Correlating transmission and local electronic structure in planar junctions: A tool for analyzing spin-dependent transport calculations

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We propose to correlate transmittance maps and spectral-density maps of planar junctions, in order to analyze quantitatively and in detail spin-dependent transport calculations. Since spectral-density maps can be resolved with respect to atom, angular momentum, and spin, the resulting correlation coefficients reveal unequivocally, e.g., which layers or which orbitals determine the tunnel conductances. Our method can be used for transport calculations within the Landauer-Büttiker formalism. Its properties and features will be discussed by means of a pure bcc Fe(001) lead as well as an extensively studied Fe(001)/MgO/Fe(001) planar tunnel junction.

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I. MOTIVATION

Spin electronics—or spintronics for short—is one of the major topics in contemporary physics (see for example Refs. 1 and 2). With respect to both device applications and fundamental physics, planar junctions have been and are being investigated experimentally and theoretically with great effort. The spin-dependent transport properties of magnetic tunnel junctions show up as tunnel magnetoresistance (TMR), that is the change of the conductance upon reversal of the magnetization direction in one of the two electrodes. Replacing the insulating barrier by a ferroelectric, a tunnel electroresistance (TER) effect can be observed in addition. In this case, the conductance depends as well on the orientation of the electrical polarization in the ferroelectric.

In TMR experiments, the current that is flowing through a tunnel device is detected in dependence on external fields and device parameters (e.g. bias voltage and individual layer thicknesses). The current-voltage characteristics of tunnel devices are often interpreted within the Jullièere model, perhaps due to its simplicity. The validity of this model has been severely questioned because it relates the TMR ratio exclusively with the spin polarization of the electrodes and, thus, neglects the interface and barrier regions completely. If the Jullièere model would be valid, the tunnel conductance would not depend on the interface material at all, in contrast to observations. In other words, the interface region is essential and has to be described in theory as good as possible.

From the preceding it is evident that a reliable description of transport in planar junctions must capture the essential properties on an atomistic level. Hence, present theoretical investigations of transport rely on sophisticated first-principles approaches to the electronic and magnetic structures.

Advanced first-principles approaches to transport allow a very detailed analysis of the electronic structure and the conductance. In particular, the probably most important question—which orbitals in which layer determine the transport properties—can be answered. However, the amount of output data that is produced by modern computer codes becomes often unmanageable for human beings. Therefore, one restricts oneself to representative subsets or comprises the numerical data into manageable representations. For example, one puts the focus of the analysis on a single wavevector in the two-dimensional Brillouin zone (2BZ), typically to the 2BZ center. By doing so, one should be aware that such a restriction could fail because considerable parts of the 2BZ may contribute to the conductance. Examples for data representations are transmittance and spectral-density maps in the 2BZ (introduced in Section II) which have become established analysis tools. They allow in principle to answer the above question. Because they are compared visually, they leave space for speculation and interpretation; or phrased differently, they introduce ambiguity. Apparently, there is need for an improved analysis tool which allows to analyze transport properties unequivocally and quantitatively, rather than ambiguously and qualitatively.

In this paper, we propose a quantitative analysis of transport properties which goes beyond the approaches sketched above. We propose to correlate transmittance and spectral-density maps. The resulting correlation coefficients reveal unequivocally, for example, which layers or which orbitals determine the tunnel conductances. Our method can be used for any computer code which relies on a Landauer-Büttiker-type approach, thus being applicable in most of the present-day transport calculations. Its properties will be discussed for two junctions exhibiting a planar geometry.

The paper is organized as follows. In Section II we introduce our approach for analyzing transport calculations. Section III gives a brief overview of our numerical approach. The correlation analysis is applied in Section IV to a pure Fe(001) lead and to an Fe(001)/MgO/Fe(001) magnetic tunnel junction (MTJ). Concluding remarks are given in Section V.
II. THEORETICAL ANALYSIS OF THE TUNNEL CONDUCTANCE

We consider a planar junction which consists of a left electrode $\mathcal{L}$, an interface region $I$, and a right electrode $\mathcal{R}$. Due to the translational invariance parallel to the interface region, the Bloch states in the electrodes are indexed by the (in-plane) wavevector $k_\parallel$ in the 2BZ; $k_\parallel$ is conserved in the scattering process.

The bias voltage $V$ opens an ‘energy window of transport’; the chemical potentials $\mu_\mathcal{L}$ and $\mu_\mathcal{R}$ of $\mathcal{L}$ and $\mathcal{R}$, respectively, differ by $eV = \mu_\mathcal{L} - \mu_\mathcal{R}$. Without loss of generality we consider the case $V > 0$, for which incoming occupied Bloch states in $\mathcal{L}$ can be transmitted into outgoing unoccupied Bloch states in $\mathcal{R}$.

According to Landauer and Büttiker, the conductance $C$ is given by

$$C(V) = \frac{e^2}{h} \int_{\mu_\mathcal{L}}^{\mu_\mathcal{R}} \int_{2BZ} T^{\mathcal{L} \rightarrow \mathcal{R}}(V; E, k_\parallel) \, d^2k \, dE. \quad (1)$$

The wavevector integral is over the two-dimensional Brillouin zone. The transmittance $T^{\mathcal{L} \rightarrow \mathcal{R}}(V; E, k_\parallel)$ is the sum over the transmission probabilities of all incoming occupied states $\lambda$ in $\mathcal{L}$ and outgoing unoccupied states $\rho$ in $\mathcal{R}$. It is related to the scattering matrix $S$ of the interface region by

$$T^{\mathcal{L} \rightarrow \mathcal{R}}(V; E, k_\parallel) = \sum_{\lambda \rho} |S_{\lambda \rho}^{\mathcal{L} \rightarrow \mathcal{R}}(V; E, k_\parallel)|^2. \quad (2)$$

The above transmittance is a key quantity in the proposed analysis; it is conveniently displayed versus $k_\parallel$ at fixed $E$ and $V$, in so-called transmittance maps ($T$ maps). Note that $T$ can be regarded as a global quantity since it depends on the electronic structure of the entire junction, that is both electrodes (incoming and outgoing Bloch states) and the interface region (scattering matrix).

The local electronic structure of the device is described in terms of the spectral density

$$N_\alpha(V; E, k_\parallel) = -\frac{1}{\pi} \text{Im} \, \text{Tr}_\alpha G^+(V; E, k_\parallel). \quad (3)$$

$\alpha$ is a compound index which can comprise for example layer, atom, orbital, angular momentum, spin indices or point-group representation. For a given division of the complete index space, the subsets of $\alpha$ are disjoint. The trace $\text{Tr}_\alpha$ of the Green function $G^+$ is restricted to the given $\alpha$ and, thus, allows a detailed analysis of the electronic structure. As for the transmittance, the spectral density is displayed in maps versus $k_\parallel$ ($N$ maps).

In previous publications we have analyzed the conductance by relating pronounced features in a transmittance map with features in the associated spectral-density maps. If these features show up in both the $T$ map and in an $N_\alpha$ map we concluded that the chosen set $\alpha$ determines the transmittance in this $(V, E)$ region. This way we could show that for Fe/Mn/vacuum/Fe junctions the topmost Mn layer governs their TMR ratio. However, for more complicated systems it turned out that the visual inspection of the maps becomes ambiguous, tedious, and not very reliable. As a consequence, we propose to correlate properly normalized $T$ and $N$ maps by means of a projection (inner product). This procedure results in a set of a few unambiguous numbers which allow to determine rapidly the set of significant $\alpha$ indices.

For given energy $E$ and bias voltage $V$ we define the average value of a function $X(V; E, k_\parallel)$ of the transmittance $T(V; E, k_\parallel)$ and the spectral density $N_\alpha(V; E, k_\parallel)$ as the average over the 2BZ,

$$A_X \equiv \frac{1}{\Omega_{2BZ}} \int_{2BZ} X(V; E, k_\parallel) \, d^2k, \quad (4)$$

where $\Omega_{2BZ}$ is the area of the 2BZ. The correlation coefficient $c_\alpha(V; E)$ is then defined by

$$c_\alpha(V; E) = \frac{A_{TN_\alpha}}{\sqrt{A_{T^2}A_{N_\alpha^2}}}. \quad (5)$$

This quantity can be interpreted as an inner product of the normalized $T(V; E, k_\parallel)$ and $N_\alpha(V; E, k_\parallel)$. Since the latter are semi-positive for all $k_\parallel$, $0 \leq c_\alpha(V; E) \leq 1$.

Note that $c_\alpha(V; E)$ is invariant with respect to scaling $T(V; E, k_\parallel)$ and $N_\alpha(V; E, k_\parallel)$ (explicitly $T(V; E, k_\parallel) \rightarrow \tau T(V; E, k_\parallel)$ and $N_\alpha(V; E, k_\parallel) \rightarrow \tau N_\alpha(V; E, k_\parallel)$). Further, for a visual inspection and comparison of the $X(V; E, k_\parallel)$ on the same scale it is convenient to normalize them by

$$\tilde{X}(V; E, k_\parallel) \equiv \frac{X(V; E, k_\parallel)}{\sqrt{A_{N_\alpha}}} \quad (6)$$

The correlation coefficient, alternatively expressable as $c_\alpha(V; E) = A_{\tilde{T}_\alpha\tilde{N}_\alpha}$, is a measure for the ‘overlap’ of $T$ and $N_\alpha$ or of $\tilde{T}$ and $\tilde{N}_\alpha$. (i) Consider a constant transmittance and a constant spectral density, $T(V; E, k_\parallel) = t$ and $N_\alpha(V; E, k_\parallel) = n_\alpha$, which can be viewed as ‘completely overlapping’. Then $A_{T^2} = t^2$, $A_{N_\alpha^2} = n_\alpha^2$, and $A_{T_N} = tan_\alpha$. Consequently, $c_\alpha = 1$ which we consider as perfect correlation. (ii) Consider a $T(V; E, k_\parallel)$ which is nonzero only in a region $\Omega_T$ of the 2BZ:

$$T(V; E, k_\parallel) = T(V; E, k_\parallel) 1_{\Omega_T}(k_\parallel), \quad (7)$$

with the indicator

$$1_{\Omega_T}(k_\parallel) = \begin{cases} 1 & k_\parallel \in \Omega_T \\ 0 & k_\parallel \notin \Omega_T \end{cases}. \quad (8)$$

Likewise, $N_\alpha(V; E, k_\parallel)$ is assumed nonzero in a region $\Omega_{N_\alpha}$ which is disjoint with $\Omega_T$ ($\Omega_T \cap \Omega_{N_\alpha} = \emptyset$; ‘zero overlap’). Consequently, $A_{T^2} \neq 0$, $A_{N_\alpha^2} \neq 0$, and $A_{T_N} = 0$ giving $c_\alpha = 0$. We consider this case as perfectly uncorrelated. We note in passing that there may be other definitions of correlation coefficients, as it is the case for the correlation of random variables.

Finally, the partial density of states PDOS$_\alpha = A_{N_\alpha}$ and the total density of states TDOS = $\sum_\alpha A_{N_\alpha}$ ($\equiv A_{N_{2BZ}}$) are computed based on $N_\alpha$, respectively.
III. CONDUCTANCE CALCULATIONS

Because our theoretical approach to spin-dependent tunneling has been described in detail elsewhere[11],[17] we restrict ourselves to a brief survey here. The electronic structure of a tunnel junction is computed within the local spin-density approximation to density-functional theory, as is formulated in multiple-scattering theory. Our spin-polarized relativistic layer Korringa-Kohn-Rostoker (KKR) method[19],[20] provides on the one hand the Green function of the entire system, from which the spectral densities $N_\alpha(V; E, k_{||})$ can be computed, eq. (2). On the other hand, the Green function can be used to calculate the transmission $T(V; E, k_{||})$, eq. (3), within the framework of the Landauer-Büttiker theory. We can also follow the approach introduced by MacLaren and Butler[21] in which the Bloch states in the electrodes and the scattering matrix of the interface region are computed by means of layer-KKR algorithms[22]. Here, the Green function is not computed explicitly.

The $T$ and $N$ maps have been computed on identical $k_{||}$ meshes in the entire 2BZ, with at least 40 000 points. In the following applications we restrict ourselves to the case of zero bias ($V = 0$ and $\mu_L = \mu_R$).

IV. APPLICATIONS

A. Fe(001)

The properties of the proposed correlation analysis are best introduced by an—admittedly—trivial case: the spin-resolved Sharvin conductance[23] of Fe(001). Because the three regions of the junction—$L$, $T$, and $R$—are identical, the scattering matrix in eq. (2) is $S_{\lambda\rho} = \delta_{\lambda\rho}$ and $T(k_{||})$ is an integer. Accordingly, the $N$ map is a projection of the Fermi surface onto the (001) plane. Without spin-orbit coupling, spin is a good quantum number; hence, we treat the majority and minority channels separately.

Figure 4 displays the normalized $k_{||}$-resolved transmission and spectral density maps. According to Table I, the later are ordered based on their $\{s, p, d\}$ or $\{\Delta_1, \Delta_5, \Delta_2+\Delta_2'\}$-like orbitorb contributions. The assignment of the angular momentum orbitals to the different subsets $\alpha$ is motivated by the irreducible representations of the $C_{4v}$ symmetry group. This decomposition is given in Table I.

(i) The map of the total spectral density agrees nicely with the associated transmission map in the majority channel (top row). In particular, all features are present and the correlation is consequently sizable ($c_5 = 0.802$).

(ii) Other maps which essentially capture all features within the majority channel are the $\tilde{N}_d$ and $\tilde{N}_{\Delta_5}$-like maps. A visual comparison of both with the transmission could lead to the conclusion that the former matches slightly better than the latter. The correlation analysis, however, shows that this may be a misinterpretation; both coefficients indicate sizeable correlations ($c_5 = 0.798$ and $c_{\Delta_5}$-like = 0.828) but that of the $\Delta_5$-like subset is slightly larger.

(iii) As a result of the relatively small correlation coefficients of $s$ ($c_5 = 0.365$) and $p$ ($c_5 = 0.432$) we identify the $d$ majority states as the dominating conducting channels. Further, with the help of Table I and the $c_5$ of the $\Delta$-like maps, a hierarchy of conducting $d$ states can be specified. Since $c_{\Delta_1}$-like = 0.484 is quite small, the $d_{3z^2-\text{r}^2}$ states seem to play no significant role. Due to the large $c_{\Delta_1}$-like the $d_{3xz}$ and $d_{3yz}$ orbitals appear to form the leading transport channels, followed by the $d_{2y^2-r^2}$ and $d_{xy}$ states ($c_{(\Delta_2+\Delta_2')}$-like = 0.656).

(iv) Similar observations can be made for the minority channel (bottom row). Again, the $d$ states represent the main conducting channels. But in comparison to the majority channel, the role of $(d_{3xz}$, $d_{3yz}$) and $(d_{2y^2-r^2}$, $d_{xy}$) orbitals is interchanged.

This example shows that the correlation analysis provides a powerful analysis tool which on one hand fits nicely to the visual interpretation of $T$ and $N$ maps. On the other hand, it clearly reveals possible misinterpretations, as has become evident in point (ii).

With 94% (majority) and 66% (minority) the $d$ states constitute by far the main contributions to the total density of states (TDOS). In this example the hierarchy of correlation coefficients often reflects the hierarchy of partial contributions to the TDOS (see Fig. 4). This ordering becomes incorrect for instance in the case of $\Delta_5$-like and $(\Delta_2+\Delta_2')$-like states in the minority channel. Here, the $\Delta_5$-like states represent with 64% most of the TDOS, but exhibit with a $c_{\Delta_5}$-like of 0.788 a smaller correlation than the $(\Delta_2+\Delta_2')$-like contributions (26%, $c_{\Delta_2+\Delta_2'} = 0.847$).

This last finding indicates already that a one-to-one mapping of partial density of states (PDOS) hierarchies and correlation coefficients is not viable. In general, transmittances depend not only on the number of available states but rely also on other conditions like e.g. the wavefunction matching at interfaces. Hence, as a prototype which exhibits more complicated correlations between transport and electronic structures properties,

| $\alpha$   | $\ell$ | $m$ | orbitals       |
|------------|--------|-----|----------------|
| $\Delta_1$-like | 0, 1, 2 | 0   | $s$, $p_x$, $d_{3z^2-\text{r}^2}$ |
| $\Delta_5$-like | 1, 2   | -1, 1| $p_x$, $p_y$, $d_{3z^2}$, $d_{3yz}$ |
| $\Delta_2$-like | 2      | -2  | $d_{2y^2-r^2}$ |
| $\Delta_2'$-like | 2      | 2   | $d_{xy}$       |
Let us suppose briefly that the Julli`ere model is valid and that the transport properties can be interpreted exclusively based on the available PDOS\textsubscript{\textalpha}. Then the spin-polarized conductances are estimated with the product of the densities of states at the Fermi energy, strictly speaking with the PDOS\textsubscript{\textalpha} inside the left (\textL) and right lead (\textR). In this picture, the conducting channels would be, according to the previous discussion of iron, mainly determined by d-like or \{\Delta_5, \Delta_2 + \Delta_2\}\textprime-like Bloch states of the Fe electrodes. But a visual inspection and comparison with the majority maps in Fig. 1 reveals at first glance no similarity in the structures with neither the \(\overline{T}(\mathbf{k}_\parallel)\) maps nor the \(\overline{\Delta}_{\text{M}}(\mathbf{k}_\parallel)\) maps.

Consequently, one could ask which states are essential for the transport processes if the predominant Fe bulk states do not play a decisive role. A closer look at the \(\overline{\Delta}_{\text{s}}\) and \(\Delta_{5}\)-like maps in Fig. 1 leads to the identification of centrosymmetric blobs like that in Fig. 2. But the associated Bloch states exhibit small \(c_\alpha\) and marginal contributions to the TDOS in Fe bulk. Do these states play a decisive role for the transport within the MTJ?

To answer this question we consider in a next step the layer-wise contributions of the PDOS\textsubscript{\textalpha} to the respective TDOS at the Fermi energy (see Fig. 3). In particular, the \(\Delta_{\text{s}}/\Delta_{\text{M}}\) percentages are shown for one half of the symmetric MTJ and are classified again by means of \{s, p, d\} or \{\Delta_1, \Delta_5, \Delta_2 + \Delta_2\}\textprime-like orbital decompositions.

The values for the outermost Fe layers in Fig. 3 (a) and (b) are identical to those for the pure Fe lead in Fig. 1, indicating the bulk-like character of those layers far from the interfaces. The corresponding d states represent with 80%-95% the most numerous parts of the TDOS up to the
tributions of the partial density of states 
the junction, i.e. the MgO barrier, s and ∆
the transmittance map in Fig. 2 with the respective 

might indeed characterize the transport. But whether 

(a) s, p, d, and (b) \{Δ1, Δ3, Δ2 + Δ2′\}-like orbital decompositions.

second Fe layers adjacent to the MgO interfaces. At these interfaces the number of d states is drastically reduced. Within the MgO film the decrease is continued down to about 10% inside the middle region of the tunnel barrier.

On the other hand, the s and p contributions which are apparently vanishingly small within the Fe electrodes, obtain substantial weight inside the MgO spacer. In particular, the p states exhibit a maximal percentage of 60% within the 1. MgO monolayer. Deeper inside the MgO, this fraction reduces to about 40%. In contrast, the s fractions reach a level of 20% at the Fe/MgO interfaces and increase monotonously to roughly about 40%. Thus, in the middle of the MgO the number of p and s states are comparably large, with a slight advantage of the former.

Further, a decomposition in \{Δ1, Δ3, Δ2 + Δ2′\}-like contributions reveals completely different characteristics in Fig. 3. Here, the Δ1-like contributions, which are of minor importance within the Fe leads, experience a massive increase at the Fe/MgO interfaces and reach levels of about 80% within the tunnel barrier. The remaining 20% are predominantly occupied with Δ3-like and few (Δ2 + Δ2′)-like states. This hierarchical order of PDOS\(\alpha\) within the MgO reflects the well known fact of symmetry-selective decay lengths of the evanescent Bloch states within the tunnel barrier \(\delta_{\alpha}\).

Due to their sizable presence within the bottle neck of the junction, i.e. the MgO barrier, s and Δ1-like states might indeed characterize the transport. But whether this predominance also results in a dominance of the conducting channels can only be answered by an analysis of the transmittance map in Fig. 2 with the respective \(\bar{N}\) maps. In order to specify exactly which layer-resolved spectral densities fits best the structures of the transmittance map, the \(\bar{N}\) maps of the whole Fe/MgO/Fe tunnel junction have to be inspected. These maps are shown in Fig. 4.

One can see immediately that \(\bar{N}_S\), \(\bar{N}_s\), \(\bar{N}_p\), and \(\bar{N}_{\Delta_1}\)-like within the MgO layers exhibit a great similarity with the structure of \(\bar{T}(\mathbf{k}_\parallel)\) in Fig. 2. On the other hand, the similarities of \(\bar{N}_d\), \(\bar{N}_{\Delta_3}\)-like and \(\bar{N}_{(\Delta_2 + \Delta_2')}\)-like within the same layers appear rather small. Due to the great dissimilarities of the spectral density maps within the Fe layers it is reasonable to expect low correlations there. But, based on visual comparisons it is hard to make definitive statements about similarities of the structures and hence which states provide the largest contributions to the electronic transport of the whole MTJ.

At this point, the tool of the correlation analysis provides the potential to gain clearer statements. The computed correlation coefficients which represent a measure for the similarity of two maps are summarized in Fig. 4 and 5.

(i) Considering Figure 4a, it turns out that s states exhibit the most prominent correlations in all layers. For each Fe layer the \(c_s\) can be quantified with about 0.1-0.2 as nearly double as large as those of p and d states. Together with the significantly high correlations of 0.7 (1. MgO layer) up to 0.95 (3. MgO layer) inside the tunnel barrier, the previously assumed dominant role of the s states can be regarded as proven for the entire MTJ.

(ii) However, inside the MgO layers the p and d states exhibit sizeable increases of their correlation coefficients, too. In particular, the \(c_p\) are with 0.2 (1. MgO layer), 0.4 (2. MgO layer) and 0.7 (3. MgO layer) approximately twice as high as the \(c_d\). In the discussion of the \(c_{\Delta_1}\)-like coefficients below it will become evident that the increasing \(c_p\) and \(c_d\) are mainly related to states exhibiting \(p_z\) and \(d_{3z^2-r^2}\) orbital character.

(iii) Since the TDOS maps comprise structures of s states closely correlated to the transmission map and less correlated p and d states, the correlation values of \(c_p\) are always lower than those for the s states.

(iv) Along the atomic layers of the MTJ, the characteristics of the \(c_{\Delta_1}\)-like coefficients in Fig. 4 show a qualitatively similar dominance as it was found for the \(c_s\) coefficients in Fig. 4. Within the Fe electrodes the correlations of the \(\Delta_1\)-like states are just slightly but noticeable larger than those of the s states in these layers, indicating an additional relevance of \(p_z\) and \(d_{3z^2-r^2}\) orbitals in the electronic transport. This finding is substantiated by relatively small correlations of both other \(\Delta\)-like representations inside the tunnel barrier. Since the latter exhibit only \{\(p_x\), \(p_y\), \(d_{3z^2}\), \(d_{3y^2}\)\} and \{\(d_{x^2-y^2}\), \(d_{xy}\)\} orbital character (see Table 1), it is reasonable to assume that the rising importance of p and d states inside the MgO is identical to an increasing significance of \(p_z\) and \(d_{3z^2-r^2}\) orbitals.

The comparison of the results of the correlation analysis with the discussion of available PDOS\(\alpha\) in Fig. 3 shows common features but reveals also significant differences. A common outcome of both approaches is the principal importance of the tunnel barrier for the electronic transport of the MTJ. In particular, both discussions end up with a conclusion that \(\Delta_1\)-like states—i.e. s, p and \(d_{3z^2-r^2}\) orbitals which are preferentially aligned along the transport direction—tunnel most effectively and conse-
Figure 4. Correlation analysis for the majority channel of an Fe(001)/6MgO/Fe(001) MTJ in parallel magnetic configuration. (a) Layer- and orbital-wise ordered spectral density maps $\tilde{N}_\alpha$ (left → right) are shown for the entire 2BZ with decompositions $\alpha$ according to Table I (top → bottom). Correlation coefficients $c_\alpha$ for contributions (a) with $\alpha = s, p, d$ and (b) $\alpha = \Delta_1$-like, $\Delta_5$-like, $(\Delta_2 + \Delta_2')$-like. Color scales for $\tilde{N}_\alpha$ are logarithmic.

V. CONCLUSIONS AND REMARKS

The analysis of transport properties within contacts that exhibit planar geometries is often accompanied with a visual comparison of large ensembles of $k_\parallel$-resolved lo-
cal spectral density and transmission maps. In this article we presented an analysis tool which helps to avoid laborious inspections and potential misinterpretations by providing exact measures. Applying the proposed correlation analysis the contributions of atoms or orbitals can be quantified unambiguously. The dominance of the s states in the tunnel current of Fe/MgO/Fe MTJs could be proven even for the states in the Fe leads, where the contribution of states to the TDOS is only marginal.

Further, the method extends the popular discussion of transport properties at the $\bar{\Gamma}$ point in Fe/MgO/Fe MTJs to a more comprehensive analysis which comprises the entire two-dimensional Brillouin zone. In principle, the technique is not restricted to planar junctions. Besides more complex layered structures it can be applied to other nano structures like point contacts or nano wires. For these atomic-sized contacts, we expect that the corresponding correlation coefficients provide the same physical insights as one would obtain from an analysis of the conduction eigenchannels [28].

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