Tight-binding theory of tunneling giant magnetoresistance

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A unified theory of the tunneling magnetoresistance (TMR) and of the ballistic-current perpendicular-to-plane giant magnetoresistance (CPP GMR) is developed. It is based on the Kubo-Landauer formula and fully realistic tight-binding bands fitted to an *ab initio* band structure. The theory is first applied to a single-orbital tight-binding model to investigate analytically a continuous transition from the CPP GMR of a metallic system to the TMR of a tunneling junction. The transition takes place when either hopping of electrons between the ferromagnetic electrodes is gradually turned off or the on-site potentials in the nonmagnetic spacer are varied so that the Fermi level in the spacer moves into the band gap. It is shown that the TMR approaches rapidly the same saturation value when either the interelectrode hopping decreases or the height of the insulating barrier increases. When the insulating barrier is high (band gap is large), the TMR depends only weakly on the thickness of the insulating layer. However, when the band gap is small compared to the conduction band width, the TMR decreases rapidly with increasing thickness of the insulator. The numerical results for a Co(001) junction, based on a fully realistic band structure of the Co electrodes, show a very similar behavior. As the tight-binding hopping matrix between the Co electrodes is gradually turned off, the TMR ratio drops initially very rapidly from its value of 280% in the metallic regime to about 40% but then stabilizes in the range 40–65 %. This is in a very good agreement with the observed value of 40%. The polarization of the current flowing across the Co junction in the metallic regime is negative (antiparallel to the magnetization) but becomes positive in the tunneling regime. The sign of the calculated polarization is, therefore, in agreement with the sign observed in all the experiments on tunneling from transition-metal ferromagnets.
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I. INTRODUCTION

Two ferromagnetic metals separated by an insulating oxide layer exhibit a giant magnetoresistance[1–3] of up to 40% due to tunneling across the insulating layer. The tunneling magnetoresistance (TMR) effect was observed by Julliere[4] (see also Maekawa and Gäfvert[5]) but the magnitude of the TMR in these early experiments was very small.

Theoretical interpretation of the TMR effect has been based on the conventional theory of tunneling (see, for example, Refs. 6, 7). The main conclusion of the conventional theory of tunneling is that the tunneling current is proportional to the product of the densities of states in the left and right electrodes. This conclusion is arrived at by treating tunneling as a quantum transition from one electrode to the other. The two electrodes between which the transitions take place are regarded as two separate systems described by different Hamiltonians.[8] Such a separation is clearly impossible in the closely related problem of the current perpendicular-to-plane giant magnetoresistance (CPP GMR) since the two ferromagnets are strongly coupled in the metallic regime via a nonmagnetic metallic spacer. Given that the CPP GMR and TMR seem to require different theoretical treatment, one might conclude that they are qualitatively different effects. It is, therefore, rather remarkable that the observed magnitudes of the CPP GMR and TMR are comparable despite the fact that the individual resistances of a tunneling junction in its ferromagnetic and antiferromagnetic configurations are several orders of magnitude higher than those of a metallic trilayer. Experimentally, the two effects seem to be closely related.

To establish a theoretical link between the TMR and CPP GMR, it is necessary to develop a nonperturbative theory of tunneling that treats the two electrodes together with the tunneling barrier as a single quantum-mechanical system. This is, indeed, the method one uses to solve the textbook problem of tunneling through a rectangular barrier. The rectangular barrier model was already applied by Slonczewski[9] to calculate the TMR. However, Slonczewski's approach is based on a direct calculation of the wave function and this method is not easily generalizable beyond a simple parabolic band.

The extension of Slonczewski's model to a realistic band structure I propose is motivated by a tight-binding description of the conventional model of tunneling due to Harrison.[10] He argues that one should start with two electrodes separated by an insulator so thick that no tunneling occurs. The two electrodes are thus regarded as completely independent systems. When they are brought closer together so that their wave functions begin to overlap, tunneling occurs. The overlap matrix elements correspond directly to the hopping integrals of the tight-binding method and are used to calculate by perturbation theory the probabilities of transition. Note that it is again assumed in this method that the states between which tunneling takes place are those of the electrodes unperturbed by the tunneling process (electrodes separated by an infinitely thick insulator).

To develop a unified theory of the TMR and CPP GMR, it is necessary to reverse the process adopted by Harrison, i.e., start with strongly interacting electrodes (metallic CPP GMR regime) and obtain the tunneling regime as a limit in which the influence of one electrode on the other is weak. It is

useful to explain first the physical picture on which the present method is based. One starts with two identical ferromagnetic electrodes in direct contact (no barrier) and assumes that there is a bias applied to them. At this stage, having two electrodes simply means that we have drawn a fictitious cleavage plane separating a single ferromagnet into two halves. The electronic structure of the ferromagnet is described by a tight-binding Hamiltonian. Since the two electrodes are in direct contact, the tight-binding hopping integrals across the fictitious interface are, of course, the same as in the bulk of the ferromagnets and the interface offers no resistance to electrons moving between the electrodes. Let us now assume that the magnetization of the right ferromagnet is rotated to become antiparallel to that of the left ferromagnet. We have thus created in this thought experiment an abrupt (infinitely narrow) domain wall. Electrons of a given spin orientation impinging on the interface will see the potential of electrons of the opposite spin on the other side of the interface and thus experience a spin-dependent scattering. It follows that the resistance due to such interfacial scattering in the antiferromagnetic configuration of the two electrodes is higher than in the ferromagnetic configuration, i.e., magnetoresistance effect occurs. This is completely analogous to the CPP GMR in a metallic trilayer. The abrupt domain wall mechanism of the GMR is also the origin of the TMR. The role of an insulating barrier is merely to decouple magnetically the left and right ferromagnets so that an abrupt rotation of the magnetization is possible.

I shall be comparing frequently the metallic and tunneling regimes of the magnetoresistance refering to the metallic regime as CPP GMR. To avoid misunderstanding, I wish to stress that CPP GMR in this context means CPP GMR in the ballistic regime in which the effect of impurities is negligible. While it is legitimate to neglect the effect of impurities in the tunneling limit (for reasons discussed in Sec. II), the situation in the metallic limit is different in that the CPP GMR observed in conventional samples is not in the ballistic but in the diffusive (ohmic) regime. One would expect to be in the ballistic regime only for mesoscopic samples. Nevertheless, since the origin of the CPP GMR in the diffusive and ballistic regimes is the same, i.e., scattering from spin-dependent potentials at the interfaces, comparison of the tunneling limit with the ballistic metallic limit is relevant.

To relate quantitatively the TMR to the metallic CPP GMR, it is necessary to have a realistic model of tunneling which allows us to pass continuously from strongly coupled ferromagnets (CPP GMR) to the tunneling limit of weakly coupled ferromagnets (TMR). The method I propose is to introduce a real cleavage plane between the ferromagnets and move them apart thus creating a vacuum gap between them. Tunneling of electrons across the vacuum gap results in tunneling magnetoresistance and the effect is qualitatively the same as for tunneling through an insulating barrier since in both cases electron wave functions decay exponentially in the region between the two electrodes.[10] In fact, it will be demonstrated in Sec. IV that the two models are equivalent but tunneling across a vacuum gap is physically more transparent. Following Harrison,[10] I shall model the effect of a vacuum/insulator gap by tight-binding hopping integrals across the cleavage plane that are made to decrease gradually from their bulk values to zero as the thickness of the gap increases. However, in contrast to the conventional theory of tunneling, the two ferromagnets are, in the present approach, always connected by a weak hopping and form, therefore, a single quantum-mechanical system described by a common tight-binding Hamiltonian.

Viewed in this way, there is no fundamental difference between tunneling magnetoresistance and CPP GMR of a metallic system. In both cases, one first calculates the exact one-electron wave functions of an insulating (metallic) layer sandwiched between two electrodes in their ferromagnetic (FM) and antiferromagnetic (AF) configurations and then determines the current flowing between the electrodes from the transmission coefficient of the structure. This is, indeed, in the spirit of the scattering theory of transport proposed by Landauer[11] which is applicable to both metallic and insulating systems. I shall, therefore, apply the Landauer scattering theory cast in a Green's function formalism to the tight-binding model of tunneling formulated above.

The plan of the paper is as follows. In Sec. II, the calculation of the transmission coefficient in terms of local one-electron Green's functions is described for a general multi-orbital tight-binding band structure. The general formalism of Sec. II is first applied in Sec. III to a single-orbital tight-binding model of tunneling across a vacuum gap since this model allows one to follow analytically the transition from the strongly coupled (CPP GMR) regime to the tunneling regime. In Sec. IV, the single-orbital tight-binding model is used to demonstrate that the TMR due to tunneling across a wide vacuum gap and TMR due to tunneling through a high insulating barrier are equivalent. Having established the equivalence between the two models of tunneling, the TMR due to tunneling between two Co(001) electrodes separated by a vacuum gap is investigated in Sec. V using fully realistic tight-binding bands fitted to a first-principles band structure of ferromagnetic fcc Co.

II. GENERAL EXPRESSION FOR THE TUNNELING CURRENT IN TERMS OF ONE-ELECTRON GREEN'S FUNCTIONS

Following Landauer,[11] we can write the conductance in a spin channel σ of any sample (metallic or insulating) sandwiched between two electrodes in terms of its transmission coefficient

$$\Gamma^{\sigma}=\frac{e^2}{h}\sum_{\mathbf{k}_{\parallel}} T^{\sigma}(\mathbf{k}_{\parallel}), \tag{1}$$

where $T^{\sigma}(\mathbf{k}_{\parallel})$ is the transmission coefficient in the channel $(\mathbf{k}_{\parallel},\sigma)$, $\mathbf{k}_{\parallel}$ is the wave vector parallel to the layer structure, and the sum in Eq. (1) is over all $\mathbf{k}_{\parallel}$ in the two-dimensional Brillouin zone. As in all the theories of tunneling, it is assumed in Eq. (1) that the electron spin and $\mathbf{k}_{\parallel}$ are conserved in the tunneling process. The conservation of spin is not a serious issue since inelastic spin-flip scattering at the ferromagnet/insulator interface is unlikely at low temperatures. However, interfacial roughness could destroy conservation of $\mathbf{k}_{\parallel}$ in samples with poor interfaces. Finally, it is assumed implicitly in Eq. (1) that the resistance of the electrodes is negligible compared with the resistance of the

sample. This is obviously satisfied in the case of tunneling and, therefore, the ferromagnetic electrodes can be regarded as perfect conductors. In the strong-coupling limit of CPP GMR when the spacer is metallic, the electrodes have to be included in the calculation of the transmission coefficient, in which case, the whole structure (the electrodes and spacer) is assumed to be placed between two ideal leads (see, e.g., Mathon *et al.*[12]). Experimentally, this is achieved in the CPP geometry with superconducting contacts.[13]

The Landauer formula is valid rigorously in the limit of a weak bias (linear-response theory) and is known to be equivalent[14] to the Kubo formula. The Kubo/Landauer fromula is, of course, applicable both to insulating and metallic spacers and is exact within the linear-response theory. To calculate the transmission coefficient for a realistic multiorbital band structure, it is most convenient to start from the Kubo formula[12,15] for the frequency-dependent conductance at zero temperature

$$\Gamma(\omega)=\frac{\pi}{\omega N^2}\int dE\sum_r\sum_{n,m}|\langle n|j_r|m\rangle|^2\delta(E+eV-E_m)\times\delta(E-E_n)\lim_{T\to 0}f(E)[1-f(E+\hbar\omega)], \quad (2)$$

where the spin index σ has been suppressed. The quantity j_r in Eq. (2) is the operator of current flowing from an atomic plane r parallel to the electrodes to the neighboring plane, the sum over r is over all N atomic planes in the sample, the sum over n,m is over the complete set of energy eigenstates $|n\rangle,|m\rangle$ of the system with energies E_n, E_m, and f is the Fermi function. Since the current is conserved and, hence, independent of r, the sum over r in Eq. (2) is trivially performed and the matrix elements of the current operator j_r can be calculated anywhere in the structure. In particular, they will be evaluated between any two neighboring atomic planes labeled 0 and 1. Assuming that both the electrodes and sample are described by a tight-binding Hamiltonian in a basis which is Bloch-like in the direction parallel to the layers and atomiclike in the perpendicular direction, we can write the current operator in the form

$$j_0=\frac{ie}{\hbar}\sum_{\mathbf{k}_\parallel}\sum_{\alpha,\beta}[t_{0\alpha,1\beta}(\mathbf{k}_\parallel)c^\dagger_{0\alpha}(\mathbf{k}_\parallel)c_{1\beta}(\mathbf{k}_\parallel)-t_{1\beta,0\alpha}(\mathbf{k}_\parallel)c^\dagger_{1\beta}(\mathbf{k}_\parallel)c_{0\alpha}(\mathbf{k}_\parallel)], \quad (3)$$

where $c^\dagger_{i\alpha}(\mathbf{k}_\parallel)$ $[c_{i\alpha}(\mathbf{k}_\parallel)]$ is the creation (annihilation) operator of a one-particle state $|i,\alpha,\mathbf{k}_\parallel\rangle$ in an atomic plane i, α is an orbital index, and $t_{0\alpha,1\beta}(\mathbf{k}_\parallel)$ is the matrix of tight-binding hopping integrals between the planes 0 and 1. Using Eq. (3) for the current operator and inserting complete sets of one-electron states $|i,\alpha,\mathbf{k}_\parallel\rangle$ in the current matrix elements, we can rewrite Eq. (2) in terms of the advanced and retarded one-electron Green's functions $G^\pm_{i\alpha,j\beta}(E,\mathbf{k}_\parallel)=\langle i,\mathbf{k}_\parallel,\alpha|(E-H\pm i\epsilon)^{-1}|j,\mathbf{k}_\parallel,\beta\rangle$. This is achieved by noting that

$$\tilde{G}_{i\alpha,j\beta}(E,\mathbf{k}_\parallel)=\frac{1}{2i}[G^-_{i\alpha,j\beta}-G^+_{i\alpha,j\beta}]=\pi\sum_n\langle\mathcal{A}|n\rangle\langle n|\mathcal{B}\rangle\delta(E-E_n), \quad (4)$$

where script letters have been used to label one-electron states of the type $|i,\alpha,\mathbf{k}_\parallel\rangle$ and ϵ is a small positive number. Taking the limit $\omega\to 0^+$, it is now easy to show that the total conductance in a spin channel σ is given by

$$\Gamma^\sigma=\frac{e^2}{h}\sum_{\mathbf{k}_\parallel}\Gamma^\sigma(\mathbf{k}_\parallel)=\frac{4e^2}{h}\sum_{\mathbf{k}_\parallel}\mathrm{Re\ Tr}(\tilde{G}^\sigma_{00}t^\sigma_{01}\tilde{G}^\sigma_{11}t^\sigma_{10}-t^\sigma_{01}\tilde{G}^\sigma_{10}t^\sigma_{01}\tilde{G}^\sigma_{10}). \quad (5)$$

Here, the trace is over all orbital indices that are contained implicitly in the layer indices 0 and 1 and all the Green's functions are evaluated at the Fermi energy E_F.

For simplicity, we derived Eq. (5) assuming hopping to nearest neighbors only. However, Eq. (5) holds also in the case of hopping to more distant neighbors provided atomic planes are replaced by principal layers.[16] For a fully realistic tight-binding parametrization of a first-principles band structure of transition metals, s,p,d bands with hopping to second neighbors are required, in which case each principal layer contains typically two atomic planes and all the Green's functions and hopping matrices in Eq. (5) are, therefore, 18×18 matrices.

No assumptions about the nature of the sample have been made in the derivation of Eq. (5) and it is, therefore, valid generally for any model of tunneling. In particular, it can be used to discuss tunneling through an insulating barrier. Alternatively, it can be applied to the tight-binding model of tunneling across a vacuum gap discussed in the Introduction. In that case, it is convenient to choose the plane labeled by 0 in Eq. (5) as the surface plane of the left electrode and the plane 1 as the surface plane of the right electrode. The matrix of tight-binding hopping integrals t^σ_{01} connecting the left and right electrodes then plays the role of the tunneling matrix elements. It is determined by the overlap of electron wave functions in the vacuum gap.

Both for calculational purposes and physical interpretation, it is useful to express all the one-electron Green's functions in Eq. (5) in terms of the surface Green's functions g^σ_{00} and g^σ_{11} of completely disconnected left and right electrodes (no electron hopping between the planes 0 and 1). The matrix elements G^σ_{00}, G^σ_{11}, and G^σ_{10} of the Green's function for the connected system are then obtained from the Dyson equation

$$G^\sigma_{00}=(I-g^\sigma_{00}t^\sigma_{01}g^\sigma_{11}t^\sigma_{10})^{-1}g^\sigma_{00},$$

$$G^\sigma_{11}=(I-g^\sigma_{11}t^\sigma_{10}g^\sigma_{00}t^\sigma_{01})^{-1}g^\sigma_{11},$$

$$G^\sigma_{10}=g^\sigma_{11}t^\sigma_{10}G^\sigma_{00}, \quad (6)$$

where I is a unit matrix.

Equations (5) and (6) provide a rigorous basis for a realistic calculation of the tunneling magnetoresistance and will be now applied to specific systems.

III. EVOLUTION OF THE CURRENT PERPENDICULAR-TO-PLANE MAGNETORESISTANCE INTO TUNNELING MAGNETORESISTANCE

The general formulation of Sec. II is first applied to a single-orbital tight-binding model of tunneling across a vacuum gap. The model allows us to investigate a continuous transition from the magnetoresistance of two electrodes separated by an abrupt domain wall to the magnetoresistance of a tunneling junction. The transition takes place as the tight-binding hopping integral connecting the two electrodes is gradually turned off.

Consider two ferromagnetic electrodes described by a simple cubic tight-binding Hamiltonian with nearest-neighbor hopping $t^{\rm bulk}$. They are parallel to an (001) plane and connected by a nearest-neighbor hopping integral t_{01}. The one-electron Green's functions that are required in Eqs. (5) and (6) are calculated assuming that electrons experience exchange-split potentials in the ferromagnets. The positions of the centers of the ferromagnet majority-spin ($\uparrow$) and minority-spin ($\downarrow$) bands are, therefore, given by $\epsilon_{\uparrow,\downarrow}=\epsilon_{\rm FM} \mp \Delta/2$, where $\epsilon_{\rm FM}$ is the spin-independent on-site potential in the ferromagnet and Δ is the exchange splitting of the bands. All the band energies are measured from the Fermi energy ($E_F=0$) in units of the bulk hopping $t^{\rm bulk}$.

Using Eqs. (5) and (6), it is easy to show that the conductance in a spin channel σ for the single-orbital tight-binding model is given by

$$\Gamma^{\sigma}=\frac{4e^2}{h}\sum_{\mathbf{k}_{\parallel}} t_{01}^2 \frac{{\rm Im}\, g_L^{\sigma}(E_F,\mathbf{k}_{\parallel}){\rm Im}\, g_R^{\sigma}(E_F,\mathbf{k}_{\parallel})}{|1-t_{01}^2 g_L^{\sigma}(E_F,\mathbf{k}_{\parallel}) g_R^{\sigma}(E_F,\mathbf{k}_{\parallel})|^2}, \quad (7)$$

where $g_L^{\sigma}(E_F,\mathbf{k}_{\parallel})$ and $g_R^{\sigma}(E_F,\mathbf{k}_{\parallel})$ are the surface Green's functions of the completely disconnected left and right electrodes. To determine the magnetoresistance ratio $R_{\rm TMR}$, it is necessary to evaluate from Eq. (7) the conductances Γ^{σ} of the junction in the ferromagnetic (FM) and antiferromagnetic (AF) configurations of the magnetic electrodes. The usual magnetoresistance ratio $R_{\rm TMR}$ is then defined by

$$R_{\rm TMR}=\frac{\Gamma_{\rm FM}^{\uparrow}+\Gamma_{\rm FM}^{\downarrow}-\Gamma_{\rm AF}^{\uparrow}-\Gamma_{\rm AF}^{\downarrow}}{\Gamma_{\rm AF}^{\uparrow}+\Gamma_{\rm AF}^{\downarrow}}. \quad (8)$$

The qualitative behavior of the TMR ratio can already be deduced from the structure of Eq. (7). The principal factor that determines the dependence of the conductance on the hopping integral t_{01} across the vacuum gap is the multiplicative factor t_{01}^2 in the numerator. Since we expect t_{01} to decrease exponentially with increasing separation between the electrodes, the conductance Γ^{σ} for any given configuration of the magnetic layers (FM or AF) decreases rapidly with decreasing t_{01}. On the other hand, since the term t_{01}^2 enters the numerator of Eq. (7) as a multiplicative factor, it cancels out in the GMR ratio. The transition from a metallic regime $t_{01}\approx t^{\rm bulk}$ to the tunneling regime $t_{01}\rightarrow 0$ is, therefore, determined entirely by the behavior of the denominator in Eq. (7). As electron hopping t_{01} between the two electrodes decreases, the denominator in Eq. (7) reaches a constant value in the limit $t_{01}\rightarrow 0$. It follows that the GMR ratio $R_{\rm TMR}$ approaches a saturation value $R_{\rm TMR}^{\rm sat}$, which can be identified with the tunneling magnetoresistance.

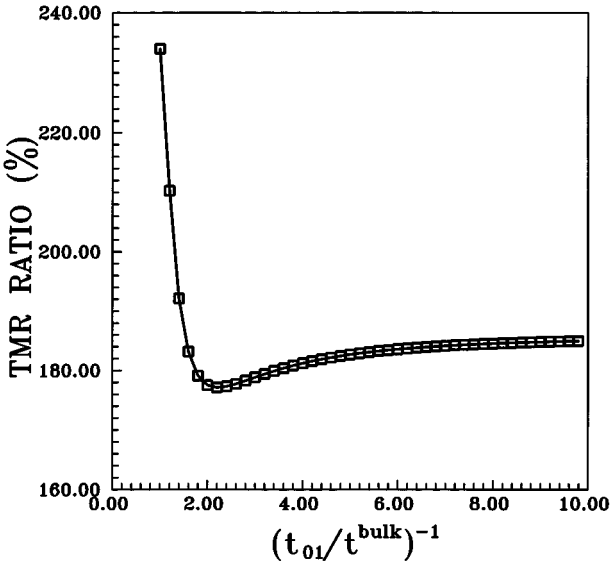

FIG. 1. Dependence of the tunneling magnetoresistance on the reciprocal of the electron hopping between the ferromagnetic electrodes. Single-orbital tight-binding model.

The individual conductances Γ^{σ} and the TMR ratio itself can be easily determined from Eqs. (7) and (8) for any value of t_{01} since the surface Green's functions are known analytically.[18] The dependence of the TMR ratio $R_{\rm TMR}$ on the reciprocal of the hopping $(t_{01}/t^{\rm bulk})^{-1}$ across the vacuum gap is shown in Fig. 1. The reciprocal of the hopping is used as a measure of the width of the gap since $(t_{01}/t^{\rm bulk})^{-1}$ increases with increasing separation between the electrodes. The values of the ferromagnet parameters $\epsilon_{\rm FM}=5.1$ and $\Delta=1.0$ (in units of $t^{\rm bulk}$) used in Fig. 1 were chosen to mimic a junction with cobalt electrodes which is discussed in Sec. V. However, the qualitative behavior of the TMR ratio is quite insensitive to the choice of the electrode parameters.

It can be seen from Fig. 1 that the TMR ratio depends only very weakly on the hopping t_{01} across the vacuum gap and a saturation value of the tunneling magnetoresistance $R_{\rm TMR}^{\rm sat}\approx 180\%$ is reached very rapidly for values of t_{01} of the order of $5-10\%$ of the bulk hopping $t^{\rm bulk}$. This is in sharp contrast to the behavior of the individual conductances $\Gamma_{\rm FM}^{\uparrow}$, $\Gamma_{\rm FM}^{\downarrow}$, and $\Gamma_{\rm AF}^{\uparrow,\downarrow}$, shown in Fig. 2, which decrease very rapidly with decreasing t_{01}. A very useful consequence of the rapid approach of TMR to saturation is that one does not require the knowledge of the hopping integrals across the interface to calculate the TMR in the tunneling regime. In fact, there are two points on the curve $R_{\rm TMR}(t_{01})$ that can be determined accurately without any model assumptions about t_{01}, i.e., the perfect metallic limit of GMR $t_{01}=t^{\rm bulk}$ (abrupt domain wall) and the strict tunneling limit $t_{01}\rightarrow 0$. It is interesting that the values of the GMR ratio for an abrupt domain wall (metallic limit) and for a tunneling junction predicted by a single-orbital tight-binding model of tunneling are very close to one another. It will be shown in Sec. V that the difference between the two values of the GMR ratio is much larger for a realistic multiorbital band structure.

Although Eq. (7) is a rigorous result of the scattering theory of transport, its formulation in terms of one-electron Green's functions is not very illuminating. However, Eq. (7)

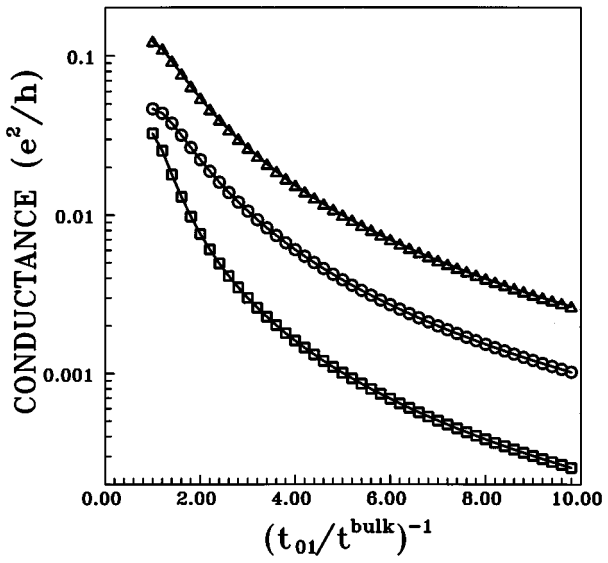

FIG. 2. Dependences of the conductances of the majority (squares) and minority (triangles) electrons in the ferromagnetic configuration and of the electrons of either spin orientation in the antiferromagnetic configuration (circles) on the reciprocal of the electron hopping between the ferromagnetic electrodes. Single-orbital tight-binding model.

can be given a very simple physical interpretation. First of all, we note that the total conductance of the junction is the sum of partial conductances in one-dimensional $\mathbf{k}_\parallel$ channels. This is, of course, a direct consequence of the assumed conservation of the parallel momentum. Moreover, $-(1/\pi)\mathrm{Im}\, g_L^\sigma(E_F,\mathbf{k}_\parallel)$ and $-(1/\pi)\mathrm{Im}\, g_R^\sigma(E_F,\mathbf{k}_\parallel)$ are the one-dimensional surface densities of states (DOS's) in a channel $\mathbf{k}_\parallel$ for the isolated left and right electrodes. It follows that the current in every channel $\mathbf{k}_\parallel$ is proportional to the product of the one-dimensional surface DOS's of the two electrodes but the product is scaled by the denominator in Eq. (7). A close link between the present linear-response theory and the conventional theory of the tunneling GMR is now obvious. If the scaling denominator is set equal to unity, Eq. (7) reduces exactly to the expression for the conductance obtained in the conventional theory of tunneling.[6] Note, however, that we are referring here to tunneling in a single $\mathbf{k}_\parallel$ channel. The correspondence appears to be complete since t_{01} plays the role of the usual tunneling matrix element.[6] Since t_{01} is very small in the tunneling regime, it is tempting to conclude that the denominator in Eq. (7) can always be approximated by unity, which would then lead to the conventional theory of tunneling. However, this simple argument breaks down when there are surface states in the electrodes since the one-dimensional surface DOS contains δ function peaks and the factor $t_{01}^2 g_L^\sigma g_R^\sigma$ in the denominator cannot be neglected no matter how small is the hopping integral t_{01}. There is, of course, no problem in reaching the tunneling limit numerically, as has been done in Fig. 1, provided due care is taken to achieve convergence of the $\mathbf{k}_\parallel$ sum. However, to use indiscriminately the approximation in which the denominator in Eq. (7) is simply replaced by unity is dangerous.

IV. TUNNELING MAGNETORESISTANCE DUE TO TUNNELING THROUGH AN INSULATING BARRIER

The general formulation of Sec. II will be now applied to a junction with an insulating barrier to demonstrate that tunneling across a vacuum gap and through an insulating layer lead to the same saturation value of the TMR. As in Sec. III, a single-orbital tight-binding model is used to describe a tunneling junction. The junction consists of two ferromagnetic electrodes separated by N atomic planes of an insulator with an on-site potential V_{ins} chosen so that the Fermi level E_F lies outside its band of allowed energies. The same nearest-neighbor hopping parameter t^{bulk} is used in the ferromagnetic electrodes and in the insulating layer, and all the band energies are again measured in units of t^{bulk}.

Formally, the calculation of the TMR from Eqs. (5) and (8) for such a system is identical to the calculation of the ballistic CPP GMR of a metallic trilayer.[12,19] One can, therefore, use directly the results derived for the metallic trilayer. It was shown by Mathon *et al.*[19] that the conductance of two semi-infinite ferromagnetic layers separated by N atomic planes of a metallic spacer is given by

$$\Gamma^\sigma=\frac{4e^2}{h}\sum_{\mathbf{k}_\parallel}\frac{\sin^2(k_\perp a)\,\mathrm{Im}\, g_L^\sigma\,\mathrm{Im}\, g_R^\sigma}{|\sin(N+1)k_\perp a-(g_L^\sigma+g_R^\sigma)\sin(Nk_\perp a)+g_L^\sigma g_R^\sigma\sin(N-1)k_\perp a|^2}. \tag{9}$$

As in Eq. (7), $g_L^\sigma(E_F,\mathbf{k}_\parallel)$ and $g_R^\sigma(E_F,\mathbf{k}_\parallel)$ are the surface Green's functions of the completely disconnected left and right electrodes, $k_\perp(E_F,\mathbf{k}_\parallel)$ is the perpendicular wave vector in the spacer, and a is the lattice constant. In the case of a metallic spacer, $k_\perp$ is real and determined from the bulk dispersion $E_F=V_{\mathrm{sp}}+2\cos(k_\perp a)+w(\mathbf{k}_\parallel)$, where $w(\mathbf{k}_\parallel)=2[\cos(k_x a)+\cos(k_y a)]$ is the in-plane dispersion and V_{sp} is the on-site potential in the spacer. In the case of an insulating spacer considered here, $k_\perp(E_F,\mathbf{k}_\parallel)$ is pure imaginary, $k_\perp=i\kappa$, and all the sine functions in Eq. (9) should, therefore, be replaced by hyperbolic sine functions. Since E_F lies outside the insulator band, the imaginary perpendicular wave vector is now determined from $E_F=V_{\mathrm{ins}}+2\cosh(\kappa a)+w(\mathbf{k}_\parallel)$.

The qualitative behavior of the TMR for a junction containing an insulator with a large band gap can be easily determined from Eq. (9). When the Fermi level lies well below the insulator conduction band (the barrier V_{ins} is high), κa is large and the decaying exponentials in all the hyperbolic sine functions in Eq. (9) can be neglected, which yields

$$\Gamma^{\sigma} \approx \frac{4e^2}{h} \sum_{\mathbf{k}_\parallel} \frac{e^{-2\kappa a N} \,\mathrm{Im}\, g_L^{\sigma} \,\mathrm{Im}\, g_R^{\sigma}}{|1-(g_L^{\sigma}+g_R^{\sigma})e^{-\kappa a}+g_L^{\sigma} g_R^{\sigma} e^{-2\kappa a}|^2}. \tag{10}$$

Moreover, when the distance between the Fermi level and the bottom of the insulator conduction band is much larger than the in-plane dispersion $w(\mathbf{k}_\parallel)$, the dependence of κ on $\mathbf{k}_\parallel$ can be neglected. This condition is satisfied when $V_{\mathrm{ins}} > W$, where W is the width of the insulator conduction band. In that case, the factor $\exp[-2\kappa(\mathbf{k}_\parallel)aN]$ can be taken outside the $\mathbf{k}_\parallel$ sum in Eq. (10) and replaced by $\exp[-2\kappa_0 aN]$, where κ_0 is the value of $\kappa(\mathbf{k}_\parallel)$ averaged over the two-dimensional Brillouin zone. The conductance of a junction with an insulator having a large band gap is, therefore, well approximated by

$$\Gamma^{\sigma} \approx \left(\frac{4e^2}{h}\right) e^{-2\kappa_0 aN} \times \sum_{\mathbf{k}_\parallel} \frac{\mathrm{Im}\, g_L^{\sigma} \,\mathrm{Im}\, g_R^{\sigma}}{|1-(g_L^{\sigma}+g_R^{\sigma})e^{-\kappa_0 a}+g_L^{\sigma} g_R^{\sigma} e^{-2\kappa_0 a}|^2}. \tag{11}$$

The structure of Eq. (11) is virtually identical to that of Eq. (7) for tunneling across a vacuum gap. The multiplicative factor $e^{-2\kappa_0 aN}$, which determines the strong dependence of the conductance on the height and width of the insulating barrier, again cancels out from the TMR ratio. Moreover, in the absence of surface states, the denominator in Eq. (11) tends to unity in the limit of a large insulator gap $\exp(-\kappa_0 a) \ll 1$. It follows that the TMR ratio approaches a saturation value which is determined entirely by the convolution of the one-dimensional densities of states $-(1/\pi)\mathrm{Im}\, g_L^{\sigma}(E_F,\mathbf{k}_\parallel)$ and $-(1/\pi)\mathrm{Im}\, g_R^{\sigma}(E_F,\mathbf{k}_\parallel)$ of the left and right ferromagnetic electrodes. The saturation value of the TMR ratio is, therefore, exactly the same as the saturation value of the TMR due to tunneling across a vacuum gap obtained from Eq. (7) in the limit $t_{01}/t^{\mathrm{bulk}} \ll 1$.

The TMR ratio R_{TMR} can be easily determined numerically from Eq. (9) for any height of an insulating barrier V_{ins}. The dependence of R_{TMR} on V_{ins}/W (W is the band width) is shown in Fig. 3 for three thicknesses of the insulating barrier $N=1$, 3, and 5 atomic planes. The values of the ferromagnet parameters $\epsilon_{\mathrm{FM}}=5.1$ and $\Delta=1.0$ (in units of t^{bulk}) are the same as in Sec. III. We recall that they were chosen to mimic a junction with Co electrodes.

It can be seen from Fig. 3 that a saturation value of the TMR is reached for barrier heights V_{ins} of the order of the band width (saturation is reached most rapidly for the narrow barrier $N=1$). It follows that for such values of the insulating barrier height, Eq. (11) provides a good estimate of the TMR. Moreover, the same estimate of the TMR ratio is obtained from Eq. (7) for tunneling across a vacuum gap. One can, therefore, conclude that tunneling across a vacuum gap and through an insulating barrier lead to the same saturation value of the TMR provided the insulator gap is of the order of or larger than the conduction band width. This argument will be used in Sec. IV to estimate the TMR of a Co(001) junction.

However, there is one important feature of the TMR due to tunneling through an insulating barrier that cannot be reproduced by the vacuum gap model. This is the dependence

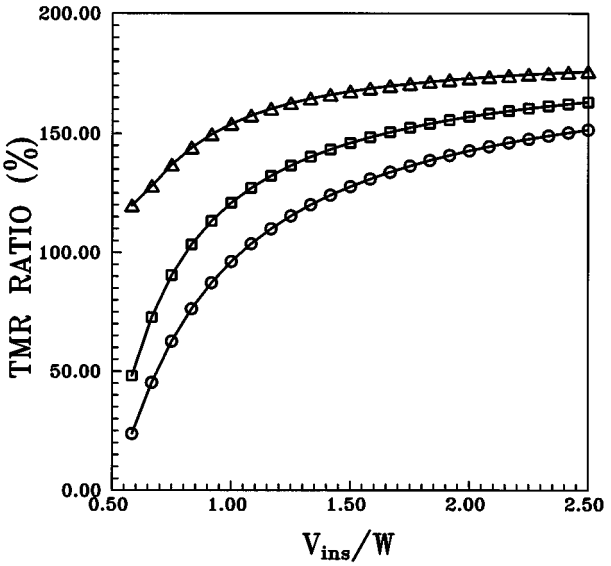

FIG. 3. Dependence of the tunneling magnetoresistance on the height of an insulating barrier between the ferromagnetic electrodes for a barrier whose thickness is one (triangles), three (squares), and five (circles) atomic planes. Single-orbital tight-binding model.

of the TMR on the barrier width. The width of a vacuum gap is equivalent to the height of a barrier but there is no equivalent of the barrier width in the tight-binding model of tunneling across a vacuum gap. The dependence of the TMR on the width of an insulating barrier can, of course, be determined numerically from Eq. (9). The results are shown in Fig. 4 for three heights of the tunneling barrier: $V_{\mathrm{ins}}/W = 1.0,\ 2.0$, and also for a very low barrier $V_{\mathrm{ins}}/W = 0.58$ (E_F just outside the band). It should be noted that the TMR ratio for the spacer thickness $N=0$ is that of a ferromagnet with an abrupt domain wall (no insulating barrier).

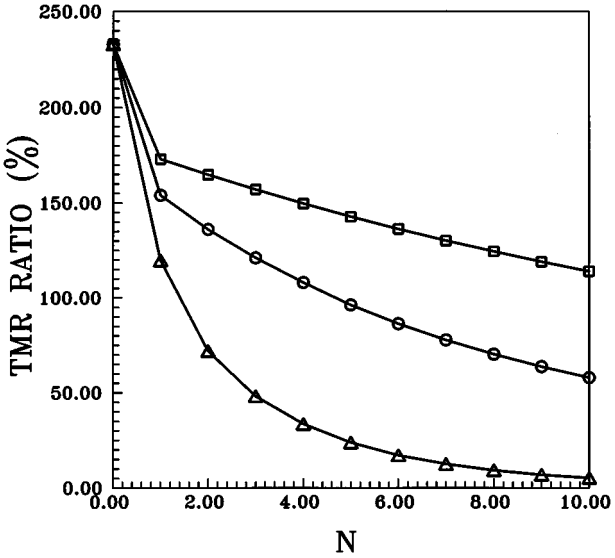

FIG. 4. Dependence of the tunneling magnetoresistance on the number of atomic planes in an insulating barrier for three heights of the barrier V_{ins} measured in units of the band width W: $V_{\mathrm{ins}}/W = 2.0$ (squares); $V_{\mathrm{ins}}/W = 1.0$ (circles); $V_{\mathrm{ins}}/W = 0.58$ (triangles). Single-orbital tight-binding model.

As expected from Eq. (11), the dependence of the TMR ratio on N is weak for a high potential barrier ($V_{\rm ins}/W=2.0$). In fact, the TMR is quite independent of N in the limit $V_{\rm ins}\rightarrow\infty$. However, it is most interesting that the TMR ratio depends strongly on the width of the barrier and, in fact, decreases rapidly with N when the insulating barrier is very low ($V_{\rm ins}/W=0.58$). The reason for this behavior is easy to understand. The weak dependence of the TMR on the barrier width predicted by Eq. (11) relies on the validity of the approximation $\exp[-2\kappa(\mathbf{k}_\parallel)aN]\approx\exp[-2\kappa_0 aN]$ which has been used to derive Eq. (11) from Eq. (10). This approximation is always valid for small N as long as E_F lies outside the insulator conduction band. However, it breaks down for large N. In fact, $\exp(2\kappa Na)\approx[(E_F-V_{\rm ins})/2]^{2N}[1-w(\mathbf{k}_\parallel)/(E_F-V_{\rm ins})]^{2N}$, where $w(\mathbf{k}_\parallel)/(E_F-V_{\rm ins})$ is a small parameter. It follows that $\exp(2\kappa Na)\approx[(E_F-V_{\rm ins})/2]^{2N}[1-2Nw(\mathbf{k}_\parallel)/(E_F-V_{\rm ins})+\ldots]$ and it is, therefore, clear that the dependence of the factor $\exp[-2\kappa(\mathbf{k}_\parallel)aN]$ on $\mathbf{k}_\parallel$ cannot be neglected for large N.

In the light of the above results, the conclusion that tunneling across a vacuum gap and through an insulating barrier leads to the same TMR needs to be qualified as follows. The two theoretical models of tunneling (vacuum gap and an insulating barrier) lead to the same TMR provided the barrier is at least as high as the conduction band width and the barrier is narrow, not wider than a few atomic planes.

V. TUNNELING MAGNETORESISTANCE DUE TO TUNNELING BETWEEN Co(001) ELECTRODES

The single-orbital tight-binding model of tunneling used in Secs. III–IV is too simple to provide quantitative estimates of the magnitude of the TMR ratio. However, the principal result of the model that the TMR ratio reaches a saturation value in the tunneling limit $t_{01}\rightarrow 0$ implies that the TMR can be determined without knowing the precise value of the tunneling matrix element t_{01}. It is, therefore, worthwhile to investigate whether this result carries through to a fully realistic multiorbital tight-binding description of TMR.

Consider two thick (semi-infinite) cobalt electrodes with (001) orientation of the surface. To determine the tunneling magnetoresistance across a vacuum gap, we start again with the well-defined case of an abrupt domain wall. The magnetoresistance can be determined exactly in this limit from Eqs. (5), (6), and (8) since the values of the tight-binding parameters for ferromagnetic fcc Co are readily available from a fit to a first-principles band structure,[20] and the matrix $t_{01}^{\sigma}(\mathbf{k}_\parallel)$ of hopping integrals across the interface is, of course, the same as in bulk Co. The only input required in the calculation are the matrix elements g_{00}^{σ} and g_{11}^{σ} of the one-electron Green's function at the surface of the semi-infinite left and right Co electrodes. They are usually generated by an iterative decimation technique[21] in which the surface Green's function is approximated by that at the surface of a thick stack of atomic planes. However, to obtain a truly surface Green's function, it is necessary to add in the decimation method a small imaginary part ϵ to the energy to disrupt quantum interference between the two surfaces of the slab. When ϵ is small, the convergence of the decimation method becomes poor. This might lead to complications since ϵ must be small in a transport calculation (if ϵ were not small, it would not be possible to discriminate accurately between propagating and localized states). I have, therefore, used a new noniterative technique for generating the surface Green's function[22] in which the convergence problem does not arise. A value $\epsilon=10^{-8}$ Ry, which was used in all the calculations, is so small that it has no effect on the conductance.

As in Sec. III, the aim is to reach the tunneling limit by turning off gradually the hopping integrals $t_{01}^{\sigma}(\mathbf{k}_\parallel)$ connecting the left and right Co electrodes. Compared with the single-orbital model of Sec. III, there is, however, a number of complications for a multiorbital band structure. First of all, the hopping integrals $t_{01}^{\sigma}(\mathbf{k}_\parallel)$ depend on the parallel momentum $\mathbf{k}_\parallel$, which means that they cannot be simply factored out of the $\mathbf{k}_\parallel$ sum in Eq. (5). It is, therefore, not immediately obvious that TMR saturates. The second problem is that the matrix elements $t_{0\alpha,1\beta}^{\sigma}(\mathbf{k}_\parallel)$ connecting different orbitals α, β across the vacuum gap scale differently with the separation r between the electrodes. To investigate the transition from the metallic to the tunneling regime, one needs, therefore, to know explicitly the dependences of all the matrix elements $t_{0\alpha,1\beta}^{\sigma}(\mathbf{k}_\parallel)$ on r.

I first address the second problem. Using s,p,d orbitals and hopping to first and second nearest neighbors, the tight-binding parameters for fcc ferromagnetic Co were obtained from the parameters for paramagnetic Co (Ref. 17) by adjusting self-consistently the on-site energies to achieve the best agreement with the first principles band structure[20] of fcc ferromagnetic Co. The matrix elements of the interplanar hopping matrix $t_{01}^{\sigma}(\mathbf{k}_\parallel)$ are, therefore, independent of the spin. They are all generated from the Slater-Koster two-center integrals $ll'm$ whose values for paramagnetic cobalt were obtained by Papaconstantopoulos.[17] Here, $l,l'=s,p,d$ are the usual orbital indices and $m=\sigma,\pi,\delta$ denotes the projection of the angular momentum.

To calculate the dependence of the GMR on the width of the gap between the Co electrodes, we require the dependence of the Slater-Koster parameters on the interatomic distance r. It is possible to include such a dependence without performing new first principles calculations. Andersen[23] proposed that the distance dependence of the tight-binding matrix elements $V_{ll'm}$ is given by

$$V_{ll'm}=C_{ll'm}r^{-(l+l'+1)}, \tag{12}$$

where $C_{ll'm}$ are distance-independent material constants. This expression suggests that the matrix elements for s-s interactions vary as r^{-1}, s-p interactions as r^{-2}, s-d and p-p interactions as r^{-3}, p-d interactions as r^{-4}, and d-d interactions as r^{-5}. The scaling law (12) was confirmed by Papaconstantopulos[17] for deviations of r from their equilibrium values as large as 5%.

For small deviations from the bulk interplanar distance $r_{\rm bulk}$ between the two Co electrodes, the GMR due to electron hopping across a gap $r>r_{\rm bulk}$ can be determined from Eqs. (5), (6), and (8) quite rigorously using the scaling law (12). For large values of r, the power-law scaling (12) is not expected to be valid. However, the key feature of the scaling law (12) that only the s-s interaction survives for large r is clearly valid generally in the tunneling limit $r\gg r_{\rm bulk}$. Since we are interested here only in the metallic and tunneling regimes, I propose to use the scaling law (12) for all values

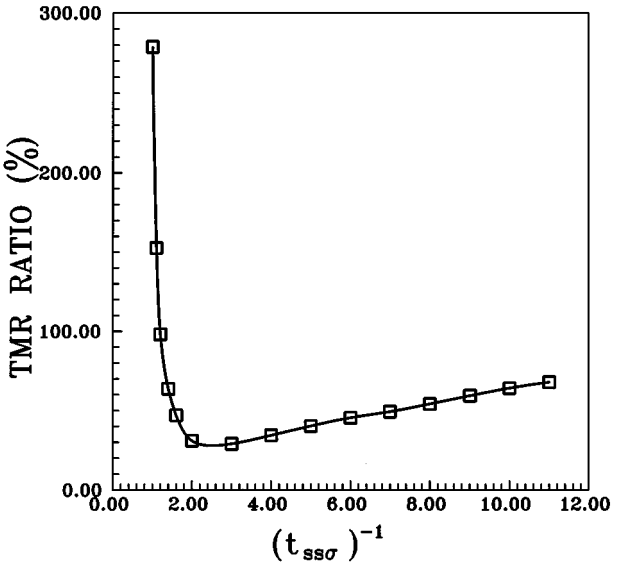

FIG. 5. Dependence of the tunneling magnetoresistance of a Co(001) junction on the reciprocal of the reduced s-s hopping between the Co electrodes.

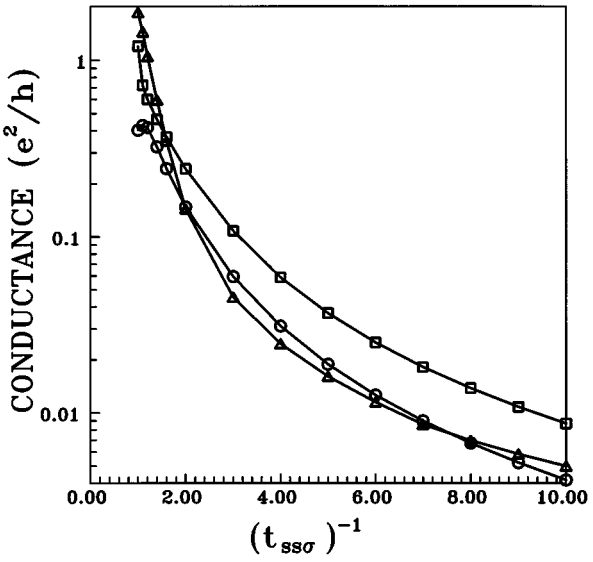

FIG. 6. Dependences of the conductances of the majority (squares) and minority (triangles) electrons in the ferromagnetic configuration and of the electrons of either spin orientation in the antiferromagnetic configuration (circles) on the reciprocal of the reduced s-s hopping between the Co electrodes.

of r treating it as an *ad hoc* interpolation scheme between the metallic limit $r \approx r_{\text{bulk}}$ and the tunneling limit $r \gg r_{\text{bulk}}$. Given that only the s-s interaction $V_{ss\sigma}$ survives in the tunneling regime, it is appropriate to use it as a measure of the width of the vacuum gap between the Co electrodes. It is, therefore, convenient to introduce a dimensionless reduced s-s hopping parameter $0 \leqslant t_{ss\sigma} \leqslant 1$ by $t_{ss\sigma} = V_{ss\sigma}/V_{ss\sigma}^{\text{bulk}}$, where $V_{ss\sigma}^{\text{bulk}}$ is the bulk s-s interaction in Co.

The dependence of the TMR ratio on the reduced reciprocal s-s hopping $(t_{ss\sigma})^{-1}$ between two Co(001) electrodes is shown in Fig. 5. The corresponding dependences of the conductances $\Gamma_{\text{FM}}^{\uparrow}$, $\Gamma_{\text{FM}}^{\downarrow}$, and $\Gamma_{\text{AF}}^{\uparrow,\downarrow}$ on $(t_{ss\sigma})^{-1}$ are shown in Fig. 6. It can be seen from a comparison of Figs. 1 and 5, that the qualitative behavior of the GMR ratio for the Co(001) junction is very similar to that of the single-orbital model of tunneling discussed in Sec. III. While the individual conductances Γ^{σ} decrease by more than two orders of magnitude when the s-s hopping $t_{ss\sigma}$ is reduced to 10% of its bulk value, the TMR ratio drops initially rather rapidly from its metallic CPP GMR value of 280% ($t_{ss\sigma}=1$) to about 40% but then increases only slowly to reach about 65% for $t_{ss\sigma}=0.1$. The rapid initial decrease of the GMR ratio for a Co junction did not occur in the single-orbital model of Sec. III. It occurs for the Co junction because, in the metallic limit $t_{ss\sigma} \approx 1$, a significant proportion of the current in Co is carried by d electrons that are highly spin polarized. This explains a large GMR ratio in the metallic regime (abrupt domain wall). In the tunneling regime, the current is carried only by s-p electrons which are weakly spin polarized and, hence, the TMR ratio is much smaller. This switching from d electrons to s-p electrons, as one moves from the metallic to tunneling regime, cannot be reproduced by a single-orbital model.

Another very interesting feature related to the aforementioned switching from d electrons to s-p electrons is that the polarization of the tunneling electrons changes sign as one moves from the metallic to the tunneling regime. This can be clearly seen in Fig. 6. In the metallic regime ($t_{ss\sigma}=1$), the conductance $\Gamma^{\downarrow}$ of the minority-spin electrons (triangles) is higher than the conductance $\Gamma^{\uparrow}$ of the majority-spin electrons (squares). However, a crossover takes place at about $t_{ss\sigma}=0.5$ and the conductance of the majority-spin electrons in the tunneling regime becomes higher than that of the minority-spin electrons ($\Gamma^{\uparrow}/\Gamma^{\downarrow} \approx 1.75$ for $t_{ss\sigma}=0.1$). The polarization of the tunneling electrons has, therefore, the same sign as the magnetization, i.e., opposite to that one would expect from the conventional density-of-states argument. This is in complete agreement with the results of all the experiments on tunneling from transition metal ferromagnets.[6]

I now return to the question of saturation of TMR in the tunneling regime. The slow variation of TMR after the initial rapid drop can be traced to the structure of Eq. (5) for the conductance. We first note that it is a good approximation to set in the tunneling regime $t_{01}^{\sigma}(\mathbf{k}_{\parallel}) \to 0$ all the tight-binding matrix elements equal to zero except for the s-s interaction $V_{ss\sigma}$. It follows that all the remaining nonzero matrix elements of the tunneling matrix $t_{01}^{\sigma}(\mathbf{k}_{\parallel})$ in Eq. (5) are proportional to $V_{ss\sigma}$, and this is the only parameter in the problem which depends on the gap width r. The conductance (5) contains, therefore, a scalar multiplicative factor $V_{ss\sigma}^2(r)$ which is independent of the parallel momentum $\mathbf{k}_{\parallel}$, and hence, cancels out in the GMR ratio (8). As for the single-orbital model, the entire variation of the TMR ratio in the tunneling regime is, therefore, determined by a weak dependence of the denominators in Eq. (6) on the gap width r. We recall that the denominators describe a mutual influence of the Co electrodes on one another, which is very weak in the tunneling regime. In fact, in the absence of surface states, $\lim_{r\to\infty} G_{01}^{\sigma} = 0$ and $\lim_{r\to\infty} G_{ii}^{\sigma} = g_{ii}^{\sigma}$, where g_{ii}^{σ} are the surface Green's function of completely disconnected left (i

$=0$) and right ($i=1$) Co electrodes. It follows from this argument that saturation of the TMR in the tunneling limit $t_{01}^{\sigma}(\mathbf{k}_{\parallel}) \rightarrow 0$ is inevitable.

The only question that remains is whether the TMR ratio in Fig. 5 has reached its saturation value for $t_{ss\sigma} \approx 0.1$. Unfortunately, the numerical evaluation of the conductances Γ^{σ} requires a very large number of $\mathbf{k}_{\parallel}$ points ($\approx 10^5$) to achieve convergence in the Brillouin zone sum in Eq. (5) and the number of $\mathbf{k}_{\parallel}$ points needed increases with decreasing hopping $t_{ss\sigma}$. Convergence could, therefore, be achieved only for $t_{ss\sigma} \geqslant 0.1$. Since the TMR ratio still increases for $t_{ss\sigma} \approx 0.1$, the value for TMR of about 65% obtained from Fig. 5 should, therefore, be regarded as a theoretical lower bound on the TMR of a Co(001) junction. The calculated saturation value of the TMR of 40–65% for a Co(001) junction is in a remarkably good agreement with the TMR ratio of about 40% observed[3] for a Co junction with an Al_2O_3 barrier.

Finally, I wish to emphasize that the dependence of the TMR ratio on the vacuum gap width shown in Fig. 5 should not be confused with the dependence of the TMR on the width of an insulating barrier. As discussed in Sec. IV, the width of the vacuum gap is related instead to the height of a narrow insulating barrier. The calculated values of the TMR for a Co(001) junction should, therefore, be relevant only to experiments with narrow insulating barriers.

VI. CONCLUSIONS

The tunneling magnetoresistance was investigated using a unified theory of the TMR and CPP GMR based on the Kubo-Landauer formula and a multiorbital tight-binding band structure of the ferromagnetic electrodes. The only assumptions of the theory are that the spin and parallel momentum are conserved in tunneling and the applied bias is low (linear-response theory). Under these assumptions, the nonperturbative Kubo-Landauer theory allows one to investigate a continuous transition from the CPP GMR of a metallic system to the TMR of a tunneling junction, which takes place as the band structure parameters of the nonmagnetic spacer are varied. Within a tight-binding scheme, there are two alternative ways of describing the transition from the CPP GMR to TMR. In the first approach, used in Secs. III and V, the overlap matrix elements between the ferromagnetic electrodes are gradually turned off to reach the tunneling regime (tunneling across a vacuum gap). The second method, explored in Sec. IV, is to vary the on-site potentials in the spacer so that the Fermi level in the spacer layer moves into the band gap (tunneling through an insulating barrier).

The TMR due to tunneling across a vacuum gap was first investigated in Sec. III for a single-orbital tight-binding model of the ferromagnetic electrodes. It was demonstrated in Sec. III both analytically and numerically that the TMR ratio depends only weakly on the overlap matrix element across the vacuum gap and approaches very rapidly a saturation value when the tight-binding hopping integral t_{01} connecting the ferromagnetic electrodes is decreased to 5–10 % of its value t^{bulk} in the ferromagnet. The saturation value of the TMR is very close to the value of the CPP GMR in the metallic regime $t_{01} \approx t^{\text{bulk}}$. The present theory of tunneling across a vacuum gap reduces in the limit $t_{01} \rightarrow 0$ to the classical theory of tunneling[6,8,10] with two important modifications. First, contrary to popular belief, the tunneling current is not proportional to the product of the densities of states of the ferromagnetic electrodes. It is determined instead by the convolution over the parallel momentum of the spectral densities of the left and right electrodes. Moreover, all the surface states are excluded from the convolution and, therefore, make no contribution to tunneling.

The TMR due to tunneling through an insulating barrier was investigated in Sec. IV using the same single-orbital tight-binding model as in Sec. III. Starting with a metallic spacer, the on-site potential in the spacer was gradually increased until the Fermi level moved out of the spacer conduction band, and thus the tunneling regime was reached. It was again found, both analytically and numerically, that the TMR ratio depends only weakly on the on-site potential in the spacer and reaches a saturation value when the insulating barrier height is of the order of the conduction band width. The saturation values of the TMR due to tunneling across a vacuum gap and due to tunneling through an insulating barrier are exactly the same. One can, therefore, conclude that the two models of the TMR are physically equivalent. However, this conclusion holds only for thin insulating barriers.

The dependence of the TMR on the width of an insulating barrier was also investigated in Sec. IV. The results are rather interesting in that the dependence on the thickness of the insulating layer, predicted by the single-orbital model, is weak when the barrier is high but becomes very strong when the barrier is low (the Fermi level lies close to the conduction band edge). In fact, the TMR for a low insulating barrier decreases very rapidly with increasing thickness of the insulating spacer. This may have implications for the experiment since the height of the barrier in a very thin oxide may be lower than in the bulk material, particularly if oxidation is imperfect.

Having established an equivalence between the two models of tunneling (vacuum gap and insulating barrier), the TMR due to tunneling between two Co(001) electrodes separated by a vacuum gap was investigated in Sec. V using fully realistic tight-binding bands fitted to a first-principles band structure of ferromagnetic fcc Co. It is found that, when the tight-binding hopping integrals between the two Co electrodes are gradually turned off, the TMR ratio drops initially rather rapidly from its metallic CPP GMR value of 280% to about 40% but then increases only slowly to reach about 65% when the dominant s-s hopping is of the order of 10% of the s-s hopping in Co. The rapid initial decrease of the GMR ratio for a Co junction occurs because, near the metallic limit, a significant proportion of the current in Co is carried by d electrons that are highly spin polarized. This explains a large GMR ratio in the metallic regime (abrupt domain wall). In the tunneling regime, the current is carried only by s-p electrons which are weakly spin polarized and, hence, the TMR ratio is much smaller.

Another very interesting feature related to the aforementioned switching from d electrons to s-p electrons is that the polarization of the tunneling electrons changes sign as one moves from the metallic to the tunneling regime. In the metallic regime, the conductance $\Gamma^{\downarrow}$ of the minority-spin electrons is higher than the conductance $\Gamma^{\uparrow}$ of the majority-spin electrons. However, a crossover takes place when the s-s

hopping drops to about half of its bulk value and the conductance of the majority-spin electrons in the tunneling regime becomes higher than that of the minority-spin electrons ($\Gamma^{\uparrow}/\Gamma^{\downarrow} \approx 1.75$). The polarization of the tunneling electrons has, therefore, the same sign as the magnetization, i.e., opposite to what one would expect from the conventional density-of-states argument. This is in complete agreement with the results of all the experiments on tunneling from transition metal ferromagnets.[6]

The calculated saturation value of the TMR for a Co(001) junction in the tunneling regime ranges from 40 to 65%. This is in a remarkably good agreement with the TMR ratio of about 40% observed[3] for a Co junction with a thin Al_2O_3 insulating barrier.

Finally, I wish to emphasize yet again that the dependence of the TMR ratio on the vacuum gap width, that was calculated in Sec. V, should not be confused with a dependence of the TMR on the width of an insulating barrier. As shown in Sec. IV, the width of the vacuum gap is related instead to the height of a narrow insulating barrier. The calculated values of the TMR for a Co(001) junction are, therefore, relevant only to experiments with narrow insulating barriers.

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