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2000 J. Phys.: Condens. Matter 12 7933

(http://iopscience.iop.org/0953-8984/12/36/308)

J. Phys.: Condens. Matter **12** (2000) 7933–7943. Printed in the UK PII: S0953-8984(00)14082-2

The transport properties of quasi-one-dimensional double-chain systems in a magnetic field

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Received 22 May 2000, in final form 25 July 2000

Abstract. We present numerical results on transport properties in quasi-one-dimensional (1D) double-chain systems in a magnetic field obtained by the use of the transfer-matrix technique. The two chains are coupled with bonds in random positions which mimic the topological disorder in the quasi-1D polymer system. There are two scattering mechanisms: the random positions of the interchain coupling and the random flux through the loops. We find that the former is suppressed by quantum interference if the interchain coupling at every link is formed by double-bond hopping, leading to the existence of extended states in the absence of a magnetic field. These states do not exist in the case of single-bond coupling. This difference between the two cases disappears in a strong field. The formula for the transmission coefficient is obtained from the numerical results in both cases.

1. Introduction

Conjugated polymers have been extensively studied recently because of their increasing importance in both fundamental and applied research. It has been predicted from the scaling theory that all the states are localized in one dimension (1D) with a small amount of disorder [1]. However, extended states have been verified in several specific 1D models. Completely reflectionless states, which have unit transmission and zero reflection, exist in the 1D random-dimer model [2]. Similar delocalized states, or completely unscattered states, have also been found in other 1D systems with correlated disorder [3–6]. The electronic transport properties of quasi-1D winding chains with random loops display groups of states with very long localization lengths which can lead to high values of the conductance [7]. The electronic diffusion in quasi-1D systems with double chains and randomly placed interchain bonds can support high conductance [8].

The delocalization features of the above-mentioned states are mainly determined by the specific interference of waves scattered by the impurities. As an example, for the resonance states in the random-dimer model the waves scattered by two impurities in a dimer are cancelled by the destructive interference, resulting in complete transmission. In the presence of a magnetic field the phases of electron waves depend also on the magnetic flux in a quasi-1D double-chain system. It would be interesting to know how the properties of states in such systems in which nearly extended states exist will be changed if a magnetic field is applied. In this paper we study the transport properties of double-chain systems in a magnetic field. The positions of interchain links are random, leading to topological disorder. In the absence of a magnetic field the systems in which the interchain coupling is formed with double-bond coupling exhibit delocalized properties, while the systems with single-bond interchain

0953-8984/00/367933+11$30.00

coupling show insulating behaviour [8]. In the presence of a magnetic field the condition for the destructive interference of backward-scattered waves in the double-bond case is violated, leading to the destruction of the extended states. On changing the magnetic field, the Aharonov–Bohm (AB) oscillations exist only in the periodic systems. With disordering of the distribution of the bonds, the AB oscillations are suppressed in both single-bond and double-bond situations. From the results of numerical calculations, we obtain a formula for the dependence of the transmission coefficient (TC) on energy, field, strength of interchain coupling and system size in random systems with both double-bond and single-bond interchain coupling. The present model can be related to the transport properties of two coupled polymer chains and other quasi-1D systems of quantum wires or nanotubes for which it has become possible to artificially separate the chains from each other in recent years.

In this paper we describe our model and the basic formulae in the next section, the numerical data obtained are analysed in the third section, and the conclusions are summarized in the last section.

2. Model and formula

The topological structure of the two-chain system is illustrated in figure 1. The two chains are wound, and cross each other to form many loops. We suppose that these loops are in the same plane and the enclosed area of a loop is proportional to its perimeter. The magnetic field is perpendicular to the plane. The tight-binding Hamiltonian of the system can be written as

$$H = H_0 + H_c \tag{1}$$

where H_0 is the Hamiltonian of the isolated chains:

$$H_0 = \sum_{l=1,2} \sum_{i=1}^{N_l-1} t_0 (c^{\dagger}_{i+1,l} c_{i,l} + \text{H.c.}) \tag{2}$$

with $c_{i,l}$ being the annihilation operator of an electron on the ith site of the lth chain, and H_c the coupling Hamiltonian of the two chains. Here N_l is the site number of the lth chain. We omit the spin index of the electrons. For the interchain coupling we consider two situations: the single-bond and double-bond coupling. For the case of single-bond coupling, the two chains

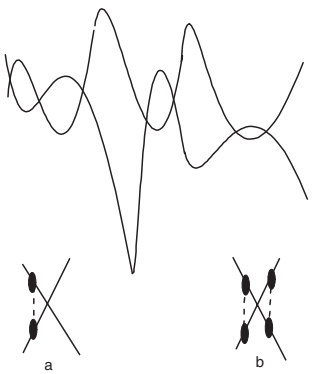

Figure 1. The topological structure of the double-chain system. The single bond and double bonds at a crossing point are shown in panels (a) and (b), respectively.

are coupled with one bond at every crossing point and H_c can be written as

$$H_c = H_{sb} = \sum_{n=1}^{N_b} (t_n c^{\dagger}_{j_{n1},1} c_{j_{n2},2} + \text{H.c.}) \tag{3}$$

where n is the index of interchain bonds, j_{n1} and j_{n2} are the positions of the nth interchain bond in the first and second chains, respectively, t_n is the hopping integral of the nth interchain bond. In the case of double-bond coupling we have

$$H_c = H_{db} = \sum_{n=1}^{N_b} [t_n (c^{\dagger}_{j_{n1},1} c_{j_{n2},2} + c^{\dagger}_{j_{n1}+1,1} c_{j_{n2}+1,2}) + \text{H.c.}]. \tag{4}$$

In both cases the positions of the nth interchain link j_{n1} and j_{n2} are random. We assume that $j_{1l} < j_{2l} < \cdots < j_{N_b,l}$ and the lengths of the chain segments between the nth and the $(n+1)$th interchain bonds are denoted as $\lambda_{nl} \equiv j_{n+1,l} - j_{nl}$ for $l = 1, 2$ and $1 \leqslant n \leqslant N_b$. In this paper we use a uniform distribution for random variables λ_{nl}:

$$P(\lambda_{nl}) = \begin{cases} \dfrac{1}{\delta\lambda} & \text{for } \lambda_0 - \delta\lambda/2 \leqslant \lambda_{nl} \leqslant \lambda_0 + \delta\lambda/2 \\ 0 & \text{otherwise} \end{cases}$$

where λ_0 is the average segment length and $\delta\lambda$ is the degree of topological disorder.

In the presence of a magnetic field the flux threaded in every loop produces a phase shift of the wave function in the two chains. We use a special gauge in which the phase produced by the flux appears only in the interchain coupling terms of the Hamiltonian. Thus the t_0 in H_0 is unchanged by the field and t_n in H_c becomes

$$t_n = t\mathrm{e}^{\mathrm{i}\phi_n} \tag{5}$$

where ϕ_n is determined by $\phi_{n+1} - \phi_n = 2\pi(-1)^n \Phi_n/\Phi_0$ with Φ_n being the flux threaded through the loop enclosed by the n and $(n+1)$th crossing points and Φ_0 the flux quantum. The sign in this expression is due to the alternating exchange of positions of the two chains in successive loops. In the case of $t = 0$, the phase of $\mathrm{e}^{\mathrm{i}\phi_n}$ is directly introduced into the coefficients of the wave functions at the crossing points to account for the effect of flux. Owing to the topological disorder, the positions of the interchain links are random variables which determine the values of ϕ_n.

We employ the transfer-matrix technique [8] to calculate the transmission coefficient of an electron moving through the system. The system contains two chains with finite lengths. We use an open boundary condition: that is, the four ends of the two finite chains of the system are respectively connected to four semi-infinite perfect chains without interchain coupling which serve as the incoming and outgoing leads. In each of the leads there are two channels corresponding to two semi-infinite chains. The N_b interchain links divide the whole system, including the leads, into $2(N_b + 1)$ segments. In each of the segments the wave function can be expressed as plane waves because the structure is regular within the segment. Thus, in the case of single-bond links we can write the coefficients of the wave function as

$$\Psi_{i,l} = A_{n,l}\mathrm{e}^{\mathrm{i}k(i-j_{n-1,l})} + B_{n,l}\mathrm{e}^{-\mathrm{i}k(i-j_{n-1,l})} \qquad \text{for } j_{n-1,l} \leqslant i \leqslant j_{n,l} \tag{6}$$

where

$$k = \cos^{-1}\frac{E}{2t_0}$$

is the wave vector with E the energy of the electron. Thus, $A_{n,l}$ and $B_{n,l}$ specify the wave function in the segment between the $(n-1)$th and the nth interchain bonds in the lth chain. This expression can be extended to $n = 1$ and $n = N_b + 1$ by including the leads. In the case of

double-bond coupling, equation (6) is still valid on changing the limit to $j_{n-1,l}+1 \leqslant i \leqslant j_{n,l}$. The Schrödinger equation is used to determine the relations between the coefficients $A_{n,l}$, $B_{n,l}$ and $A_{n+1,l}$, $B_{n+1,l}$ which can be written in the transfer-matrix form

$$\begin{pmatrix} A_{n,1} \\ B_{n,1} \\ A_{n,2} \\ B_{n,2} \end{pmatrix} = \hat{T}_n \begin{pmatrix} A_{n-1,1} \\ B_{n-1,1} \\ A_{n-1,2} \\ B_{n-1,2} \end{pmatrix}.$$

With the recursive use of the transfer matrices we obtain

$$\begin{pmatrix} A_{N_b,1} \\ B_{N_b,1} \\ A_{N_b,1} \\ B_{N_b,1} \end{pmatrix} = \prod_{n=1}^{N_b} \hat{T}_{N_b-n+1} \begin{pmatrix} A_{0,1} \\ B_{0,1} \\ A_{0,2} \\ B_{0,2} \end{pmatrix} \equiv \hat{T} \begin{pmatrix} A_{0,1} \\ B_{0,1} \\ A_{0,2} \\ B_{0,2} \end{pmatrix}.$$

In the case of single-bond coupling, the transfer matrix $\hat{T}_{n+1}$ is

$$\hat{T}_{n+1} = \frac{1}{2\mathrm{i}t_0 \sin(k)} \begin{pmatrix} a_1 & 0 & -b_2 \mathrm{e}^{\mathrm{i}\phi_n} & -b_2^* \mathrm{e}^{\mathrm{i}\phi_n} \\ 0 & -a_1^* & b_2 \mathrm{e}^{\mathrm{i}\phi_n} & b_2^* \mathrm{e}^{\mathrm{i}\phi_n} \\ -b_1 \mathrm{e}^{-\mathrm{i}\phi_n} & -b_1^* \mathrm{e}^{-\mathrm{i}\phi_n} & a_2 & 0 \\ b_1 \mathrm{e}^{-\mathrm{i}\phi_n} & b_1^* t \mathrm{e}^{-\mathrm{i}\phi_n} & 0 & -a_2^* \end{pmatrix} \tag{7}$$

where

$$a_l = 2\mathrm{i} \sin(k) \mathrm{e}^{\mathrm{i}k(j_{n,l}-j_{n-1,l})} t_0 \qquad b_l = t \mathrm{e}^{\mathrm{i}k(j_{n,l}-j_{n-1,l})}.$$

For the double-bond coupling the transfer matrix becomes

$$\hat{T}_{n+1} = \frac{1}{2\mathrm{i}t_0 \sin(k)} \begin{pmatrix} a_1 & 0 & -2b_2 \mathrm{e}^{\mathrm{i}\phi_n} & -2c_2 \mathrm{e}^{\mathrm{i}\phi_n} \\ 0 & -a_1^* & 2c_2^* \mathrm{e}^{\mathrm{i}\phi_n} & 2b_2^* \mathrm{e}^{\mathrm{i}\phi_n} \\ -2b_1 \mathrm{e}^{-\mathrm{i}\phi_n} & -2c_1 \mathrm{e}^{-\mathrm{i}\phi_n} & a_2 & 0 \\ 2c_1^* \mathrm{e}^{-\mathrm{i}\phi_n} & 2b_1^* t \mathrm{e}^{-\mathrm{i}\phi_n} & 0 & -a_2^* \end{pmatrix} \tag{8}$$

where

$$c_l = t \mathrm{e}^{-\mathrm{i}k(j_{n,l}-j_{n-1,l}-1)} \cos(k).$$

Since there are two channels in every lead, the transmission of the electrons from the incoming lead to the outgoing lead is characterized by the 2×2 transmission matrix $\hat{M}$ in which every element stands for the probability of transmission of a plane wave from one incoming channel to an outgoing channel. After a straightforward calculation, the transmission matrix can be expressed as

$$\hat{M}_{i,j} = \frac{\hat{T}_{i4}\hat{T}_{i'j'}\hat{T}_{4j} - \hat{T}_{i2}\hat{T}_{i'4}\hat{T}_{4j} - \hat{T}_{i4}\hat{T}_{i'j}\hat{T}_{4j'} + \hat{T}_{ij}\hat{T}_{i'4}\hat{T}_{4j'} + \hat{T}_{ij'}\hat{T}_{i'j}\hat{T}_{44} - \hat{T}_{ij}\hat{T}_{i'j'}\hat{T}_{44}}{(-1)^{i+j+1}(\hat{T}_{22}\hat{T}_{44} - \hat{T}_{24}\hat{T}_{42})} \tag{9}$$

where

$$i' = \begin{cases} 2 & \text{for } i = 1 \\ 3 & \text{for } i = 2 \end{cases} \qquad j' = \begin{cases} 2 & \text{for } j = 1 \\ 3 & \text{for } j = 2. \end{cases}$$

The conductance is proportional to TC which can be expressed as

$$\mathrm{TC} = \mathrm{Tr}\, \hat{M}^\dagger \hat{M}. \tag{10}$$

Since there are two channels in this open system, the maximum value of TC is 2.

3. Calculated results for the single-bond and double-bond cases

The topological disorder of the present systems is due to the random positions of the interchain coupling. Thus, in the absence of the magnetic field the degree of disorder depends on the strength of the interchain hopping t. In the calculations, we generate the random configurations from the probability $P(\lambda_{nl})$. The results are averaged over 100 runs and the variance is shown by error bars in the figures. In figure 2 we plot the dependence of the transmission coefficient on the strength of t. We can see that TC generally decreases with the increase of $|t|$ for both the double- and single-bond cases. This is expected from the fact that the degree of disorder is increased with $|t|$. However, there is an essential difference between the double- and single-bond cases. In the double-bond case, TC is almost unchanged by increasing $|t|$ when $|t|$ is smaller than $0.75t_0$. In the absence of a magnetic field the transmission of electrons is almost complete in this range of t, reflecting the existence of extended states as illustrated in reference [8]. On applying the magnetic field, TC decreases from the value for perfect transmission due to the increase of randomness caused by the random flux threaded through the loops, but the dependence of TC on the strength of t is still weak. This implies that the effect of scattering of electrons by the interchain coupling is almost cancelled by the quantum interference from the double-bond structure as indicated in reference [8], even in the presence of the magnetic field. In the magnetic field the spreading of TC for random configurations under the same distribution is much wider because of the large fluctuations of flux through the loops. In the case of single-bond coupling, TC is rapidly decreased by increasing $|t|$, as expected from the localization of electrons due to the topological disorder. For small $|t|$ one has $(1 - \mathrm{TC})/\mathrm{TC} \propto t^2$. This relation suggests that the strength of the scattering at every crossing point is proportional to t^2. In the presence of a magnetic field this relation is still valid, but the value of TC decreases because of the additional disorder due to the randomness of the flux. In this case the spreading for the random configurations is narrower than that of the double-bond case, reflecting that the role of the scattering by the crossing points is dominant over the role of random flux in the case of the single-bond coupling and relatively small field.

In figure 3 we plot TC as a function of the energy E of the incident electron. It can be seen that the E-dependence is similar to the t-dependence of TC. In the absence of a magnetic field the reflectionless states exist over a wide range of energy for the double-bond case, while the value of TC is much smaller and linearly decreases with E^2 in the case of single-bond coupling. On applying a magnetic field, TC decreases in both cases due to the additional disorder of the random flux. In the double-bond case, TC is almost independent of E but the spreading of TC for random configurations is much wider. In the single-bond case, the linear dependence of TC on E^2 is still valid.

In figure 4 we display the dependence of TC on the strength of the magnetic field. We can see clearly that the transmission coefficient exponentially decreases with the square of the magnetic field in both the double-bond and single-bond cases. The B-dependence of TC is the same for the two cases due to the fact that the magnetic field causes randomness in the flux which is independent of the structure of the interchain bonds. In the single-bond case the value of TC is reduced due to the scattering at the crossing points. In order to investigate the scaling behaviour of the electronic states, in figure 5 we show the dependence of TC on the size of the system. In the case of double-bond coupling, except for slight oscillations as shown in the inset, TC is on average independent of the system size in the absence of a magnetic field, verifying again the existence of the extended states. On applying the magnetic field, the disorder from the random flux of the loops is introduced and TC exhibits strictly exponential decay with the system size, implying the destruction of the extended states by the magnetic field. In the case of single-bond coupling there is no essential difference in scaling behaviour

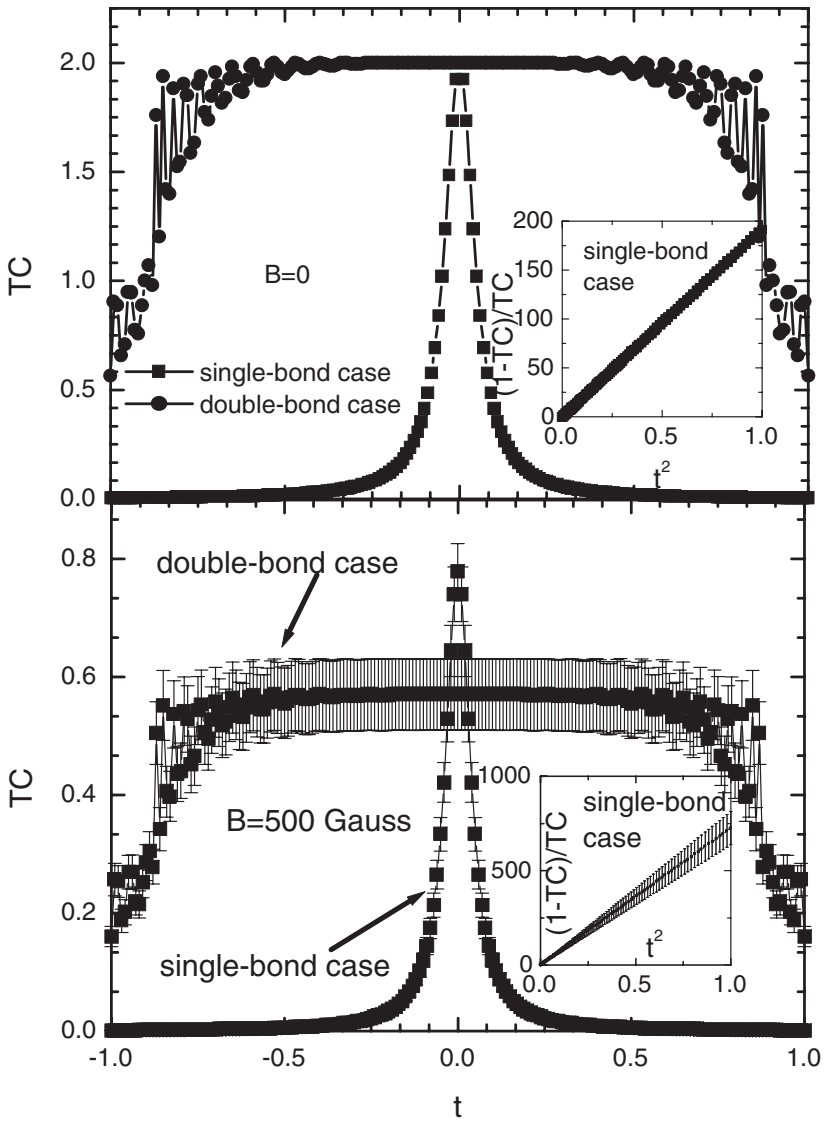

Figure 2. The transmission coefficient (TC) as a function of the interchain hopping potential t in units of t_0 (main panel). $E = 0.2t_0$, $N = 40$, $\lambda_0 = 300$, and $\delta\lambda = 200$. The curves correspond to averages over 100 random configurations and the variances are shown by error bars. The lattice spacing for calculation of the flux is 3 Å. We show the dependence of $(1 - \mathrm{TC})/\mathrm{TC}$ on t^2 in the insets.

between the cases for the presence and absence of the magnetic field, indicating that the states were already localized before the field was applied.

By summarizing the results of figures 2, 3, 4, and 5, we obtain an expression for TC in the case of double-bond coupling:

$$\mathrm{TC} \propto \exp(-\alpha_1 N B^2) \tag{11}$$

where α_1 is a constant and $N \equiv N_b - 1$ is the number of loops. Because in this case the scattering is mainly from the random flux in the loops, this formula reflects the behaviour of

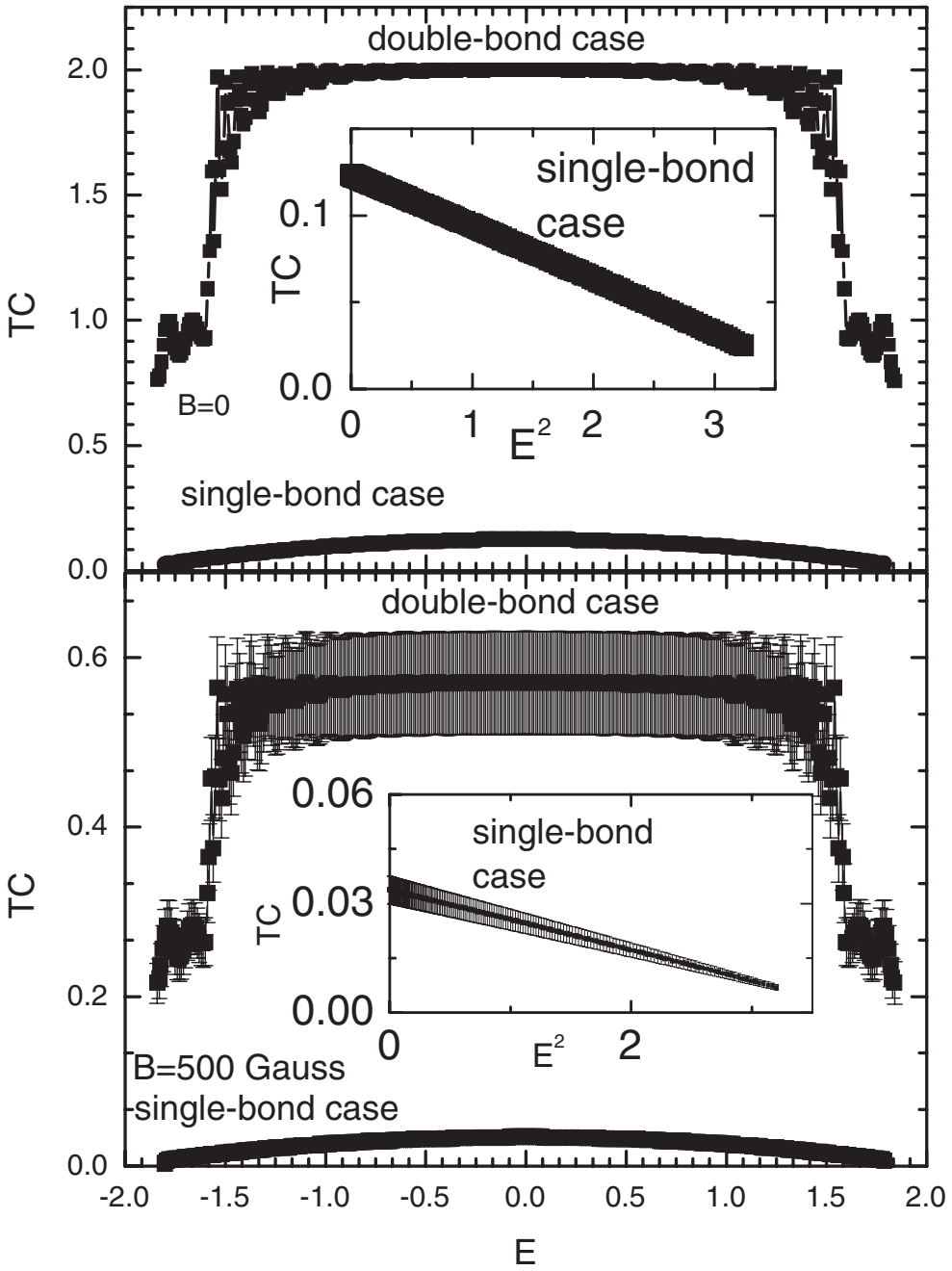

Figure 3. The transmission coefficient (TC) as a function of the energy of the electron E. The unit of E is t_0. $t = 0.2t_0$ and the other parameters are the same as those for figure 2. In the insets we show the dependence of the transmission coefficient on E^2.

states in a quasi-1D system with a series of random fluxes. For this double-chain system in a small magnetic field, the mean free path for the scattering of the random flux can be estimated

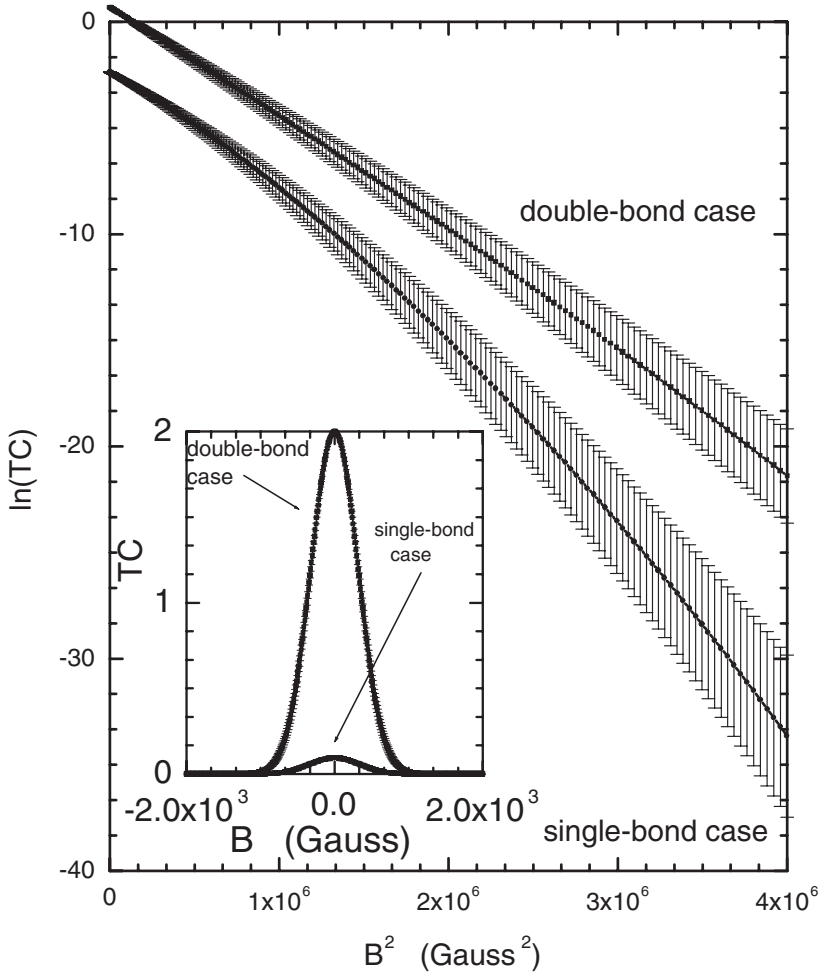

Figure 4. The dependence of the logarithmic transmission coefficient on the square of the intensity of the magnetic field B^2. The inset is a linear plot of the transmission coefficient as a function of B. $E = 0.2t_0$ and the other parameters are the same as for figure 3.

with the aid of the Fermi's golden rule as

$$\frac{1}{\bar{l}} = \frac{\pi N \lambda_0}{2t_0^2 \sin^2(k_F)} \left\langle |\langle k_{1F}|[H - \langle H\rangle]|k_{2F}\rangle|^2 \right\rangle \tag{12}$$

where $|k_{lF}\rangle$ is the state at the Fermi level in the lth pure chain, k_F is the Fermi vector, $\langle \cdots \rangle$ denotes the ensemble average over the random structure, and the mean free path is in units of the lattice spacing. The localization length ξ in quasi-1D systems is the mean free path times the number of channels. From this relation one has

$$\frac{1}{\xi} = \frac{N B^2 t^2 \delta\lambda^4}{288 t_0^2 \lambda_0 \Phi_0^2 \sin^2(k_F)}. \tag{13}$$

By comparison of equation (13) and equation (11), we have

$$\alpha_1 = \frac{t^2 \delta\lambda^4}{144 t_0^2 \lambda_0 \Phi_0^2 \sin^2(k_F)}. \tag{14}$$

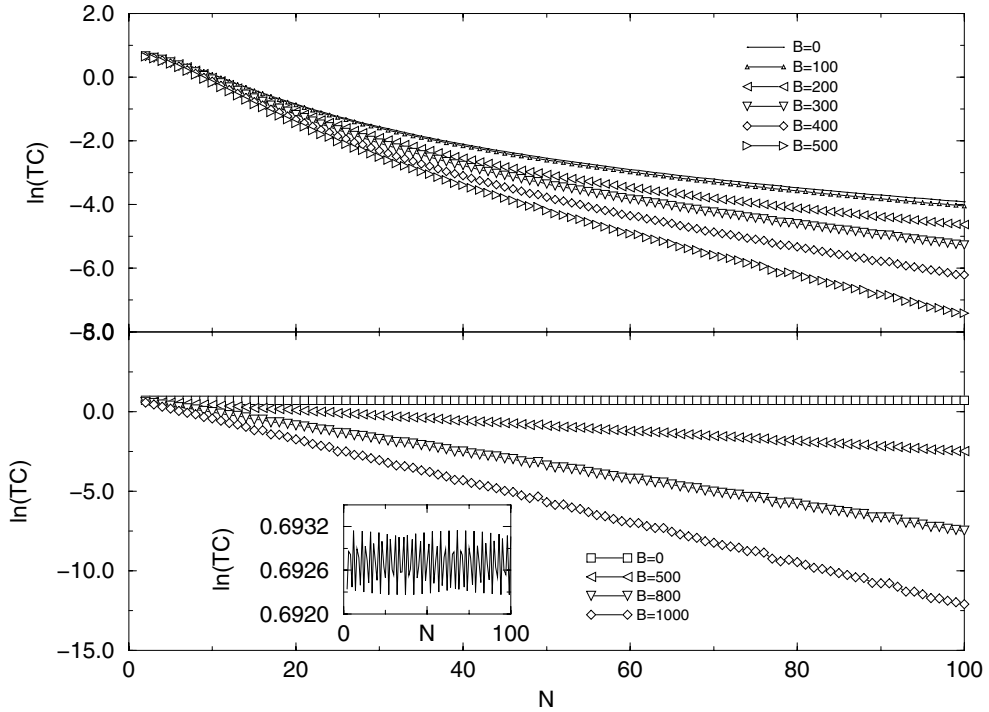

Figure 5. The dependence of the logarithmic transmission coefficient on the number of loops. The upper panel is for the case of single-bond coupling and the lower panel for the case of double-bond coupling. The other parameters are the same as for figure 4. The inset shows the details of oscillations of the transmission coefficient with varying N for the case of double-bond coupling in the absence of a magnetic field.

In the case of single-bond coupling, the transmission coefficient depends on E, t, and B. For small values of E, t, and B, one can estimate TC from equation (12) as

$$\mathrm{TC} \propto \frac{1}{1 + t^2(\alpha_2 B^2 + \beta_2 E^2 + \gamma_2)} \tag{15}$$

with

$$\alpha_2 \sim \frac{N B^2 \delta\lambda^4}{144 t_0^2 \lambda_0 \Phi_0^2} \qquad \beta_2 \sim \frac{\pi N \delta\lambda^2}{80 t_0^4 \lambda_0} \qquad \gamma_2 \sim \frac{\pi N \delta\lambda^2}{120 t_0^2 \lambda_0}.$$

The numerical results are fitted by this formula, as can be seen from the figures.

In the above figures the AB oscillations are not seen because in order to observe AB oscillations the magnetic field has to be as large as 10^4 G in systems with loops containing 400 to 800 sites. To investigate the behaviour of AB oscillations, in figure 6 we show TC as a function of B for systems with loops containing 4000 to 8000 sites. It can be seen that for both single- and double-bond cases the regular AB oscillations can be observed only if the system is periodic in the structure of the loops. In the disordered structure the peaks become random and the height of these peaks oscillates and generally decays as the field increases. The decay rate increases with the system size. There is no difference in behaviour between the single- and double-bond cases, because in a large magnetic field the randomness of the flux is dominant.

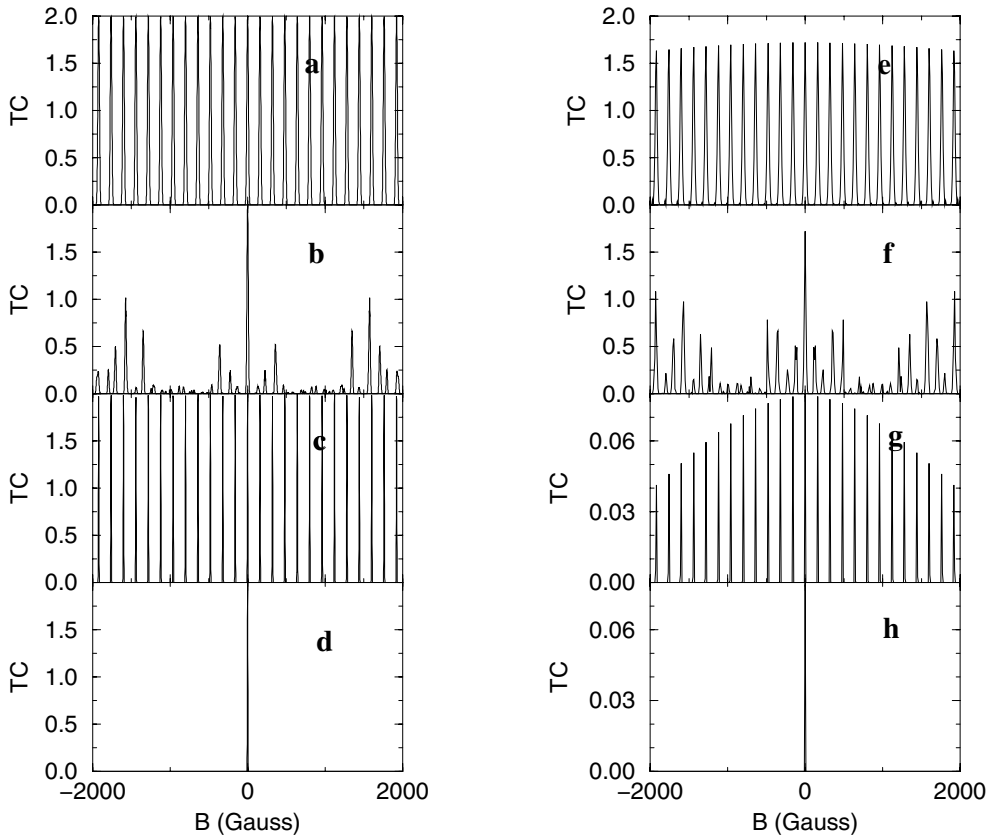

Figure 6. The dependence of the logarithmic transmission coefficient on the intensity of the magnetic field. Graphs (a), (b), (c), and (d) correspond to the case of double-bond coupling; the others correspond to the single-bond case. For graphs (a), (b), (e), and (f) $N = 5$, and for the others $N = 50$. For graphs (a), (c), (e), and (g) the number of sites in every loop is 6000, and for the others the number of sites in every loop is randomly distributed from 4000 to 8000. $E = 0.2t_0$ and $t = 0.2t_0$. The lattice spacing is 3 Å.

4. Conclusions

We investigate the transport properties of electrons in double-chain systems with random topological structure in the presence of a magnetic field. We discuss two types of interchain coupling: the single-bond coupling and double-bond coupling. The electrons are scattered by two disorder factors: (i) the random distribution of the interchain hopping integrals; (ii) the randomness of the flux through the loops. The former is suppressed in the case of double-bond coupling due to the quantum interference; thus the behaviour of TC in these systems purely shows the effect of a quasi-1D sequence of random fluxes. As a result, there exist extended states in the absence of a magnetic field but they are destroyed by applying the field and TC is exponentially reduced by increasing N and B^2. In the case of single-bond coupling, both randomness factors have effects on the states and the states are localized in both the absence and the presence of a magnetic field. We obtain an expression for TC from the numerical calculations. The results may shed light on the study of quasi-1D systems with disordered topological structure and random flux.

Acknowledgments

This work was supported by the National Foundation of Natural Science in China, Grant No 69876020, and by the China State Key Projects of Basic Research (G1999064509).

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