Magnetoconductance through a small nonlinear one-dimensional system

2002 J. Phys.: Condens. Matter 14 12477

(http://iopscience.iop.org/0953-8984/14/47/320)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 12477–12484 PII: S0953-8984(02)38126-8

Magnetoconductance through a small nonlinear one-dimensional system

H Bahlouli and A AlSunaidi

Department of Physics, KFUPM, Dhahran 31261, Kingdom of Saudi Arabia

E-mail: bahlouli@kfupm.edu.sa and asunaidi@kfupm.edu.sa

Received 13 June 2002
Published 15 November 2002
Online at stacks.iop.org/JPhysCM/14/12477

Abstract

We study the effect of Coulomb correlation on the transmission properties of a one-dimensional chain connected to two perfect leads in the presence of a static magnetic field. Due to the presence of a strong on-site nonlinear interaction between two opposite spins within the chain, the zero-voltage conductance exhibits strong correlations between parallel and antiparallel spin conduction channels which results in a substantial spin polarization for small chain sizes.

1. Introduction

Spin-polarized electron tunnelling has become a very active area of research due to its potential in the manufacture of magnetic field sensors and digital storage devices [1]. Usually these applications deal with nanostructure devices and consequently the mutual Coulomb interaction between electrons due to their strong confinement plays an important role. This gives rise to a nonlinear interaction which will certainly affect the transport properties of the system. Nonlinear effects have been the subject of intensive research in condensed matter physics, both from the theoretical and experimental points of view [2]. This is due, in part, to the wide range of potential applications in the design of new optical and electronic devices for computing and communications. For instance, it has been shown that nonlinearity gives rise to multistability and noise, and might originate a chaotic behaviour in certain systems. Transport properties of nonlinear chains of atoms and double-barrier structures under applied electric fields have been recently examined by Cota *et al* [3]. Their work shows that resonances shift in the presence of nonlinearity and that their width decreases as the nonlinearity becomes stronger. Nonlinearity is also relevant to transport problems in nanoscale devices [4]: it is known that the electron–electron interaction is important in any serious study of the transport properties of small systems such as quantum dots and few-impurity models [5]. Generally speaking, the Coulomb interaction gives rise to a nonlinear term in the Schrödinger equation. In this case the Coulomb interaction is modelled by a cubic, nonlocal term in the equation of motion of the corresponding fermionic field operators. To proceed further, a Hartree–Fock

approximation for the nonlinear term is used [6]. One can also use a perturbative approach in the Coulomb interaction [7].

In this work we take the alternative approach of modelling the effect of the electron–electron interaction by a nonlinear local term in the Schrödinger equation. One can look at such an approximation as being a Hartree-like approximation of the original many-body problem. We examine a one-dimensional (1D) problem where the source of the nonlinearity is due to the presence of a strong on-site Coulomb interaction between the two opposite spins at the same site, rather than to a strong electron–phonon coupling. Since the spin degree of freedom plays an important role in the correlated transport through the system, a study of the magnetic field dependence of the linear conductance will exhibit a lift of the degeneracy of the two spin states when a strong magnetic field is applied. That is why we will focus on the zero-voltage conductance and conductance polarization as a function of the external magnetic field.

In this paper we report on the numerical calculation of the two-probe conductance and the transmission coefficient of a finite interacting 1D system connected to two perfect leads. Since in our present study we are not concerned with the charging effect, which is of primary importance for quantum dots, we will not take into consideration the confining potential of the chain. In section 2 we introduce our model and explain the principle of our numerical approach. In section 3 we evaluate the transmission coefficient in the presence of nonlinear interaction and study the effect of magnetic field and interaction with the leads. In section 4 we present the numerical results for the finite-temperature conductance and study the effect of the magnetic field on the conducting properties of the finite chain. Finally in section 5 we present our conclusions with a summary of our basic results.

2. Theoretical model

In this paper we would like to investigate the effect of the magnetic field on the transmissive properties of a nonlinear chain described by an Anderson Hamiltonian. We use the standard Anderson model to describe this system. The model consists of three regions: a finite chain of strongly interacting atoms at sites $1 \leqslant i \leqslant N+1$, and two semi-infinite leads on the left, $-\infty < i \leqslant 0$, and on the right, $N+2 \leqslant i < +\infty$.

We consider the problem of the transmission of an electron incident with energy E upon a strongly interacting region where electron–electron interaction is important. In the interacting region we impose a strong-local-interaction term that mimics the on-site Coulomb interaction $U\rho_{i\sigma}\rho_{i-\sigma}$ which is proportional to both spin-up and spin-down local densities, $\rho_{i\sigma} = |\Psi_{i\sigma}|^2$ where $\Psi_{i\sigma}$ is the probability amplitude for finding an electron at the ith site. U is a parameter measuring the strength of the local Coulomb interaction. This repulsive interaction arises from the charge accumulation and shifts the energy levels of the opposite spin states. Thus we expect our model to adequately describe the nonlinear effects due to charge accumulation:

$$H = \sum_{n,\sigma}\left[\epsilon_{n,\sigma}\Psi^*_{n,\sigma}\Psi_{n,\sigma} + \sum_{m\neq n} V_{n,m}\Psi^*_{n,\sigma}\Psi_{m,\sigma} + \tfrac{1}{2}U|\Psi_{n,\sigma}|^2|\Psi_{n,-\sigma}|^2\right] \tag{1}$$

where $\Psi_{n,\sigma}(t)$ is the complex amplitude and $\epsilon_{n,\sigma} = \epsilon_n - \sigma B$ is the energy at site n ($n = 1, 2, \ldots, N+1$, N being the size of the chain) of an electron with spin σ. U is the strength of the on-site interaction within the chain and $V_{n,m}$ is the overlap integral which depends, in general, only on the distance between the two sites m and n, so $V_{n,m} = V_{m,n}$. Note that $\Psi_{n,\sigma}$ and $\mathrm{i}\Psi^*_{n,\sigma}$ form canonically conjugate variables and $\frac{\mathrm{d}}{\mathrm{d}t}\Psi_{n,\sigma} = -\frac{\partial H}{\partial(\mathrm{i}\Psi^*_{n,\sigma})}$ is the corresponding equation of motion. From the above Hamiltonian we then obtain

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Psi_{n,\sigma} + \sum_m V_{n,m}\Psi_{m,\sigma} + (\epsilon_{n,\sigma} + U|\Psi_{n,-\sigma}|^2)\Psi_{n,\sigma} = 0 \tag{2}$$

where $\Psi_{n,\sigma}(t)$ and $\epsilon_{n,\sigma}$ are the probability amplitude for finding the electron at site n and the corresponding local energy, respectively, at site n for an electron with spin σ. The on-site energy $\epsilon_{n,\sigma} = \epsilon_n - \sigma B$ is defined in terms of the zero-field on-site energy level ϵ_n shifted by the Zeeman energy. 'Spin-up' designates the electron spin direction in which the electron magnetic moment is in the direction of the applied magnetic field and has a lower energy than that of the spin-down electron whose magnetic moment is directed oppositely to the field. The above equation is a variant of the discrete nonlinear Schrödinger (DNLS) equation whose properties have been studied extensively in recent years. The origin of the nonlinearity, in our case, is the local Coulomb interaction which exists only within the small system and shifts the energy levels of opposite spins. However, the local nature of this interaction term makes it inadequate to describe the long-range Coulomb interaction. Thus, our model (2) does not correspond to the well-known Hubbard model, often used as a model Hamiltonian to describe nanostructure devices. Also, equation (2) does not even correspond to the classical Hartree approximation of the Hubbard model. In the Hartree approximation, the nonlinear term is described not by a single orbit as described in equation (2), but rather by the sum of all orbits below the Fermi level. Nevertheless, the DNLS equation (2) does contain some essential features of the interacting system, such as the repulsive and nonlinear nature of the interaction.

Let us find the stationary states of (2), i.e. we look for solutions of the type $\Psi_{n,\sigma}(t) = \mathrm{e}^{\mathrm{i}Et}\Psi_{n,\sigma}(E)$ where E is the associated eigenvalue. We restrict ourselves to a nearest-neighbour tight-binding approximation. Let $V_{n,n+1}$ be the hopping integral between the nth and the $(n+1)$th site; under these assumptions our previous equation becomes

$$(E - \epsilon_{n,\sigma})\Psi_{n,\sigma} = V_{n,n-1}\Psi_{n-1,\sigma} + V_{n,n+1}\Psi_{n+1,\sigma} + U|\Psi_{n,-\sigma}|^2\Psi_{n,\sigma}. \tag{3}$$

We now choose the hopping integrals as follows:

$$V_{n,n+1} = \begin{cases} V_L & \text{for } n < 0 \text{ or } n \geqslant N+2 \\ V_0 & \text{for } n = 0 \text{ and } N+1 \\ V_S & \text{for } 1 \leqslant n \leqslant N. \end{cases} \tag{4}$$

That is, the hoppings within the lead and the interacting system are V_L and V_S, respectively, while the links of the interacting system with the left and right leads are V_0. From now on we use a parameter defined as $y = V_0/V_L$ that expresses the degree of hybridization of the small-chain states with the extended states at the leads.

3. Transmission features

We consider first the problem of transmission of an electron incident on the quantum wire in the presence of a nonlinear interaction and magnetic field. To study the scattering properties of our system, we send a plane wave from the right and study its transmission. Thus, we assume a solution of the form

$$\Psi_{n,\sigma} = \begin{cases} (I_\sigma \mathrm{e}^{-\mathrm{i}kn} + R_\sigma \mathrm{e}^{\mathrm{i}kn})\chi_\sigma & \text{for } n \geqslant N+1 \\ T_\sigma \mathrm{e}^{-\mathrm{i}kn}\chi_\sigma & \text{for } n \leqslant 0. \end{cases} \tag{5}$$

Here, χ_σ describes the electronic spin state which is assumed to be conserved throughout the transmission process since we are ignoring spin-flip processes. The quantities I_σ, R_σ, and T_σ represent the amplitudes of the incident, reflected, and transmitted waves, respectively.

From the computational point of view, equation (3) is very useful. It relates the values of the wavefunction at three successive discrete locations along the x-axis. It is often referred to as the Poincaré map in the literature [8, 9]. For 1D systems the discretization of the Schrödinger equation can be performed exactly [9]. It has been proven numerically that the output uniquely

defines the input but the inverse is not true [10]. That is why in our numerical computations we will fix the output amplitude to unity and iterate to find the input amplitude of the incident wave. The solution of equation (3) is done iteratively by taking our initial conditions $\Psi_0 = 1$ and $\Psi_{-1} = \exp(\mathrm{i}k)$; the lattice spacing is set to unity throughout this article. We consider here an electron having a wavevector k incident at site $N+2$ from the right (by taking the length of chain $L = N$, i.e. $N+1$ sites); the transmission coefficient can then be expressed as [8, 11]

$$\tau_\sigma = \left|\frac{T_\sigma}{I_\sigma}\right|^2 = \frac{4\sin^2 k}{|\Psi_{N+2,\sigma} - \Psi_{N+3,\sigma}\exp(-\mathrm{i}k)|^2}. \tag{6}$$

Thus the transmission coefficient depends only on the values of the wavefunction at the end sites, $\Psi_{N+2,\sigma}$ and $\Psi_{N+3,\sigma}$, which are evaluated from the iterative equation (3). In the region outside the chain, the leads are described by a noninteracting tight-binding Hamiltonian for which the dispersion relation reads

$$E = 2V_L \cos k \tag{7}$$

which relates the incident electronic energy, E, to the propagation wavenumber k. For convenience, we measure all energies in units of V_L, i.e. we set $V_L = 1$ in all of our numerical computations. Similarly, we set $V_S = 1$, so we concentrate on the interaction and magnetic field effect on the transmission properties of our system.

The numerical computations for the transmission through a single impurity ($N = 0$ in our notation, since N represents the length of the chain rather than the number of atoms) are shown in figure 1. In figure 1(a) we show how the transmission changes as we vary the strength of the binding to the leads (expressed by $y = V_0/V_L$) for $U = 0$ and $B = 0$. As expected, the transmission is low and sharply peaked at the resonant energy $E = 0$ for small values of y and then widens and increases in magnitude as y increases. In figure 1(b) we show the transmission for $B = 0$, $y = 1$ and different values of the nonlinear interaction strength, U. We see that the transmission gets more and more suppressed as U increases. Figure 1(c) shows the transmission versus the applied magnetic field for different values of y, $U = 0$, and $E = 0$. The transmission has a Gaussian-like shape while its peak decreases abruptly with decreasing values of y. Figure 1(d) shows the transmission versus B for the interacting case with $U = 1$ and one sees clearly that the presence of the nonlinear interaction lifts the degeneracy of the energy level. We see from this figure that the up-spin contribution has been increased while the down-spin contribution is being suppressed in the presence of the nonlinear interaction. In the case $y = 0.5$ we see that the down-spin contribution is completely suppressed (see figure 1(d)).

4. Coulomb interaction effect on the conductance

In order to obtain a realistic picture of our model, it is necessary to include in our study finite-temperature effects. The two-probe conductance (in units of $e^2/\hbar$) at finite temperature is defined by the thermal average of the transmission coefficient [12]:

$$G(T, \mu) = \sum_\sigma \int \mathrm{d}E \left(-\frac{\partial f(\mu, E)}{\partial E}\right)\tau_\sigma(E). \tag{8}$$

Here $f(\mu, E)$ is the Fermi–Dirac distribution function given by

$$f(\mu, E) = (\mathrm{e}^{(E-\mu)/k_BT} + 1)^{-1}, \tag{9}$$

where k_B is the Boltzmann constant and μ the chemical potential of the sample. The integration is extended over the allowed energy band, but at low temperatures the derivative of the Fermi–Dirac function is a strongly peaked function of E, which vanishes everywhere except for

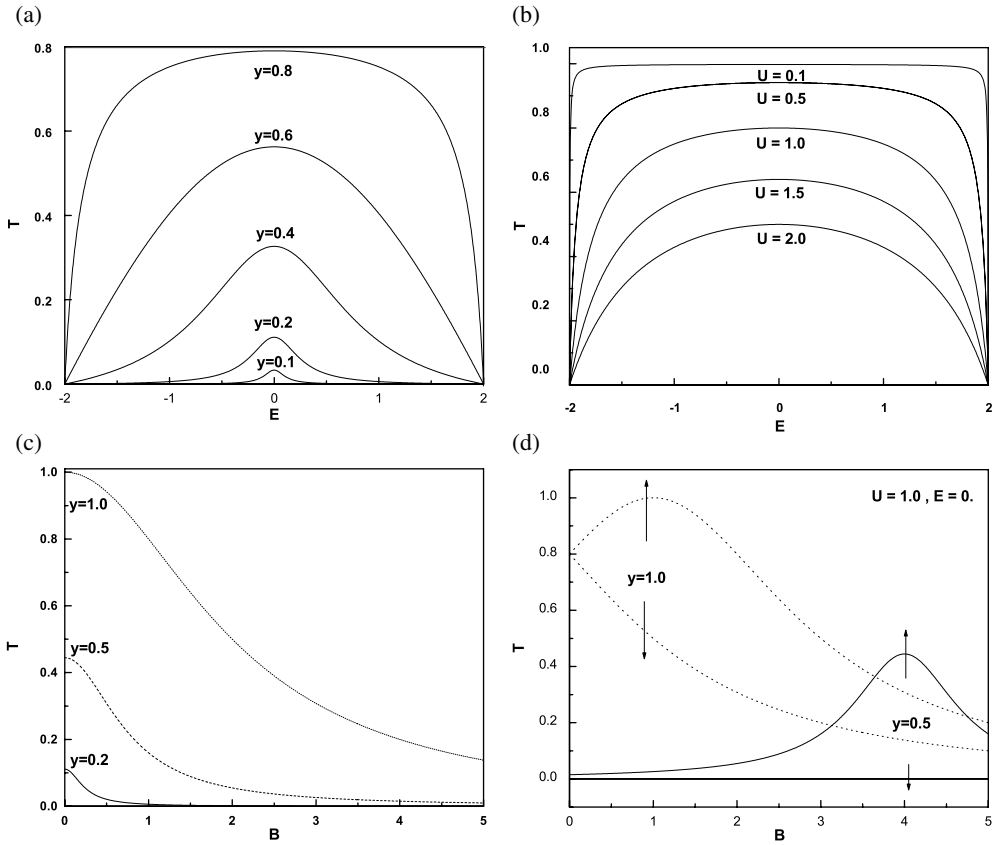

Figure 1. (a) Transmission coefficient across a single impurity as a function of the incoming plane-wave energy, for $B = 0$, $U = 0$, and different values of the system–leads interaction y. (b) Transmission coefficient across a single impurity as a function of the incoming plane-wave energy, for $B = 0$, $y = 1$, and different values of the nonlinear interaction U. (c) Transmission coefficient across a single impurity as a function of the applied magnetic field B, for $E = 0$, $U = 0$, and different values of the system–leads interaction, y. (d) Transmission coefficient for each spin across a single impurity as a function of the applied magnetic field B, for $E = 0$, $U = 1$, and different values of the system–leads interaction y.

energies close to the chemical potential, μ; the integral will be essentially zero outside an interval of width $k_B T$. At low temperatures the general form of the $G(T, \mu)$ curve depends strongly on the value adopted for the chemical potential. Thus, in general, the conductance will be enhanced if the chemical potential is close to a set of transmission peaks (resonances) and reduced when the chemical potential is away from resonant transmission peaks. Thus the conductance as a function of temperature will exhibit several characteristic structures depending on the location of the chemical potential. In our case, since we are just interested in the field dependence of the conductance and the effect of the nonlinear interaction, we will fix our chemical potential to zero in all computations. We should also keep in mind that our energies are counted in units of V_L, which in general is of the order of few meV. Thus while computing the conductance in equation (8), it should be borne in mind that temperatures of the order of $T \simeq 10^{-1}$–10^{-2} are reasonably low temperatures, while $T \simeq 1$ corresponds to high temperatures.

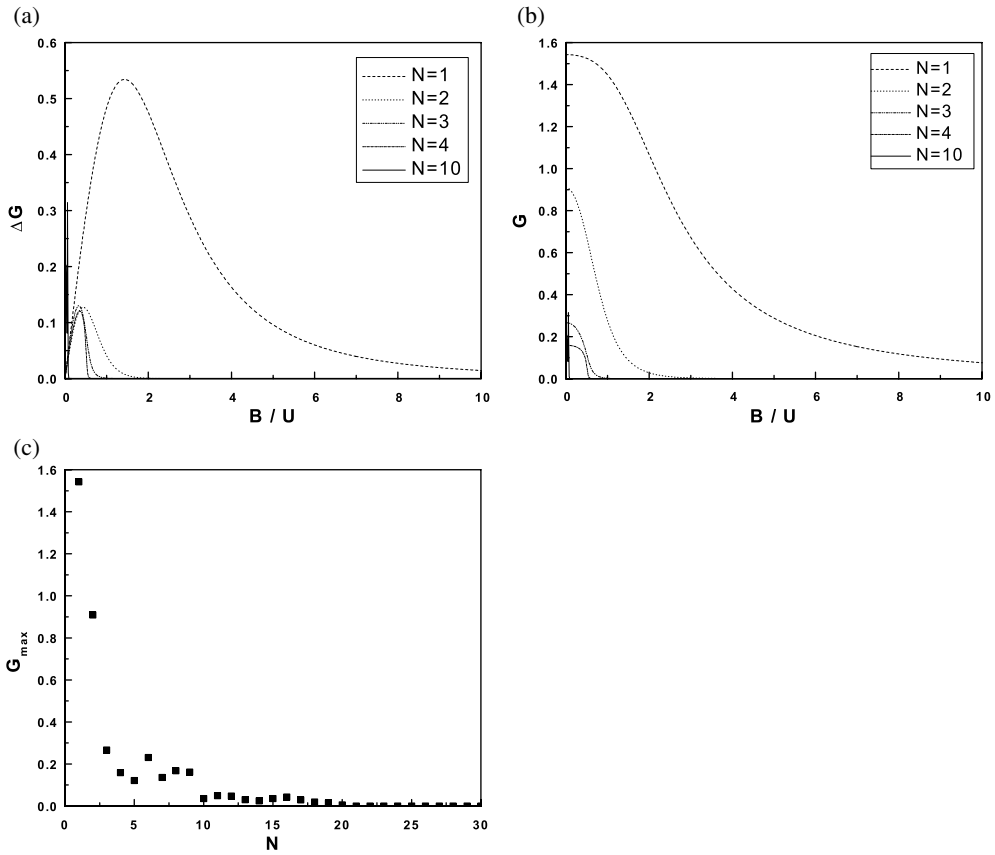

Figure 2. (a) Conductance polarization (in units of $e^2/\hbar$) as a function of the applied magnetic field B for different chain sizes (N is the number of atoms in the chain). The interaction energy is $U = 1$, the temperature is $T = 0.1$, and $y = 1$. (b) Conductance (in units of $e^2/\hbar$) as a function of the applied magnetic field B for different chain sizes (N is the number of atoms in the chain). The interaction energy is $U = 1$, the temperature is $T = 0.1$, and $y = 1$. (c) The maximum value of the conductance (in units of $e^2/\hbar$) as a function of the number of atoms in the chain. The interaction energy is $U = 1$, $B = 0$, the temperature is $T = 0.1$, and $y = 1$.

We have calculated the conductance numerically using the transmission coefficient obtained in the previous section. The total conductance is calculated as the sum of the conductances for up- and down-spin electrons while the conductance spin polarization (also called magnetoconductance) is defined as $\Delta G = G_\uparrow - G_\downarrow$. Figures 2(a), (b) show the magnetoconductance ΔG and conductance $G(B)$, respectively, as a function of B/U, for a relatively large, fixed value of U (i.e. $U/V_L = 1$). The maximum contribution to the conductance at zero field is mainly due to the fact that both spins contribute equally. At larger field the spin-down contribution starts being suppressed by the on-site Coulomb interaction and hence the conductance decreases. At very large magnetic fields $B \gg U$, both spin channels will be suppressed and so is the total conductance ($G = G_\uparrow + G_\downarrow$) as shown in figure 2(b). Thus the magnetic field dependence of the magnetoconductance exhibits a clear transition from correlated to uncorrelated transport. The up-spin channel contributes the most to the conductance at relatively low fields. We see that the polarization conductance (figure 2(a)) is peaked at values of the magnetic field which become smaller as the system size increases. In

standard Hubbard model one expects a peak in the conductance at $B = U$, but in our case the Coulomb interaction is weighted by the probability amplitude $|\Psi_{i\sigma}|^2$ and, due to the continuous nature of this amplitude, the Coulomb effect will be averaged out. In figure 2(c) we show how the maximum value of the conductance changes with the length of the chain (for each value of N we evaluate the conductance for different values of B and choose the maximum value, called G_{max}). It is clear from this figure that the conductance decays very rapidly with length, so the magnetoconductance effect that we are interested in will not be observable for $N \geqslant 10$ (in figures 2(a), (b) the $N = 10$ contribution is almost unobservable; it is basically a very small spike at very low field) and its magnitude decreases rapidly with length. This behaviour of the conductance for long chains is expected, because the effect of the on-site Coulomb interaction is basically to push the resonances of the transmission by an amount, roughly speaking, of the order of U. Thus if the Coulomb interaction is of the order of the width of the energy band, then almost all resonant energies have been boosted outside the allowed energy region and consequently no transmission and hence no conduction occurs.

5. Conclusions

We have studied in this article a simple alternative model for the properties of transmission through a small interacting system connected to perfect leads and subject to a static magnetic field, based on an extension of the DNLS equation. The results show that the transmission for an electron with spin parallel to the external field is always greater than the transmission for the antiparallel spin. The conductance $G(B)$ shows a single maximum as a function of the external field, which occurs at zero field; then it decreases quickly at large fields due to the presence of the Coulomb interaction. A substantial tunnelling magnetoresistance has been evaluated whose magnitude decreases with the size of the system. This effect has potential applications in the manufacture of magnetic field sensors and digital storage devices. However, it is clear that the magnitude of this effect depends strongly on two parameters, the strength of the on-site Coulomb interaction U and the length of the chain N. The imbalance between up- and down-spin contributions is enhanced for larger values of U. On the other hand, the conduction is suppressed for longer chains due to the cumulative Coulomb effect along the chain. The term $U|\Psi_{n,-\sigma}|^2$ in the Schrödinger equation creates an effective potential repulsive to the incident electron, an effect which builds up very rapidly along the chain and hence suppresses conduction for long chains. Our elementary model does not take into account the generally important complications such as spin-flip processes, interface effect, and bias dependence. However, it does provide a basis for the understanding of the effect of electron–electron correlations on the magnetic transport properties of small systems.

Acknowledgment

We would like to acknowledge the support of King Fahd University of Petroleum and Minerals during the progress of this work.

References

[1] Prinz G A 1998 *Science* **282** 1660
[2] Abdullaev F, Bishop A R and Pnevmatikov S (ed) 1992 *Disorder with Nonlinearity* (Berlin: Springer)
[3] Cota E, Jose J V, Maytorena J and Monsivais G 1995 *Phys. Rev. Lett.* **74** 3302
[4] Averin D V and Likharev K K 1991 *Mesoscopic Phenomena in Solids* ed B L Altshuler *et al* (Amsterdam: Elsevier)

[5] Johnson N F 1995 *J. Phys.: Condens. Matter* **7** 965
[6] Apenko S M, Blanter Ya M and Losovik Yu E 1993 *Phys. Lett.* A **176** 137
[7] Oguri A 1999 *Phys. Rev.* B **59** 12240
Oguri A 1997 *Phys. Rev.* B **56** 13422
Oguri A 2000 *Physica* B **284–288** 1932
[8] Cota E and Ulloa S E 1995 *Phys. Rev.* B **51** 10875
[9] Sanchez A, Macia E and Dominguez-Adame F 1994 *Phys. Rev.* B **49** 147
[10] Delyon F, Levy Y E and Souillard B 1986 *Phys. Rev. Lett.* **57** 2010
[11] Economou E N and Soukoulis C M 1981 *Phys. Rev. Lett.* **46** 618
[12] Azbel M Ya, Harstein A and DiVincenzo D P 1984 *Phys. Rev. Lett.* **52** 1641