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Scattering theory of perpendicular transport in metallic multilayers (invited)

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Electronic transport in metallic multilayers is discussed in the language of the Landauer–Büttiker scattering formalism. The semiclassical conductance through a disordered interface can be unambiguously separated into specular and diffuse scattering contributions. Analytical results are derived for the perpendicular conductance of multiple disordered interfaces. Predictions for the transport properties of interfaces with dilute but strongly scattering defects should be accessible to verification by experiments. First results of first-principles calculations of ballistic transport in magnetic multilayers are presented.

I. INTRODUCTION

The giant magnetoresistance or spin-valve effect found in antiferromagnetically coupled metallic multilayers[1] has recently been studied in the so-called CPP (current perpendicular to the interface plane) geometry, both experimentally[2,3] and theoretically.[4–14] One of the many advantages of this configuration compared to the more conventional CIP (current in plane) geometry is its high symmetry, which simplifies the physics and allows more insight into the electronic transport through heterointerfaces. The importance of interface scattering in many areas of metal and semiconductor physics is reflected by numerous articles since the seminal work by Fuchs,[15] which are mainly concerned with transport parallel to an impenetrable rough interface, e.g., in the two-dimensional electron gas.[16] In the present article interface scattering is discussed for metallic transport normal to the interfaces on the basis of the Landauer–Büttiker formalism.[17] We show that in a semiclassical approximation the diffuse scattering is unequivocally connected to the impurity scattering correction to the electric field vertex. Our approach gives a simple relation between the specular and diffuse part of the transmitted wave. The conductance of a multilayer is found by a semiclassical concatenation of single interfaces. The theory can be applied to find the magnetoconductance in magnetic multilayers, where spin-dependent interface scattering is generally believed to be responsible for the spin-valve effect.

In Sec. II the Landauer–Büttiker formalism is introduced with emphasis on its relation to the conventional linear response theory. In Sec. III we review our previous results for disordered interface scattering in the semiclassical and effective mass approximations.[6,12,13] A critical assessment of the validity of our results is given in Sec. IV, where evidence is presented for the importance of quantum interference and band-structure effects beyond the semiclassical approximation.

II. LANDAUER–BÜTTIKER FORMALISM

The Landauer conductance formula[17] can be derived directly from the Kubo formula for the two-terminal configuration as sketched in Fig. 1.[18] It is required that (i) the sample is connected to the contacts via two low-impedance leads and (ii) the contacts are at thermodynamic equilibrium with a small electrochemical potential difference $\Delta\mu=\mu_1-\mu_2$. According to the Kubo linear response formalism the current can be calculated in terms of a nonlocal conductivity tensor $\underline{\sigma}(\mathbf{r},\mathbf{r}')$ and the local electric field $\mathbf{E}_{\rm loc}(\mathbf{r})$. The total current passing through an arbitrary plane S with normal $\hat{\mathbf{n}}_S$ is given as

$$J_S=\int_S d\mathbf{r}\,\hat{n}_S(\mathbf{r})\cdot\mathbf{j}(\mathbf{r})=\int_S d\mathbf{r}\int_\Omega d\mathbf{r}'\;\hat{\mathbf{n}}_S\underline{\sigma}(\mathbf{r},\mathbf{r}')\mathbf{E}_{\rm loc}(\mathbf{r}'). \tag{1}$$

We may choose S to cut through one of the leads and to be part of the surface defining the total volume Ω which encloses the sample (see Fig. 1). The local electric field is the gradient of the electrochemical potential $\mathbf{E}_{\rm loc}(\mathbf{r})=\nabla\mu(\mathbf{r})/e$ which vanishes in the leads according to our assumption (i). The chemical potentials in the leads are supposed to be identical to the ones in the contacts [assumption (ii)]. The divergence theorem and the condition of local charge conserva-

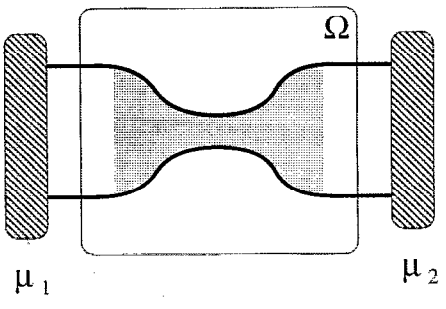

FIG. 1. Transport experiment described by Landauer's formula in the two-terminal configuration. A current flows through the sample due to an electrochemical potential difference $\mu_1-\mu_2$ between the contacts which are indicated by heavy shading. Ω is the volume encircled by the thin line, which includes the shaded sample region and part of the low-impedance leads to the equilibrated contacts.

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tion, $\nabla\cdot\mathbf{j}(\mathbf{r})=0$, can then be employed to transform the volume integral in Eq. (1) into a surface integral,

$$J_2=-J_1=G\Delta\mu/e, \tag{2}$$

where J_1 and J_2 are the currents through the two leads and G is the conductance,

$$G=\int d\mathbf{r}\int d\mathbf{r}'\ \hat{\mathbf{n}}_1(\mathbf{r})\underline{\sigma}(\mathbf{r},\mathbf{r}')\hat{\mathbf{n}}_2(\mathbf{r}'). \tag{3}$$

This result shows that the current through the sample depends only on the *total* potential drop over the sample and it is not necessary to know the *local* current and electric-field distribution to obtain the transport properties. It can then be shown[18] that the conductance is proportional to the sum of the transmission probabilities $|t_{m,n}|^2$ between the different modes m and n at the Fermi energy in the left- and right-hand side leads (spin-degeneracy assumed),

$$G=\frac{2e^2}{h}\sum_{m,n}|t_{m,n}|^2. \tag{4}$$

The transmission amplitude $t_{m,n}$ can be calculated via the Schrödinger equation.[13,19]

In many experiments it is not possible to cleanly separate "contacts," "leads," and the "sample." However, the Landauer–Büttiker formalism can be applied also when the conductance is limited by a well-defined narrow sample region as sketched in Fig. 1, where the contribution of the contact/lead region, and inaccuracies of its theoretical treatment, can be safely disregarded. In macroscopic samples the effects of the contacts may be neglected anyway. One might also wonder if the formalism may be applied to the spin-valve effect. It is well known that a ferromagnetic layer causes a nonequilibrium spin polarization of the outgoing current.[20,21] On the other hand, the equilibrated contacts are an essential ingredient in the derivation of Landauer's formula. However, this problem is of no concern as long as the spin-flip relaxation length is sufficiently longer than the length of the narrow sample section which limits the conductance. If the spin flip takes place in a wide sample section or in the contacts itself, it will not significantly contribute to the conductance. The spin-flip-induced degradation of the giant magnetoresistance with increasing temperature[8,22] cannot be treated by our theory, however.

III. DISORDERED INTERFACE SCATTERING

We consider the configuration in Fig. 2(a), i.e., a relatively narrow pillar of metallic material which limits the current in the circuit, as fabricated by Gijs *et al.*,[3] although macroscopic devices as investigated by Pratt *et al.*[2] can be treated as well. The de Broglie wavelength in high-density metals is only a few Å and quantum effects due to lateral confinement can be neglected for pillars wider than, say, 0.01 μm. In this regime the sample boundaries also have a negligible effect. Let us first consider scattering at a single interface. The interface roughness is modeled by short-range scatterers that are randomly distributed over the interface. The incoming and outgoing electron states are in this section approximated by plane waves with an effective parabolic dispersion. The wave function at an energy E is determined by the Schrödinger equation,

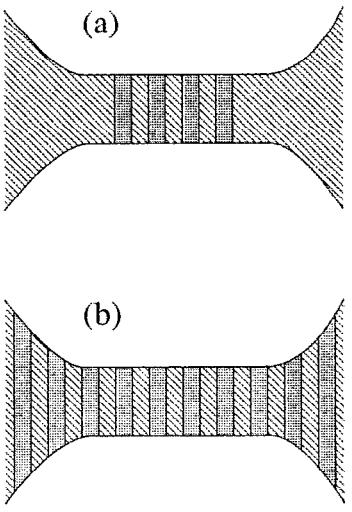

FIG. 2. (a) Sample geometry considered in the first part of the article, where the leads are made from a bulk metal, and the conductance is limited by the narrow region containing a heterostructure. (b) Pillar made from a superlattice, a configuration which is accessible to band-structure calculations.

$$\left(-\frac{\hbar^2}{2}\nabla\frac{1}{m^*(x)}\nabla+U_C(x)+V(x,y,z)\right)\psi(x,y,z)$$
$$=E\psi(x,y,z). \tag{5}$$

The conduction-band profile, $U_C(x)$, and the effective mass of the electron $m^*(x)$, are approximated by step functions at $x=0$. The interface roughness is represented by the potential $V(x,y,z)$. Landauer's conductance formula for this situation reads (spin degeneracy assumed)

$$G=\frac{2e^2}{h}\sum_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'}^{\text{prop}}|t_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'}|^2. \tag{6}$$

$\mathbf{k}_\parallel$ and $k_\perp$ are the transverse and longitudinal components of the wave vectors related by

$$k_\perp^L=[(2m_L^*/\hbar^2)(E_F-U_L)-k_\parallel^2]^{1/2},$$
$$k_\perp^R=[(2m_R^*)/\hbar^2)(E_F-U_R)-k_\parallel^2]^{1/2}.$$

The transmission (reflection) coefficient from state $\mathbf{k}_\parallel'$ to state $\mathbf{k}_\parallel$ is $t_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'}(r_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'})$ and the summation is over propagating modes. In the following we set $\Delta U_C=0$ and $\Delta m^*=0$, which considerably simplifies the analytical treatment (see Ref. 13 for generalizations of the following equations). Current conservation and the continuity of the wave function relate the transmission probabilities and the transmission coefficients by an optical theorem,[23]

$$\sum_{\mathbf{k}_\parallel}^{\text{prop.}}|t_{\mathbf{k}_\parallel,\mathbf{k}_\parallel'}|^2=\text{Re}(t_{\mathbf{k}_\parallel',\mathbf{k}_\parallel'}). \tag{7}$$

The diagrams contributing to the transmission probability can be classified as crossing or non-crossing. The crossing

diagrams[13] describe phase coherence phenomena like weak (Anderson) localization of the wave function.[24] Neglecting crossing diagrams, i.e., phase coherent scattering between different defects, it is possible to find the transmission probability in terms of the irreducible self-energy Σ (Ref. 13),

$$\langle |t_{k_\parallel,k'_\parallel}|^2\rangle = \delta_{k_\parallel,k'_\parallel} \frac{k_\perp^2}{\left|k_\perp + i\frac{m^*}{\hbar^2}\Sigma\right|^2} + \frac{k_\perp}{\left|k_\perp + i\frac{m^*}{\hbar^2}\Sigma\right|^2} \times \frac{\frac{-m^*}{\hbar^2}\,\mathrm{Im}(\Sigma)}{\Sigma^{\text{prop.}}_{k''_\parallel} \frac{k''_\perp}{\left|k''_\perp + i\frac{m^*}{\hbar^2}\Sigma\right|^2}} \frac{k'_\perp}{\left|k'_\perp + i\frac{m^*}{\hbar^2}\Sigma\right|^2}. \quad (8)$$

Our approximation is called semiclassical and valid for $|\Sigma|/E_F \ll 1$. Otherwise it breaks down when the distance between dephasing inelastic collisions becomes larger than the average separation between scatterers. Electrons are scattered specularly at the interface if the transverse component of the wave vector is conserved, which is the first term on the right-hand side of Eq. (8). The second term clearly represents the diffuse scattering contribution, which vanishes if the vertex correction is not taken into account.

To lowest order in the self-energy $m^*\Sigma/(\hbar^2 k_F)$ the conductance is independent of the real part of the self-energy,

$$G = G^0(1 - 4\eta_{IR} + 2\eta_{IR}), \quad (9)$$

where $\eta_{IR} = -m^*\ \mathrm{Im}(\Sigma)/(\hbar^2 k_F)$. $G^0 = (2e^2/h)(Ak_F^2)/(4\pi)$ is the Sharvin conductance which is proportional to the sample cross section A. The second term reduces the conductance due to specular scattering. The third, diffuse term *increases* the conductance by opening additional channels for electron transport.

We will now study the situation where all scatterers have equal magnitude of strength $\pm\gamma$ with an average $\bar{\gamma}$ which does not have to vanish. The self-energy is calculated in the single-site approximation, i.e., using the exact cross section for isolated defects, but neglecting crossed diagrams,

$$\Sigma^S = \frac{\eta_{IR}\bar{\gamma} - in_{IR}(m^*/\hbar^2)\gamma^2(k_F/2\pi)(1 - i\sqrt{\alpha^2 - 1})}{1 + [(m^*\gamma/\hbar^2)(k_F/2\pi)]^2(1 - i\sqrt{\alpha^2 - 1})^2}. \quad (10)$$

This result reduces to the Born result in the weak scattering limit $[m^*\gamma k_F/(\hbar^2\pi) \ll 1]$. For strong scattering $[m^*\gamma k_F/(\hbar^2\pi) \gg 1]$, but to lowest order in η_{IR}, we obtain the interesting result that

$$G = \frac{2e^2}{h}\left(\frac{Ak_F^2}{4\pi} - \frac{N_{IR}}{\alpha^2}\right), \quad (11)$$

where a high-momentum cutoff αk_F characterizes the spatial range of the scattering potentials. The conductance is reduced by a factor proportional to the number of defects $N_{IR} = An_{IR}$. Each scatterer effectively blocks one channel and the conductance becomes independent of the scattering strength. This blocking is somewhat reduced by a factor $1/\alpha^2$ via a "leak" of evanescent states. An experiment is proposed to test this expression: Insert a layer (or a multilayer, see below) with strong short-range scatterers between two low-impedance leads. Such a structure could be realized by the technique of δ-doping, which is routinely employed in semiconductor technology. By measuring the conductance and the number of impurities the theory can be checked and the leaking factor α can be determined which provides information about the range of the scattering potential. Note that a nonzero average of scatterers has no effect on the conductance in this limit.

Results for a single interface can be generalized to N interfaces, taking both interface scattering and bulk impurity scattering into account. Semiclassical concatenation of transmission probabilities[19] is consistent with the neglect of crossing diagrams in the single-interface scattering. The transmission properties do not change with the distance between the interfaces in this approximation. By allowing the interfaces to be infinitesimally close to each other, one can convince oneself that the relation between the transmission probabilities and the transmission coefficients, Eq. (7), still holds for the N-interface configuration. The conductance for a multilayer is

$$\frac{G^{(N)}}{G^0} = 1 - 2x_N + 2x_N^2 \ln\left(1 + \frac{1}{x_N}\right), \quad (12)$$

where $x_N = N/(2\bar{N}) = L/(2l)$. $\bar{N} = l/L_p = [2\eta_{IR} + L_p/l_{BI}]^{-1}$ is the mean free number of traversed interfaces, where L is the total sample length, $L_p = L/N$, l is the global mean free path and l_{BI} is the mean free path due to bulk impurity scattering. This relation agrees with Eq. (11) in Ref. 6 for $\Delta U_C = 0$. The two-dimensional equivalent of this expression is of interest in quasiballistic transport in semiconductor nanostructures,[25,26]

$$\frac{G^{(N)}_{2D}}{G^0_{2D}} = 1 - \frac{x_N\pi}{2} + \begin{cases} \dfrac{x_N^2}{\sqrt{1-x_N^2}} \ln\left(\dfrac{1+\sqrt{1-x_N^2}}{x_N}\right) & \text{for } x_N < 1, \\ \dfrac{x_N^2}{\sqrt{x_N^2-1}} \arccos\dfrac{1}{x_N} & \text{for } x_N > 1, \end{cases} \quad (13)$$

where $G^0_{2D} = (2e^2/h)(Wk_F/\pi)$ is the two-dimensional Sharvin conductance, proportional to the channel width W. For disordered homogeneous samples these expressions are similar but not identical to de Jong's solution for the Boltzmann equation.[26] The reason for the differences can be traced to the complete backscattering of electrons with grazing incidence in the present formalism, which in the Boltzmann approach are transmitted with probability of one-half.[26] In the large N limit a Drude-like (Ohm's law) expression is obtained for the conductivities,

$$\sigma_\infty = \begin{cases} \lim_{N\to\infty} \dfrac{NL_p G^{(N)}}{A} = \dfrac{2e^2}{h}\,\dfrac{k_F^2}{3\pi}\,l & \text{in three dimensions,} \\ \lim_{N\to\infty} \dfrac{NL_p G_{2D}^{N}}{W} = \dfrac{2e^2}{h}\,\dfrac{k_F}{2}\,l & \text{in two dimensions.} \end{cases} \tag{14}$$

For three-dimensional superlattices this limit has been treated before by Zhang and Levy.[4]

For a magnetic multilayer it is now straightforward to find the conductance by including spin-dependent interface and bulk scattering. The difference in the mean free number of traversed interfaces between both spin channels is $\Delta\bar{N}$ and the spin-averaged results is $\bar{N}$. The magnetoconductance of an antiparallel coupled multilayer is $\Delta G = G^P - G^{AP}$. The magnetoconductance depends on the parameters $\Delta\bar{N}$, $\bar{N}$, and the number of interfaces N. The spin-valve effect increases with the number of bilayers and saturates at the Drude limit for $N \gg \bar{N}$ (Ref. 4). In the limit of a magnetic superlattice the relative magnetoconductance is

$$[\Delta G/G^P]^{\text{Drude}} = (\Delta\bar{N}/2\bar{N})^2.$$

IV. VALIDITY OF SEMICLASSICAL AND EFFECTIVE-MASS THEORY

It is important to assess the accuracy of the semiclassical and the effective-mass approximations for transition-metal multilayers, which are the most interesting class of compounds for applications of the present theory. The semiclassical approximation discards quantum interference effects which are known to be important for several other properties. The oscillatory coupling of magnetic layers is a genuine quantum interference effect since it depends on the thickness of the non-magnetic layer.[27] Size-quantized states have been observed by inverse photoemission and claimed to mediate the magnetic coupling.[28] It is therefore not clear from the outset that semiclassical approximations can be used to describe transport properties. A combined theory for coupling and transport proposed in Ref. 29 is still in a formal stage. In a numerical study on disordered multilayers Asano and co-workers[9,10] provide evidence that quantum size effects can be very important for the transport properties. They proceed from a tight-binding approximation for the d electrons, which corresponds to a small bandwidth and large effects for a given potential discontinuity. The effect of the potential step is much smaller, however, when s electrons at the Fermi energy are considered to be responsible for the transport, especially in Cu/transition-metal multilayers. Zhang and Levy[14] also found rather small quantum effects of miniband formation for the small potential step sizes seen by s electrons. In reality, free electrons and d electrons are strongly hybridized. This problem cannot be solved satisfactorily within an effective-mass approximation, revealing the need for a transport theory which takes the correct band structure of the transition metal into account. s-d hybridization has been investigated in a tight-binding approximation by Itoh, Inoue, and Maekawa[30] to investigate the scattering potential of a rough Cu/Ni surface. Coehoorn[31] correlates magnetotransport with the spin-dependent occupation number differences of d orbitals at heterointerfaces obtained from first-principles band-structure calculations. Oguchi[32] employ band-structure calculations of superlattices to calculate the average Fermi velocities, i.e., the gradient of the energy dispersion at the Fermi surface, parallel and perpendicular to the interfaces. The strong anisotropies are due to quantum size effects similar to those found by Asano and co-workers.[9,10] However, transport and band structures are connected heuristically by introducing a phenomenological transport scattering time.

Here we want to emphasize that the Landauer–Büttiker formalism lends itself very well to go beyond the effective-mass and semiclassical approximations, taking into account band-structure effects rigorously. The Landauer conductance formula is easily rewritten for the case of a complicated band-structure by labeling the in- and outgoing electron states at the Fermi energy by the parallel crystal momentum $\mathbf{q}_\parallel$ inside the first Brillouin zone and band index ν (spin degeneracy assumed),

$$G = \frac{2e^2}{h} \sum_{\mathbf{q}_\parallel \nu, \mathbf{q}'_\parallel \nu'} |t_{\mathbf{q}_\parallel \nu, \mathbf{q}'_\parallel \nu'}|^2. \tag{15}$$

The calculation of the transmission probabilities is of course more difficult. In order to get a feeling for the interrelation between electronic structure and transport, we propose considering the perfectly ballistic regime of a microstructure or point contact. This regime might be realized in future devices since atomically perfect interfaces are already obtainable by molecular-beam-epitaxy crystal growth techniques. Furthermore, Asano and co-workers[9,10] pointed out that the projected density of states of unperturbed systems is strongly correlated with the conductance affected by interface roughness scattering. The finite (Sharvin) conductance is proportional to the finite cross section A and the contact conductances in the narrow sample region due to heteroinsertions.[6] The configuration in Fig. 2(a) is not directly accessible to band-structure calculations, however. We therefore concentrate on the configuration in Fig. 2(b), for which the Sharvin conductance comes down to the sum of the projections S of the Fermi surfaces for the different bands on the plane normal to the transport direction $\hat{\mathbf{n}}$,[33]

$$\begin{aligned} G_{\hat{\mathbf{n}}} &= \frac{2e^2}{h}\,\frac{A}{4\pi^2}\,\frac{1}{2} \sum_\nu S_\nu(\hat{\mathbf{n}}) \\ &= \frac{2e^2}{h}\,\frac{A}{4\pi^2}\,\frac{1}{2} \sum_\nu \int d\mathbf{q} |\hat{\mathbf{n}} \cdot \nabla_{\mathbf{q}} \epsilon_\nu(\mathbf{q})| \delta[\epsilon_\nu(\mathbf{q}) - E_F], \end{aligned} \tag{16}$$

which can be calculated given the band-structure energies $\epsilon_\nu(\mathbf{q})$ on a sufficiently fine mesh of wave vectors in the first Brillouin zone. In Fig. 3 we plot the number of conduction channels for Cu, which is proportional to the ballistic conductance through a constriction with cross section A, as calculated using first-principles band structures obtained by the linear muffin-tin orbital method (see Ref. 33 for details). To indicate the contributions from different bands the Fermi energy is varied, keeping the Cu band structure unmodified.

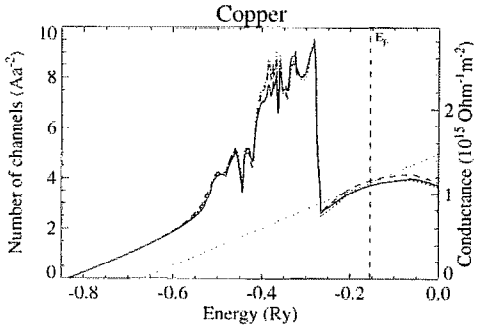

FIG. 3. Number of conducting channels in a constriction of copper with cross section A and oriented along the main crystal axes ⟨100⟩ (solid line), ⟨110⟩ (dashed line), and ⟨111⟩ (dotted line) (a=3.61 Å). The Fermi energy is varied for the (fixed) energy band structure calculated for Cu. The dashed straight line is the free-electron result.

Note that $G_{\hat{\mathbf{n}}}$ is anisotropic even for cubic crystals. By calculating Eq. (16) for magnetic superlattices with $\hat{\mathbf{n}}$ parallel and perpendicular to the interfaces a first-principles, consistent theory of transport and magnetism can be achieved. First results have been obtained for Co_1/Cu_2 ⟨111⟩-oriented superlattices forced into the spin-parallel (P) and spin-antiparallel (AP) configurations. The conductances are 1.14 (P) and 0.96 (AP) for the CIP geometry and 0.83 (P) and 0.64 (AP) for the CPP geometry, all in $10^{15}\ \Omega^{-1}\,\mathrm{cm}^{-2}$. The magnetoconductance (P-AP)/AP is therefore 19% for the CIP geometry in contrast to 30% in the CPP geometry, explaining a significant fraction of the experimental value as a purely ballistic effect. A detailed analysis will be published in due course.[33]

V. CONCLUSIONS

In summary, we have derived analytical semiclassical expressions for perpendicular transport through disordered interfaces. An experiment to check the theory is proposed which might lead to a deeper understanding of the scattering process and the microscopic structure of disordered interfaces. In the two-current model the expressions are easily generalized to describe the giant magnetoresistance in terms of the mean free number of traversed interfaces for the majority and minority spins. First results indicate the importance of taking realistic band structures into account.[33]

ACKNOWLEDGMENTS

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