

FIRST-PRINCIPLES SCATTERING MATRICES FOR SPIN-TRANSPORT

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Abstract. We describe a very efficient formalism for calculating transmission and reflection matrices from first principles in layered materials. Within the framework of spin density functional theory and using tight-binding muffin-tin orbitals, scattering matrices are determined by matching the wave-functions at the boundaries between leads which support well-defined scattering states and the scattering region. The calculation scales linearly with the number of principal layers N in the scattering region and as the cube of the number of atoms H in the lateral supercell. For metallic systems for which the required Brillouin zone sampling decreases as H increases, the final scaling goes as H^2N . In practice, the efficient basis set allows scattering regions for which $H^2N \sim 10^6$ to be handled. The method is illustrated for Co/Cu multilayers and single interfaces using large lateral supercells (up to 20×20) to model interface disorder. Because the scattering states are explicitly found, “channel decomposition” of the interface scattering for clean and disordered interfaces can be performed.

One of the most important driving forces in condensed matter physics in the last thirty years has been the controlled growth of layered structures so thin that interface effects dominate bulk properties and quantum size effects can be observed. In doped semiconductors, the large Fermi wavelength of mobile charge carriers made it possible to observe finite size effects for layer thicknesses on a micron scale. Much thinner layers must be used in order to make such observations in metals because Fermi wavelengths are typically of the order of an interatomic spacing. Nevertheless, following rapidly on the heels of a number of important discoveries in semiconductor heterostructures, interface-dominated effects such as interface magnetic anisotropy, oscillatory exchange coupling and giant magnetoresistance (GMR) were found in artificially layered transition metal materials. Reflecting the shorter Fermi wavelength, the characteristic length scale is of order nms .

Our main purpose here is to briefly outline a scheme suitable for studying mesoscopic transport in inhomogeneous, mainly layered, transition metal magnetic materials. We require that our computational scheme be (i) physically transparent, (ii) first-principles, requiring no free parameters, (iii) capable of handling complex electronic structures characteristic of transition metal elements and (iv) very efficient in order to be able to handle lateral supercells to study layered systems with different lattice parameters and to model disorder very flexibly.

A tight-binding (TB) muffin-tin-orbital (MTO) implementation of the Landauer-Büttiker formulation of transport theory within the local-spin-density approximation (LSDA) of density-functional-theory (DFT) satisfies these requirements very well.

Because wave transport through interfaces is naturally described in terms of transmission and reflection, the Landauer-Büttiker (LB) transmission matrix formulation of electron transport gained rapid acceptance as a powerful tool in the field of mesoscopic physics [1, 2], once the controversies surrounding the circumstances under which different expressions should be used had been resolved [1]. The two-terminal conductance of a piece of material is measured by attaching leads on either side, passing a current through these leads and measuring the potential drop across the scattering region. In the LB formulation of transport theory, the conductance G is expressed in terms of a transmission matrix $t = t(E_F)$

$$G = \frac{e^2}{h} \text{Tr}\{ t t^\dagger \} \quad (1)$$

where the element $t_{\mu\nu}$ is the probability amplitude that a state ν in the left-hand lead incident on the scattering region from the left (see Fig. 1) is scattered into a state μ in the right-hand lead. The trace simply sums over all incident and transmitted ‘‘channels’’ ν and μ and e^2/h is the fundamental unit of conductance. In most current work on first-principles transport [3, 6] the conductance is calculated directly from Green’s functions expressed in some convenient localized orbital representation [7]. Explicit calculation of the scattering states is avoided by making use of the invariance properties of a trace. Because we want to make contact with a large body of theoretical literature on mesoscopic physics and address a wider range of problems in the field of spin-dependent transport, we calculate the microscopic transmission and reflection matrices t and r . By using a real energy, we avoid the problems encountered,

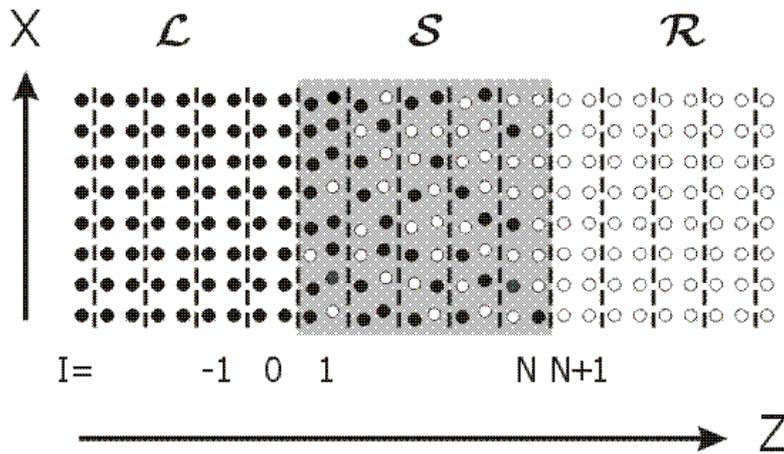


Fig. 1. Sketch of the configuration used in the Landauer-Büttiker transport formulation to calculate the two terminal conductance. A (shaded) scattering region (S) is sandwiched by left- (L) and right-hand (R) leads which have translational symmetry and are partitioned into principal layers perpendicular to the transport direction. The scattering region contains N principal layers but the structure and chemical composition are in principle arbitrary

when a small but finite imaginary part of the energy is used, in distinguishing propagating and evanescent states. The Landauer-Büttiker formalism satisfies our first requirement of physical transparency.

In developing a scheme for studying transport in transition metal multilayers, a fundamental difference between semiconductors and transition metals must be recognized. Transition metal atoms have two types of electrons with different orbital character. The s electrons are spatially quite extended and, in solids, form broad bands with low effective masses; they conduct easily. The d electrons are much more localized in space, form narrow bands with large effective masses and are responsible for the magnetism of transition metal elements. The “magnetic” electrons, however, being itinerant do contribute to electrical transport. The appropriate framework for describing metallic magnetism, even for the late $3d$ transition metal elements, is band theory [8]. An extremely successful framework exists for treating itinerant electron systems from first-principles and this is the Local Density Approximation (LDA) of Density Functional Theory (DFT). For band magnetism, the appropriate extension to spin-polarized systems, the local spin-density approximation (LSDA) satisfies our second requirement of requiring no free parameters [9].

Oscillatory exchange coupling in layered magnetic structures was discussed by Bruno in terms of generalized reflection and transmission matrices [10] which were calculated by Stiles [11, 12] for realistic electronic structures using a scheme [13, 14] based on linearized augmented plane waves (LAPWs). At an interface between a non-magnetic and a magnetic metal, the different electronic structures of the majority and minority spin electrons in the magnetic material give rise to strongly spin-dependent reflection [15, 16]. Schep used transmission and reflection matrices calculated from first-principles with an embedding surface Green’s function method [17] to calculate spin-dependent interface resistances for specular Co/Cu interfaces embedded in diffusive bulk material [18]. The resulting good agreement with experiment indicated that interface disorder is less important than the spin-dependent reflection and transmission from a perfect interface. Calculations of domain wall resistances as a function of the domain wall thickness illustrated the usefulness of calculating the full scattering matrix [19, 20]. However, the LAPW basis set used by Stiles and Schep was computationally too expensive to allow repeated lateral supercells to be used to model interfaces between materials with very different, incommensurate lattice parameters or to model disorder. This is true of all plane-wave based basis sets which typically require of order 100 plane waves per atom in order to describe transition metal atom electronic structures reasonably well.

Muffin-tin orbitals (MTO) form a flexible, minimal basis set leading to highly efficient computational schemes for solving the Kohn-Sham equations of DFT [21, 23]. For the close packed structures adopted by the magnetic materials Fe, Co, Ni and their alloys, a basis set of 9 functions (s , p , and d orbitals) per atom in combination with the atomic sphere approximation (ASA) for the potential leads to errors in describing the electronic structure which are comparable to the absolute errors incurred by using the local density approximation. This should be compared to typically 100 basis functions per atom required by the more accurate LAPW method. MTOs thus satisfy our third and fourth requirements of being able to treat complex electronic structures efficiently.

The tight-binding linearized muffin tin orbital (TB-LMTO) surface Green's function (SGF) method has been developed to study the electronic structure of interfaces and other layered systems. When combined with the coherent-potential approximation (CPA), it allows the electronic structure, charge and spin densities of layered materials with substitutional disorder to be calculated self-consistently very efficiently [24]. To calculate transmission and reflection matrices from first principles, we have combined the wave-function matching (WFM) formalism described by Ando [25] for an empirical tight-binding Hamiltonian, with an *ab-initio* TB-MTO basis [23]. The method which results has been applied to a number of problems of current interest in spin-transport: to the calculation of spin-dependent interface resistances where interface disorder was modelled by means of large lateral supercells [26]; to the first principles calculation of the so-called mixing conductance parameter entering theories of current-induced magnetization reversal [27] and the related problem of Gilbert damping enhancement in the presence of interfaces [28]; to a generalized scattering formulation of the suppression of Andreev scattering at a ferromagnetic/superconducting interface [29]; to the problem of how spin-dependent interface resistances influence spin injection from a metallic ferromagnet into a III-V semiconductor [30]. These examples amply demonstrate that our fourth requirement is well satisfied.

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