A proper ballistic calculation of tunneling conductance for real junctions

P. M. Levy\textsuperscript{a}, K. Wang\textsuperscript{a}, P. H. Dederichs\textsuperscript{b}, C. Heide\textsuperscript{a}, S. Zhang\textsuperscript{c}, L. Szunyogh\textsuperscript{d}, and P. Weinberger\textsuperscript{e}

\textsuperscript{a}Department of Physics, New York University, 4 Washington Place, New York, NY 10003

\textsuperscript{b}Forschungszentrum Jülich, Institut für Festkörperforschung, D-52425, Jülich, Germany

\textsuperscript{c}Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211

\textsuperscript{d}Department of Theoretical Physics, Technical University Budapest, H-1521 Budapest, Hungary

\textsuperscript{e}Institut für Technische Elektrochemie, Technische Universität Wien, A-1060 Wien, Austria

(March 21, 2022)

Employing an \textit{ab initio} Screened Korringa-Kohn-Rostoker (SKKR) band structure method for a metal-vacuum-metal junction, we find that the tunnel conductance is different when it is calculated across the barrier and far from it. We attribute this difference to an artefact of the ballistic approach which overestimates the role of specular reflections, and its inability to pick up contributions from localized interface states. To reconcile the ballistic approach with experiment, we propose that the tunnel conductance should be calculated as if it is measured directly across the barrier. In this case the predicted tunneling magnetoresistance is larger.

PACS numbers: 73.40.Gk, 75.70.-i, 73.20.At, 75.70.Pa

Measurements of the resistance and magnetoresistance (MR) of magnetic planar tunnel junctions are usually made by passing a current with voltage probes far removed from the interfaces between the electrodes and insulating barrier. Therefore it makes sense to calculate these transport properties as the transmission probability from propagating eigenstates in one electrode to those of the other. To maintain a steady state current the electrodes are connected to reservoirs, and it is understood that propagating eigenstates are determined far from the electrode/barrier interfaces. While this procedure is reasonable, a consensus based on data and intuitive grounds has evolved that the current in tunnel junctions is controlled by the electronic structure at the interfaces, e.g., the local density of states (LDOS)\textsuperscript{[1]}. This conflicts with the above description which uses the electronic structure in the electrodes far from the interface, which is different from that at the interface. In this letter we point out that calculations made with the Landauer-Büttiker or other formalism for purely ballistic transport over the whole junction cannot be directly compared to data on real junctions for at least two reasons. The ballistic conductance overestimates the role of specular reflections from the barrier as seen by the electrodes, and, if they are present, overlooks contributions from states localized near the interfaces that are coupled to itinerant states in the electrodes by diffusive and relaxation processes in real junctions. The first causes the ballistic conductance to decrease much more rapidly than it would with diffusive electrodes; the second provides additional conduction channels. Under these conditions the electronic structure at the electrode/barrier interfaces controls the tunneling current. As we will show, to model the conductance of real planar tunnel junctions, i.e., with diffusive electrodes, it should be calculated as if it is measured directly across the barrier. In other words, to reconcile the ballistic approach with experiment one has to change the boundary conditions on the transport calculation.

![FIG. 1. Scheme for conductance calculations across different ballistically conducting sections of a transition metal/vacuum/transition metal junction. At the points α and β the ballistic region is joined with diffusive electrodes thus forming an open system with reservoirs on each side.](image-url)

We have calculated the conductance of transition-metal/vacuum tunnel junctions by using the Caroli formalism\textsuperscript{[2]}. While real junctions have insulating barriers, we have taken a vacuum as it is the simplest insulator for which we can do an \textit{ab-initio} calculation. Normally, one sets the chemical potentials far from the barrier, i.e., deep in the leads. In such an approach one does not specify the chemical potentials at intermediate planes across which one chooses to evaluate the current, and one keeps the ballistic information about the propagators throughout the entire junction; not just between these planes. In our approach we set the chemical potentials at the
planes we are looking at \( \mu_{\alpha}(\beta) \simeq \mu_{\alpha}(\beta) \), and so far as transport is concerned we are able to isolate the region between \( \alpha \) and \( \beta \) from the remainder of the junction; see Fig.1. Thus, as we see below, one is able to talk about the conductance of a part of a full junction.

In the linear response region, the tunneling conductance is

\[
G = \frac{2e^2}{\hbar} \text{Tr} \left\{ \rho^\alpha (\epsilon_F) |t^\dagger (\epsilon_F)\rangle |\alpha \rangle \rho^\beta (\epsilon_F) \langle \beta | (\epsilon_F) \beta \alpha \right\},
\]

where \( t^{\alpha \beta} \) is the t-matrix between \( \alpha \) and \( \beta \); the trace \( \text{Tr} \) is over all (site and angular momentum, or energy level) indices; and the density of states (DOS) at the Fermi level \( \rho^\alpha \) and \( \rho^\beta \) used in this formalism are those at a surface created by cutting the junction so that the two parts thereby created are isolated from one another [4].

In order to obtain the t-matrix, we first determine the propagator \( G \) from a full junction calculation and then backward derive the t-matrix from Dyson’s equation \( G = g + gVG = g + gtg \), where \( g \) is the propagator in the absence of the perturbation \( V \). In our case, \( V \) joins diffusive electrodes with a ballistically conducting system consisting of \( p \) magnetic monolayers of a transition metal, the electrodes, on each side of a vacuum barrier of six monolayers as shown in Fig.1. We adopted an empty lattice structure for the vacuum layers which has the same properties as the metallic electrodes except that it contains no atoms. By definition \( g^{\alpha \beta} \) is zero and, due to the fact that \( V \) takes the form of a nearest neighbor interaction (in a principal layer description in which we use 2 atomic layers we have indeed nearest and next nearest neighbor interactions [3]), we find

\[
G^{\alpha \beta} = g^{\alpha \alpha} t^{\alpha \beta} g^{\beta \beta}. \tag{2}
\]

Upon inversion this yields the t-matrix, which differs for different \( \alpha \) and \( \beta \). By inserting this result in Eq. (1) to calculate the conductance we treat the transport between \( \alpha \) and \( \beta \) ballistically inasmuch as we explicitly use the propagator \( G^{\alpha \beta} \), while the transport in the regions of the electrodes to the left of \( \alpha \) and the right of \( \beta \) are treated diffusively, because we do not keep track of the momentum there. Rather their effect on conductance is taken into account in a “mean field-like” manner by a self energy term in the propagator [3]. In the limit of large \( p \) the conductance converges to a system that is independent of \( p \), i.e. the full ballistic approach.

The conductance for fcc(100) Fe/vacuum/Fe, and for fcc(100) Co/vacuum/Co tunnel junctions has been calculated from band structures obtained from the spin-polarized scalar-relativistic Screened Korringa-Kohn-Rostoker (SKKR) method [3], and the atomic sphere approximation (ASA) is used. Here we present the results for Fe; they are further corroborated by those on Co. The lattice parameter for Fe is 5.27 a.u. (atomic units). Two atomic layers are included in each screened principal layer, and the screening potential is set to 2 Ry inside each atomic cell. The Gunnarsson-Lundqvist exchange-correlation potential is used, and energy integration is performed by means of Gaussian quadrature with 16 points on a semi-circle in the upper half complex energy plane. For self-consistent calculations of the bulk metal, the free metal surface and the metal-vacuum-metal interface potentials, 45 \( k \) points are used in the irreducible wedge of two dimensional Brillouin Zone (2DBZ), which enables the Fermi level to be converged up to \( 10^{-7} \) Ry. For more details on this method see Ref. [3]. We used a small imaginary part of the energy of \( \epsilon = 0.5 m\text{Ryd} \) in the propagators in order to converge our results in a reasonable time.

![FIG. 2. Total conductance calculated in units of \( e^2/h \times 10^{-4} \) across different sections of a Fe(p)/vac(6)/Fe(p) tunnel junction with \( \epsilon = 0.5 m\text{Ryd} \).](image.png)

In Fig.2 we show the ballistic conductance for Fe(p)/vac(6)/Fe(p) tunnel junctions calculated either across the barrier, i.e. \( p = 0 \), or up to \( p = 7 \) Fe layers from the barrier. The conductance in all channels, majority, minority and antiparallel, decrease as we are increasing the number of monolayers of the electrodes we include in the ballistic calculation; this is particularly pronounced in the minority channel. Most of the decay in the ballistic conductance is between \( p = 0 \) and 1, because this is the region where the electronic structure is changing most. It stands to reason that the usual approach, in which the entire junction is treated ballistically, produces a lower conductance than the one we would calculate just across the barrier. The full ballistic approach includes the additional specular reflections near the barrier that comes from the bending of the band bottoms which represents the charge that has leaked out of the metallic electrodes into the vacuum barrier. For example, we find 0.7 of a total of 3 minority electrons leak out of the surface layer of the Fe electrode; for the majority band only 0.1 of the 5 electrons leak out. In Fig.2 one sees that the effect of the leakage is far more pronounced in the minority band than the majority, and this explains why the conductance drops much more in the minority band than the majority when we take into account the reflections due to the
bending of the band bottoms.

In real junctions transport is diffusive, particularly in the electrodes, so that the total resistance is the sum of resistances of each part; in this case one should limit a ballistic calculation to just the barrier. As the resistance of the barrier in tunnel junctions is about 10⁵ times greater than that of the electrodes, even for junctions with resistances as low as 50Ωμm², it is reasonable to say that the barrier determines the resistance (p = 0) and the electrodes give negligible contributions, i.e., in real planar junctions the conductance does not vary much as one goes away from the barrier. The decay of the ballistic conductance for increasing p is thus an artefact of having considered the transport in the electrodes ballistically.

We note that the tunneling magnetoresistance MR is larger when it is measured across the barrier. While we obtain MR ratios (G_P − G_AP)/G_P of 82% and 38% for the Fe and Co junctions when we use the conductances calculated at p → ∞, these ratios increase to 86% and 65% when measured directly across the barrier, i.e., at the interfaces p = 0.

In addition, as we will show now for the case of the Fe/vacuum junction, diffuse scattering and relaxation processes may couple localized states at the interfaces to propagating states in the electrodes. As in Fe these localized states are dominant in the minority channel close to the Fermi energy, they give an additional rise to the MR. The complete eigenvalue spectrum of a semi-infinite solid contains the continuum of bulk states as well as additional states localized at the surface \[P\]. In ferromagnetic metals such as Fe(100) the existence of localized states at the surface has been known for some time \[P\]; more recently surface states were also observed in Gd(0001) \[Q\]. If the energy of the surface states lie in Gd(0001) \[R\], the system contains a Fermi distribution even for the localized states; therefore ballistic transport will be unaffected by impurities, e.g., in Fe, was calculated by Mertig to be about 1µEmcm/atomic% \[S\]; therefore, for 1atomic% impurities, we can roughly estimate the elastic scattering rate of the order of \(1/\tau_{mp} = 10^{14} \text{sec}^{-1}\) \[T\]. For the tunnel junctions studied to date with resistances in the range of 10³−10⁶Ωμm², as well as for the Fe/vac/Fe junction we will discuss, the tunneling rate is in the range 10⁶−10¹⁰ sec⁻¹, so that the diffuse scattering in sufficient to have localized states contribute to participate in conduction. At finite temperatures relaxation processes, such electron-electron, electron-phonon, and electron-magnon interactions, can couple the localized to itinerant states; our rough estimates tell us that the relaxation is faster than the tunneling rate of 10⁶ sec⁻¹ when the temperature is below the Fermi level of 0.7K; the tunneling rate is 10²⁰ sec⁻¹. We conclude that while tunneling electrons create holes in the localized interface states, they recombine almost instantaneously due to scattering by phonons, magnons, other electrons, or interfacial disorder so that for the calculation of the current one can always assume a Fermi distribution even for the localized states. On the contrary for currents perpendicular to the plane of the layers (CPP) in metallic multilayered structures the rate at which electrons traverse a layer is determined by the Fermi velocity, which is the of the order of 10¹⁶ sec⁻¹. As the relaxation mechanisms are much slower, it is reasonable to calculate the conductance in metallic multilayers by neglecting relaxation to localized states, even though they appear at interfaces in much the same way as surface states \[U\].

At the Fe(100)/vac interface surface states exist in the minority channel at the Fermi level for \(k_\parallel \not= 0\); for \(k_\parallel \sim 0\) localized states exist above \(\epsilon_F\) \[V\]; therefore those with \(k_\parallel \sim 0\) contribute to tunneling if one applies a bias. In our ASA calculations there are only surface resonant states at \(\epsilon_F\), and we have found localized states in the minority channel about \(k_\parallel \sim 0\) just below the Fermi level at \(\epsilon \sim \epsilon_F - 0.05eV\). We also calculated the surface density of states at 0.05eV below the Fermi level, as well as the conductance 0.05eV below the Fermi level both at the interface and in the bulk, i.e., \(p = 0\) and 4 in terms of the in-plane momentum \(k_\parallel\). The large DOS at the surface about \(k_\parallel = 0\) at 0.05eV below the Fermi level, which is absent at \(\epsilon_F\) and in the bulk \(p = 4\) indicates the presence of the localized surface state. On comparing the conductances in, only the conductance for the barrier \(p = 0\) and at \(\epsilon_F - 0.05eV\) has a strong contribution from the localized states about \(k_\parallel = 0\); all the other conductances have “holes” about \(k_\parallel = 0\). One notes that the average of the conductance for \(p = 0\) at \(\epsilon_F - 0.05eV\) is four times larger than at \(\epsilon_F\). The conclusion that can be drawn is that if localized states exist about \(k_\parallel \sim 0\) for \(E \sim \epsilon_F\) they would contribute to the conductance measured across the barrier, but do not contribute to the ballistic conductance away from the interfaces. In real junctions where localized states are mixed with resonant and itinerant at the surface they contribute to the conduction as measured across electrodes far from the barrier; therefore it is only the ballistic conductance calculated for the barrier itself, \(p = 0\), that captures the contribution from localized states.
states if they exist. In general the contribution of localized states to tunneling will depend on their coupling to the states in the barrier, i.e. their chemical bonding.

In conclusion, when one compares the conductance of real magnetic tunnel junctions with diffusive electrodes to a calculation of conductance where it is assumed that transport is ballistic throughout, e.g., for large $p$, we find it overestimates the role of specular reflections as seen by the electrodes, and, if they are present, overlooks contributions from states localized near the interfaces that are coupled to itinerant states in the electrodes by diffusive and relaxation processes in real planar junctions. Both mechanisms present in all planar tunnel junctions conspire to maintain the conductance relatively constant as we go away from the barrier, i.e., the decrease in the ballistic conductance does not apply to realistic planar junctions. For these reasons the only conductance one obtains in a ballistic calculation that can be compared to real junctions is that across the barrier $p = 0$. This should not suggest that ballistic calculations far away from the barrier are meaningless; one can certainly think of systems such as two iron whiskers separated by a vacuum or MgO barrier where conductance in the electrodes is purely ballistic at very low temperatures.

We have used vacuum whereas the barriers in the tunnel junctions studied to date have been insulators; while this changes the conductance one calculates, it does not alter the conclusion we arrive at, i.e., if one does a ballistic calculation it should be that of only the barrier. For finite bias one probes a larger region about the Fermi level so that localized surface states away from $\epsilon_F$ contribute to conduction; their contribution to the conductance will be included if one does the calculation directly across the barrier rather than in the electrodes.

We would like to acknowledge and thank William Butler for sharing with us his unpublished results on the tunneling conductance of Fe/vac/Fe junctions, Matthias Bode for bringing to our attention his spin polarized tunneling results, and Phivos Mavropoulous and Nickos Papanikolaou for helpful discussions. This work was supported by the Defense Advanced Research Projects Agency and Office of Naval Research (Grant No. N00014-96-1-1207 and Contract Nos. MDA972-96-C-0014, and MDA972-99-C-0009 ), the National Science Foundation (Grant No. INT-9602192), NATO (Grant No. CRG 960340), the Hungarian National Science Foundation (OTKA T030240), and the TMR Network ERBFMXCT-960089.

[1] R. Meservey and P. M. Tedrow, Phys. Rep. 238, 173 (1994).
[2] C. Caroli, R. Combescot, P. Nozieres and D. Saint-James, J. Phys. C 4, 916 (1971); J. Phys. C 5, 21 (1972); R. Combescot, J. Phys. C 4, 2611 (1971).
[3] Kuising Wang, thesis New York University, 1999; Kuising Wang, P. M. Levy and S. Zhang, to be published.
[4] J. Pollmann and S.T. Pantelides, Phys. Rev. B 18, 5524 (1978).
[5] L. Szunyogh, B. Újfalussy, P. Weinberger, J. Kollár, Phys. Rev. B 49, 2721 (1994).
[6] S. Datta, Electronic Transport in Mesoscopic Systems (Cambridge University Press, Cambridge, England, 1995); see pp.145-162.
[7] O. Gunnarsson and B. I. Lundqvist, Phys. Rev. B 13, 4274 (1976).
[8] A. Zangwill, Physics at Surfaces, (Cambridge University Press, Cambridge, 1988) pp. 54.
[9] J.A. Stroscio, D.T. Pierce, A. Davies, R.J. Celotta and M. Weinert, Phys. Rev. Lett. 75, 2960 (1995); J.W. Gadzuk, J. Vac. Sci. Tech. 9, 591 (1979).
[10] M. Bode, M. Getzlaff and R. Weisendanger, Phys. Rev. Lett.81,4256 (1998); J.Vac.Sci. Technol.A 17, 2228 (1999).
[11] J.M. MacLaren, X.-G. Zhang, W.H. Butler and Xindong Wang, Phys. Rev. B 59, 5470 (1999).
[12] I. Mertig, P. Zahn, M. Richter, H. Eschrig, R. Zeller, and P. H. Dederichs, J. Magn. Magn. Mater. 151, 363 (1996).
[13] N. W. Ashcroft and N. D. Mermin, Solid State Physics, (Holt, Rinehart and Winston, New York, 1976) p. 9.
[14] P. Zahn, J. Binder, I. Mertig, R. Zeller, and P. H. Dederichs, Phys. Rev. Lett. 80, 4309 (1998).
[15] N. Papanikolaou, B. Nonas, S. Heinze, R. Zeller, and P.H. Dederichs, to be published.
[16] B. Heinrich, private communication.