p = 1/6000 \alpha^{-1}$ (with $\alpha$ the average carbon-carbon distance in trans-polyacetylene). Our choice of parameters is summarized in Table 5-1 and will become clear in Section 5.6. Depending on the parameters, one observes two qualitatively very different behaviors: $w(J)$ either has a pronounced peak at $J^* \approx J(r^*)$ (with $r^* = R^* d$ and $R^*$ as in Eq. (5.34)) and tends to zero for $J \to 0$, or $w(J)$ diverges for small $J$. The distinction between these two behaviors is dominated by only one parameter combination:

$$\alpha = \frac{\tilde{W}^2}{2D} \xi_0.$$ \hspace{1cm} (5.59)$$
Figure 5-6: The distribution \( w(J) \) of exchange constants as a function of \( J/J_0 \) for the four parameter sets given in Table 5-1. The curves correspond to \( \alpha = 1.5 \) (dots), 1.0 (dash-dot), 0.75 (dashes), and 0.5 (solid). For \( \alpha \geq 1.0 \) the distribution has a pronounced peak at some \( J = J^* \) and tends to zero for \( J \to 0 \). In contrast, for \( \alpha < 1.0 \), \( w(J) \) diverges when \( J \to 0 \).

In fact, Eq. (5.58) for \( J \ll J^* \) yields

\[
w(J) \propto \left( \frac{J_0}{J} \right)^{1-\alpha},
\]

which shows that the relative strength of the interchain interactions and the disorder determines whether \( w(J) \) diverges \( (\alpha < 1) \) or approaches zero \( (\alpha > 1) \) for \( J \to 0 \).

The power-law dependence of \( w(J) \) at small \( J \) gives rise to a characteristic low-temperature behavior of the magnetic susceptibility, as we will see in the next section.

5.6 Magnetic susceptibility of trans-polyacetylene

In this section we consider trans-polyacetylene as a disordered Peierls system and calculate its magnetic susceptibility due to disorder-induced soliton-antisoliton pairs as a function of temperature. The temperature dependence of the magnetic susceptibility is determined by the distribution of exchange constants Eq. (5.58). For temperatures \( T \) much larger than the typical singlet-triplet energy splitting \( J^* \), almost all spin pairs are thermally excited. Thus, we have, essentially, \( 2n_p \) free spins, which give rise to a Curie susceptibility. Indeed, Eqs. (5.9) and
(5.12) yield:
\[ \chi(T \gg J^*) \approx \frac{1}{2} g^2 \mu_B^2 \beta \int_0^\infty \text{d} |J| w(J) = \frac{1}{2} g^2 \mu_B^2 \frac{n_p}{T}, \]  
(5.61)
where the density of soliton-antisoliton pairs \( n_p \) is given by Eq. (5.56). In the opposite limit, \( T \ll J^* \), however, most of the spin pairs are in the singlet state and do not contribute to the magnetic susceptibility. Under these conditions Eqs. (5.12) and (5.58) yield:
\[ \chi(T \ll J^*) = C(T) \left( \frac{J_0}{T} \right)^{1-\alpha}, \]  
(5.62)
with \( \alpha \) as in Eq. (5.59) and logarithmic temperature corrections given by
\[ C(T) \approx \frac{4 g^2 \mu_B^2}{9 J_0 \alpha} \left( \frac{n_p \xi_0}{\pi} \right)^{\frac{1}{2}} \frac{\mu^2}{D \xi_0^2} \frac{\Gamma(1 + \alpha) \text{Li}_\alpha(\frac{1}{\tau})}{(\ln(J_0/T))^{5/2}}, \]  
(5.63)
\((\text{Li}_\nu(z) = \sum_{k=1}^{\infty} z^k/k^\nu \) is the polylogarithm function). The dominant factor in Eq. (5.62) is \( (J_0/T)^{1-\alpha} \), which basically gives the density of spin pairs with singlet-triplet splitting \( \sim T \) (cf. Eq. (5.60)).

We thus find that the low-temperature behavior of the magnetic susceptibility differs from the Curie law and is dictated by the relative strength \( \alpha \) of interchain interactions and disorder. For \( \alpha < 1 \), the susceptibility diverges as \( T \to 0 \), while for \( \alpha > 1 \) it approaches zero.

A low-temperature \((T < 30 \text{ K})\) deviation from Curie behavior has indeed been observed by Foot et al. in ESR experiments on Durham \textit{trans}-polyacetylene [5]. These authors already suggested pairing of spins as possible reason for this behavior. To see whether our model of spins associated with disorder-induced soliton-antisoliton pairs offers a microscopic explanation, we compared our result for \( \chi(T) \) (numerically calculated from Eqs. (5.12) and (5.58)) to the experimental data. In our fit procedure there are, in principle, three free parameters: \( \tilde{W}, \tilde{D}, \) and \( J_0 \) (for the correlation length we take the SSH value \( \xi_0 = 7\alpha \)). We require, however, that our parameters are also consistent with the total density of spin pairs, which is reported to be approximately \( n_p = 1/6000 \alpha^{-1} \) [2, 3, 4, 5]. This requirement imposes a relation between \( \tilde{W} \) and \( \tilde{D} \), reducing the number of free parameters to two.

In practice, we chose various values for \( \alpha \) (Eq. (5.59)). For each \( \alpha \) value, \( \tilde{W} \) and \( \tilde{D} \) are uniquely determined by \( n_p \), and \( J_0 \) is left as free parameter to fit the temperature dependence of the magnetic susceptibility. This procedure yielded the fits shown in Figure 5-7, with parameter sets given in Table 5-1. For convenience, we will refer to each parameter set by its \( \alpha \) value. We note that our values for \( J_0 \) are much smaller than the value \( J_0 = 4\Delta_0 \sim 10^4 \text{ K} \), which one would expect in the absence of Coulomb interactions. It is not known, however, how Coulomb interactions alter \( J_0 \) and (possibly) the exponent in Eq. (5.10).

The important point is now that, while all four parameter sets give rise to reasonable fits of the experimental data, they predict totally different behaviors for \( T \leq 5 \text{ K} \), where experiments have not been performed. This is shown in Figure 5-8, where we extend the four theoretical fits to 1 K. The qualitative differences in the low-temperature behavior, dictated by the value of \( \alpha \), are clearly visible below 5 K. This suggests that extending the experiments to lower temperatures may yield more information on the relative strength of interchain interactions and disorder in \textit{trans}-polyacetylene.
Figure 5-7: Fits of our theory (solid curve) to the experimental data (dots) for the magnetic susceptibility of Durham trans-polyacetylene obtained in Ref. [5]. The four parameter sets given in Table 5-1 were used to fit the same experimental data points (see text for details). The deviation from Curie behavior (straight line) below $T = 30 K$ is clearly seen and reasonably reproduced by each fit down to $T = 5 K$, below which experimental data are not available.

We conclude this section by noting that, within the context of our model, it is possible to determine the strength of the interchain interactions and the disorder independent of the fitting parameter $J_0$. For this purpose, the density $n_p$ of soliton-antisoliton pairs is to be obtained experimentally from the Curie tail of the magnetic susceptibility, while for the same sample $\alpha$ is to be determined from the asymptotic zero-temperature behavior of the magnetic susceptibility. Then, using Eqs. (5.56) and (5.59), the strength of the interchain interactions,

\[
\tilde{W} \approx 4 \alpha \frac{\mu}{\xi_0} \left[ \ln \left( \frac{4\alpha}{n_p \xi_0} \right) \right]^{-1},
\]

and the disorder strength,

\[
\tilde{D} \approx 8 \alpha \frac{\mu^2}{\xi_0} \left[ \ln \left( \frac{4\alpha}{n_p \xi_0} \right) \right]^{-2},
\]

can be calculated as a function of $n_p$ and $\alpha$. For typical values of the density $n_p$, the logarithmic factor depends only weakly on $\alpha \sim O(1)$ and can be approximated by a numerical constant. If $n_p = 1/6000 \alpha^{-1}$ and choosing again the SSH-parameter $\xi_0 = 7\alpha$, one obtains $\tilde{W} \approx 0.07 \alpha \mu / \alpha$ and $\tilde{D} \approx 0.02 \alpha \mu^2 / \alpha$. It is important to realize that Eqs. (5.64) and (5.65) do not depend on the maximal exchange constant $J_0$ which may be used as a fitting parameter for temperatures around the typical exchange $J^*$. 
5.7 Concluding remarks

To summarize, we have calculated the magnetic susceptibility of quasi-one-dimensional Peierls systems with a doubly degenerate ground state. We have related the temperature-dependent part of the susceptibility to the presence of neutral solitons and antisolitons with spin $\frac{1}{2}$ induced by disorder in the electron hopping amplitudes along the chain. We have assumed the interchain interactions to be sufficiently strong to bind the disorder-induced solitons and antisolitons into pairs and thus establish long-range bond order in the system. Using a mapping on the random-field Ising model, we have calculated the distribution of the soliton-antisoliton pair size. This allowed us to obtain the distribution of exchange constants describing the interaction between the spins of the soliton and the antisoliton within one pair. Both distributions strongly depend on the relative strength $\alpha$ of the disorder and the interchain interactions. As a result, the magnetic susceptibility deviates from the Curie law: below $T = J^*$, where $J^*$ is the most probable value of the exchange constant, the magnetic susceptibility behaves as $(1/T)^{1-\alpha}$.

We explained in Section 5.3, that this power-law temperature dependence of the magnetic susceptibility can be traced back to the fact that the pair size distribution Eq. (5.54) is exponential for pair sizes $r$ which are large compared to the typical pair size $r^*$,

$$
\tilde{p}(r \gg r^*) \propto \exp \left( -\alpha \frac{r}{\xi_0} \right).
$$

(5.66)

This exponential dependence can be interpreted as follows: For pair sizes $r \gg r^*$, the energy of the string between soliton and antisoliton exceeds the kink creation energy: $\tilde{W}r \gg \mu$. Thus, the amplitude of the optimal fluctuation is $\tilde{h}r \approx \tilde{W}r$ (see Eq. (5.33)). The Gaussian weight

Figure 5-8: As Figure 5-7, but now the four theoretical curves are shown down to $T = 1$ K. It is clearly observed that different values for $\alpha$ (the relative strength of disorder and interchain interactions) lead to qualitatively different low-$T$ ($< 5$ K) behavior of the magnetic susceptibility.
of this fluctuation,

\[ w(r) = \exp \left( -\frac{\tilde{\nu}^2 r^2}{2D} \right) \simeq \exp \left( -\frac{\tilde{W}^2 r}{2D} \right), \quad (5.67) \]

is the exponential in Eq. (5.66) and by comparison we correctly estimate the important parameter \( \alpha = \tilde{W}^2 \xi_0 / (2D) \) in agreement with Eq. (5.59). Similar arguments were used in Section 2.3 to explain the power-law dependence of the density of states in the Fluctuating Gap Model of disordered systems [23].

Our results explain the deviation of the magnetic susceptibility from Curie behavior observed in Durham \textit{trans}-polyacetylene [5], though from the experimental data it is difficult to find unambiguously the values of \( \alpha \) and \( J^* \) for this conjugated polymer. It is, therefore, important to extend the measurements to lower temperatures, where the temperature dependence of the magnetic susceptibility is extremely sensitive to the choice of parameters.

In the ordered phase, the disorder-induced soliton-antisoliton pairs show up in the x-ray spectrum as a broad incoherent peak associated with each sharp elastic peak arising from the bond length alternation. Our result for the pair size distribution allows one to calculate the intensity \( I(q) \) of this incoherent peak which simply is proportional to the Fourier transform squared of the connected correlator Eq. (5.51). With the pair size distribution Eq. (5.54) in the continuum limit, we obtain

\[ I(q) \propto \left| \int_{-\infty}^{\infty} dl \langle \sigma(0) \sigma(l) \rangle e^{-iql} \right|^2 = \left| \int_{0}^{\infty} dl \tilde{\rho}(l) \frac{1 - \cos(ql)}{q^2} \right|^2, \quad (5.68) \]

and immediately find the peak width from \( I(q') = I(0)/2 \) to be independent of the disorder strength: \( q' \sim \tilde{W}/\mu \). It should be kept in mind, however, that this calculation does not account for other broadening mechanisms, e.g., those due to the complicated morphology of polyacetylene samples.

We finally mention that our theory is only applicable when the low-temperature behavior of the susceptibility is an intrinsic property of the material and is not governed by spins of impurities. The latter situation may, in fact, be realized in Shirakawa \textit{trans}-polyacetylene, which shows Curie behavior down to \( T = 1.5 \) K [24]. Furthermore, we assumed the existence of long-range order in the system. Whether this is a reasonable assumption in the case of (partially) crystalline \textit{trans}-polyacetylene is an open question. It would, therefore, be interesting to extend our studies to the case without long-range order. At the same time, however, it should be noted that in substituted polyacetylenes, the degeneracy of the two dimerized configurations may be lifted. This leads to an extra (intrachain) source of soliton-antisoliton confinement [25] and favors long-range bond order. Our theory may be applied to these substituted polymers by simply adding to the interchain interaction per bond (\( \tilde{W}_a \)), the energy difference per bond between the two dimerized configurations. As this energy difference may be controlled by varying the substitutions, this opens interesting possibilities to study disorder-induced solitons in more detail.
Bibliography


