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Conductance quantization in ferromagnetic nanowires

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Abstract. Theoretical studies of the conductance of ferromagnetic and paramagnetic nanowires are performed within the framework of a three-dimensional s–d model. The attention is focused on spin-dependent conductance quantization, which manifests itself in a spectacular way when a circuit becomes open and the conduction goes down in discrete steps. A new approach is developed by assuming that in the last stages of the breaking of the nanocontact, there are fewer and fewer conduction paths, distributed at random and stretching across the contact region. Conductances are calculated within the quasiballistic regime, using the Kubo formula and a recursion Green's function technique. The results for weak ferromagnets (both majority and minority d bands intersect the Fermi surface) are qualitatively different from those for strong ferromagnets (only the minority d bands do), which may explain why experimental cumulative histograms of the conductance reveal more pronounced peaks in the case of Fe than for Ni, and consequently the latter are more sensitive to surface contaminations (oxidization).

1. Introduction

Conductance quantization (CQ) in ballistic point contacts was first reported in references [1,2], in the two-dimensional gas of a GaAs–AlGaAs heterostructure. The width of the point contacts in those experiments was controlled by applying a (negative) gate voltage. When the absolute value of the gate voltage is large enough, the width of the constriction (in the direction perpendicular to the current) makes the transverse modes quantize and the corresponding subbands become well separated from each other [3]. In contrast to the heterostructures, metallic point contacts are far more difficult to control and, due to high carrier concentration, extremely small constrictions (of the order of a few Å) are required to separate the subbands to the extent that makes conduction discrete steps detectable. Nevertheless, metallic point contacts may be surprisingly easily fabricated and precisely measured, e.g. by recording a conductance decay during the breaking of a circuit either by opening an electromagnetic relay or by just bringing two wires into and out of contact [4–8] (not to mention some other experimental techniques). Quantized conductance has been reported in metals (Au, Al, Pb, Na), liquid metals (Hg and Sb), amorphous metal (Co–Fe–Si–B), semi-metal (Bi) and ceramics (La–Sr–MnO_3) (see reference [7] and references therein).

Up to now, the consensus view that has emerged is that the conductance quantization, in steps of $G_0 = 2e^2/h$, is due to the ballistic transport through a nanocontact region between the paramagnetic lead wires. In the case of ferromagnetic leads the situation is more complicated and still under debate. Although it is known that single experiments on Ni

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do show conductance quantization, there is still controversy about the structure of conductance *cumulative* histograms, which have been reported to be almost featureless in references [7, 8]. This is in contrast to the case for Fe whose cumulative histograms have pronounced peaks, according to reference [7], where it has been shown that experiments performed under ambient conditions on Ni (merely mentioned) and on Fe (thoroughly discussed) lead to qualitatively different cumulative histograms of conductance.

The obvious difference between these two transition metals, which I would like to focus on, is that bulk Ni is a strong ferromagnet with its majority-spin d-electron band nearly fully filled, whereas Fe—as a weak ferromagnet—has both of the d bands open at the Fermi surface.

The aim of the present paper is to show, on the one hand, that in the case of paramagnetic metals the CQ phenomenon may be expected to be almost independent of the model parameters, like electron concentration (Fermi energy). On the other hand, I want to stress that when a system is ferromagnetic—spin degeneracy gets lifted and energy levels are less separated from one another—the conductance is more sensitive to details of the density of states. In particular, whether a ferromagnet is strong or weak is quite crucial.

2. The model and the method of computation

The widespread view of how a contact-breaking process proceeds in metals is that a junction in the form of a more and more narrow and long neck is formed, and eventually breaks (the 'chewing gum effect'). As has been recently shown, however, in the case of ceramics another scenario develops, which seems to be due to brittle fracture [7] rather than the neck formation (plastic deformation).

In this paper I propose yet another approach in an attempt to explain differences in CQ behaviour among strong and weak ferromagnets, and paramagnetic materials. On the basis of experimental facts, the following requirements have been imposed, while constructing the model nanocontact (contact-breaking region): (i) in the paramagnetic case the discrete steps G_0 in cumulative histograms should be nearly independent of the Fermi energy; and (ii) in the ferromagnetic case the spin-dependent effects due to the spin-polarized d bands should be visible. So, below I propose another way of viewing of the contact-breaking mechanism in metals, stressing the role of the asperity or roughness of the contact surfaces. It is assumed in this approach that shortly before the contact is completely broken there are only a few conduction strands or paths left, which eventually disappear. In other words, the nanocontact, in the form of a collection of strands connecting the paramagnetic or ferromagnetic electrodes, is a quasiballistic conductor responsible for the conductance quantization. Within the ballistic regime the current is carried by transverse modes and the length of the conductor does not critically influence its resistance since the voltage drops only at its ends.

I have carried out numerical studies of conductances of metallic contacts within the framework of a 'semi-realistic' s–d model with intra-atomic hybridization. The model has proved to work quite well in dealing with magnetoconductance problems in Cu/Co multilayers [9]. In the present study, however, real-space representation is used and homogeneous metals are considered, i.e. the nanocontact (regarded as a quasiballistic conductor) is sandwiched between semi-infinite ideal lead wires (LW) made of the same metal as the nanocontact itself. Of course, in contrast to the LW, the nanocontact is not ideal, but is deformed in order to mimic the contact-breaking process. The conduction paths are distributed at random over the cross-sectional area, and stretch across the junction (the transition or disordered region). The number of conduction paths is supposed to correspond to the breaking process duration (time). Only the last stages of the contact breaking matter, so the numerical simulation may be restricted

from several down to 1 and 0 (open contact) paths. It is obvious by construction that it is not a cross-sectional area which is crucial but rather a surface density of conduction channels. The results I present are based on simulations of junctions, 7×7 in area (in lattice constant units), repeated 2000 times for each number of paths. The mutual positions of individual paths are completely random and they may be, but do not have to be, close to one another.

Technically, the conduction paths have been generated by putting additional huge on-site potentials everywhere within the junction except on the paths. The lengths of the nanocontacts generated (equal to the path length) have been changed from 1 to 10 atomic spacings, and all the lengths have been assumed to occur with the same probability. The physical mechanism behind this model is that electrodes in contact have rough surfaces and touch each other by means of randomly distributed 'bridges' (strands); moreover the bridges—as ballistic conductors—have hardly length-dependent resistances (for nanoscale distances).

It is noteworthy within this context that the term *conduction path* does not have exactly the same meaning as what is usually meant by *conduction channel*; the difference is that a single conduction path contains in general a few conduction channels due to both spin and orbital degeneracy. The degeneracies may be however lifted when a system is ferromagnetic and/or when the symmetry is lowered by disorder.

In linear response theory, the dc conductance of the junction can be expressed in terms of the full Green's functions (GF) of the problem. These Green's functions, in turn, are given by means of appropriate recursion relations [9,10] (refer to reference [9] for more details, including ones related to the parameters: $t_s = -1$, $t_d = -0.2$ and $V_{sd} = 1$, i.e. the hopping integrals and hybridization). The on-site potentials are now being set as follows: $\epsilon^s_{\uparrow,\downarrow} = 0$, $\epsilon^d_{\uparrow} = -1$ and $\epsilon^d_{\downarrow} = -1$ (-0.2) for the paramagnetic (ferromagnetic) case. With these parameters and the hopping integrals given above, it is easily seen from the spin-dependent densities of states that for $E_F = -0.5$ both the $\uparrow$ and $\downarrow$ d bands are partially filled (weak ferromagnet), whereas for $E_F = 0$ the majority ($\uparrow$) d band is full (strong ferromagnet).

In order to have identical lead wires as the nanocontact (in the absence of disorder), it is necessary to include hybridization in the LW, too. This has been accomplished by solving the recursive equations within the lead wires by iteration, starting with the analytic expression with no hybridization and then switching the hybridization on [11].

Finally, the conductance Γ_σ, i.e. the contribution of electrons with spin σ to the dc conductance, reads

$$\Gamma_\sigma = \frac{4e^2}{h} \mathrm{Tr}\{\tilde{G}_\sigma(i-1,i-1)\hat{T}\tilde{G}_\sigma(i,i)\hat{T} - \hat{T}\tilde{G}_\sigma(i,i-1)\hat{T}\tilde{G}_\sigma(i,i-1)\} \tag{1}$$

where $\hat{T}$ is a diagonal hopping matrix, $\tilde{G}$ denotes the imaginary part of G and $\mathrm{Tr}\{\cdots\}$ denotes the *trace* of the matrices of rank $2L_x \times 2L_y$ (L_x, L_y stand for the dimensions in the direction normal to the current).

3. Results

The main results of the present paper are presented in figures 1 and 2. The figures show cumulative histograms of conductances. All the histograms are numerically accurate and have normalized areas; moreover all the computed points are included in the figures (not just the averages). The only adjustable parameter is a histogram step $\Delta\Gamma$ which has to be chosen so as to be in accord with the number of random configurations. In the present studies $\Delta\Gamma = 0.1$ and there were 2000 statistical samplings for each number of conduction paths, which guarantees reproducibility of the results at least for the positions of the main peaks and their relative heights. It is readily seen from figure 1 that in the paramagnetic case the histograms are roughly

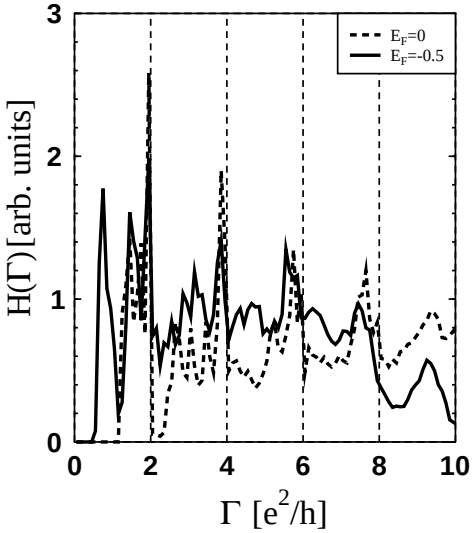

Figure 1. Cumulative histograms of the conductance in the paramagnetic case; each histogram has well defined peaks. The positions of the main peaks can be fairly accurately brought to 2, 4, 6 and 8 e^2/h if serial resistances of 230 and 292 Ω are included for $E_F = 0$ and -0.5, respectively.

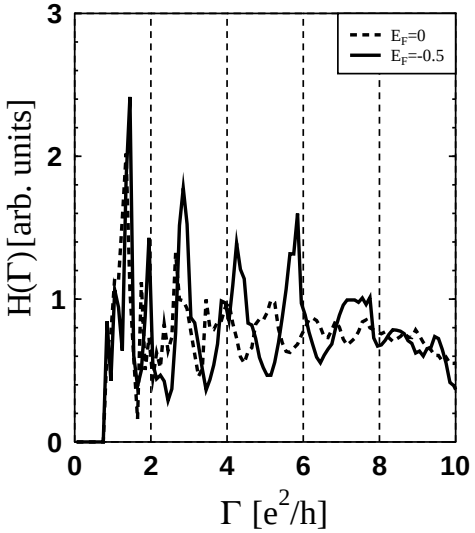

Figure 2. As figure 1, but for the ferromagnetic case. The solid curve, which corresponds to a weak ferromagnet (open d bands at E_F), has pronounced peaks. The dashed curve (a strong ferromagnet with the majority d band almost completely closed) has smaller peaks.

independent of the Fermi energy, at least as far as the existence of well defined peaks (not far away from 2, 4, 6, 8 e^2/h) is concerned. Incidentally, the positions of the peaks can be brought very close to the above-mentioned integer values if, in accordance with the usual practice [1,12], additional serial resistances (R) are taken into account. The origin of these residual resistances is a backscattering process [12]. In order to include it, it is sufficient to modify the computed conductances (Γ), as follows: $\Gamma_{\rm real}^{-1} = \Gamma^{-1} - R$. The corrections R are equal to 230 and 292 Ω for $E_F = 0$ and $E_F = -0.5$, respectively, with an uncertainty of less than ±3% for new peak positions around 2, 4, 6 and 8. In figure 2 the ferromagnetic case is displayed. This time, the histograms corresponding to a strong ferromagnet ($E_F = 0$) show small, densely distributed peaks, whereas for a weak ferromagnet ($E_F = -0.5$) the peaks are clearly more pronounced. The poorer structure of the cumulative histogram of the strong ferromagnet suggests that in the presence of surface contaminations it may be even more suppressed and possibly smoothed down to a featureless form. In contrast, the weak-ferromagnet histogram with more pronounced structure will survive the influence of some moderate disorder. In view of this, the present observations may be associated with the behaviour of strong (Ni) and weak (Fe) ferromagnets reported in the literature [7] if one assumes that the imperfections responsible for the smearing out of the structure of the cumulative histograms are due to the oxide contaminations (the experiment in question was made in an air atmosphere). More recently [13], Ni point contacts have been studied in vacuum (10^{-8}–10^{-7} Torr) and spin-dependent conductance quantization has been found at room temperature (ferromagnetic phase) and at 770 K (paramagnetic phase). Since the present theory works actually at 0 K and uses a simplified band structure, it is pointless to expect more than just qualitative agreement with the experiment. Bearing this in mind, what deserves mentioning is that the present results confirm such findings as clear spin dependence of the histograms (paramagnetic versus ferromagnetic cases) and the existence of peaks around odd multiples of the conductance quantum e^2/h (figure 2).

The present model of the nanocontact is a static one. So the time evolution of the conductance may be imitated by carrying out decompositions of the cumulative histograms into their components enumerated by the number of conduction paths (N). It is obvious that the more open a nanocontact is, the fewer the paths remaining are. Figure 3 illustrates the evolution of the first eight paths corresponding to the model strong ferromagnet. The lengths (L_z) of the nanocontacts have been assumed statistically independent and uncorrelated with the number of conduction paths. The computations presented in this paper correspond to L_z ranging from 1 to 10. This way of modelling the nanocontact is physical, since: (i) the ballistic conductance hardly depends on L_z (for a given N); and (ii) in the experimental situation of two wires brought into and out of contact, neither the forces acting nor the roughness of the colliding surfaces—i.e. the main factors which determine both L_z and N—are controllable.

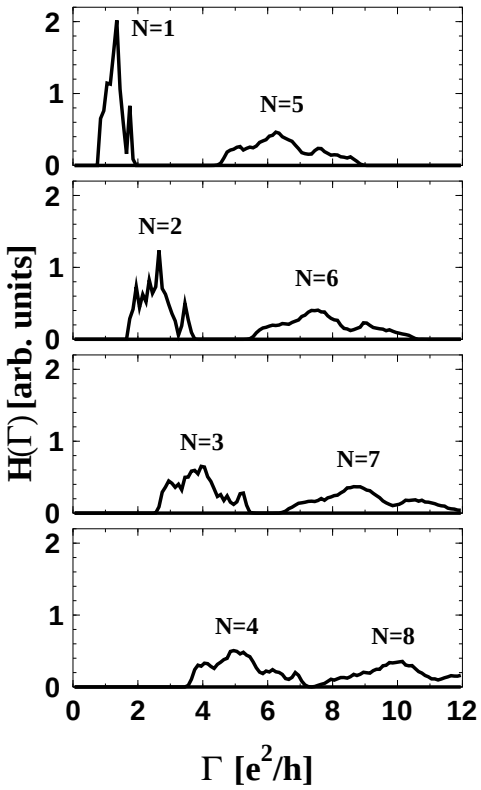

Figure 3. Decomposition of the cumulative conductance corresponding to the dashed curve of figure 2 into parts coming from the first N conduction paths. For compactness, two different partial distributions are placed in each panel.

When comparing figures 1 and 2 it can be seen that the corresponding solid lines differ from each other less than the dashed ones. For 'compact' systems with well defined subbands, this could be due to the fact that in the weak-ferromagnet case as well as in the paramagnetic case, there are both ↑-spin d electrons and ↓-spin d electrons at the Fermi surface, in contrast to the strong-ferromagnet case for which majority-spin electrons are practically absent at E_F. Presumably, reasoning along these lines may still work even when a system disintegrates into a bunch of atomic chains forming a nanocontact—explaining thereby why the fact that a parent bulk metal is a strong or weak ferromagnet is relevant.

At first glance, the present method might seem to be similar to that exploited in reference [12]. Although both the approaches use tight-binding Hamiltonians, they differ very much in the following respects: (i) the present model is a three-dimensional two-band model with s–d hybridization, whereas that in reference [12] is an s-band two-dimensional one; and (ii) in this method the nanocontact is constructed in the form of a collection of conduction paths stretching across the otherwise insulating medium (due to huge on-site potentials in the disordered region). In reference [12], in turn, the disordered two-dimensional zone is generated by letting the on-site energy take random values between $\pm$*half the bandwidth*. Another important point is that (iii) the nanowire-breaking process in the present model is put into effect, in a natural way, as soon as the last conduction paths have been gradually broken (the Fermi energy is always kept constant), whereas the authors of reference [12] proceed the other way round and control the number of conduction channels by lowering the Fermi energy and keeping the nanocontact geometry unchanged.

In conclusion, a new model of a nanocontact has been proposed to describe the conductance of colliding ferromagnetic electrodes. It has been shown that conductance quantization is spin dependent, which manifests itself in differences between the cumulative conductance histograms corresponding to paramagnetic and ferromagnetic nanocontacts. The results show that in the paramagnetic phase the main peaks are centred about even multiples of the conductance quantum (e^2/h), whereas in the ferromagnetic case odd multiples occur too. Moreover, for a given ferromagnet its cumulative conductance histograms depend on whether it is weak or strong. A strong ferromagnet has less peaked structure, which can be more easily affected by surface contaminations and degraded, unless the nanocontacts are protected against oxidization. These findings agree qualitatively with recent experiments.

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References

[1] van Wees B J, van Houten H, Beenakker C W J, Williamson J G, Kouvenhoven L P, van der Marel D and Foxon C T 1988 *Phys. Rev. Lett.* **60** 848
[2] Wharam D A, Thornton T J, Newbury R, Pepper M, Ahmed H, Frost J E F, Hasko D G, Peacock D C, Ritchie D A and Jones G A C 1988 *J. Phys. C: Solid State Phys.* **21** L209
[3] Datta S 1995 *Electronic Transport in Mesoscopic Systems* ed H Ahmed, M Pepper and A Broers (Cambridge: Cambridge University Press)
[4] Costa-Krämer J L, Garcia N, Garcia-Mochales P and Serena P A 1995 *Surf. Sci. Lett.* **342** L1144
[5] Ott F 1998 *Europhys. News* **29** (Jan/Feb) 13
[6] Hansen K, Laegsgaard E, Stensgaard I and Besenbacher F 1997 *Phys. Rev.* B **56** 2208
[7] Ott F, Barberan S, Lunney J G, Coey J M D, Berthet P, de Leon-Guevara A M and Revcolevschi A 1998 *Phys. Rev.* B **58** 4656
[8] Costa-Krämer J L 1997 *Phys. Rev.* B **55** R4875
[9] Krompiewski S and Krey U 1998 *Europhys. Lett.* **44** 661
[10] Asano Y, Oguri A, Inoue J and Maekawa S 1994 *J. Magn. Magn. Mater.* **136** L18
[11] Gebele O 1998 *Diploma Thesis* Regensburg University
[12] Garcia-Mochales P and Serena P A 1997 *Phys. Rev. Lett.* **79** 2316
[13] Oshima H and Miyano K 1998 *Appl. Phys. Lett.* **73** 2203