Temperature Dependence of Itinerant Electron Junction Magnetoresistance

A. H. MacDonald,[1] T. Jungwirth,[1,2] and M. Kasner[1]
[1]*Department of Physics, Indiana University, Bloomington, Indiana 47405*
[2]*Institute of Physics ASCR, Cukrovarnická 10, 162 00 Praha 6, Czech Republic*
(Received 18 December 1997)

In itinerant electron ferromagnets, spectral weight is transferred at finite temperatures from quasiparticle peaks located at majority- and minority-spin band energies to shadow-band peaks. For a given Bloch wave vector and band index, the majority-spin shadow-band peak is located near the minority-spin quasiparticle energy and the minority-spin shadow-band peak is located near the majority-spin quasiparticle energy. This property can explain much of the temperature dependence seen in the magnetoresistance of magnetic tunnel junctions. [S0031-9007(98)06624-1]

PACS numbers: 75.10.Lp, 75.30.Ds, 75.30.Et

Efforts [1] to achieve a complete understanding of late transition metal ferromagnets have been frustrated by fundamental difficulties associated with the band character of the electrons which carry the spontaneous magnetic moment. The itinerant character of magnetic electrons in these systems is incontrovertibly established by de Haas–van Alphen studies [2] which map out majority- and minority-spin Fermi surfaces enclosing $\vec{k}$-space volumes consistent with the measured saturation moment per atom. Nevertheless, many finite-temperature properties of these systems are inconsistent with a simple Stoner-Wohlfarth [3] mean-field theory for band ferromagnets and are more easily rationalized in a picture in which the d electrons are regarded as localized. The localized versus itinerant conundrum is often most informatively addressed by probes of the one-particle Green's function. For example, photoemission studies have [4] and continue [5] to improve insight. The present work is motivated by recent success [6] in fabricating ferromagnet-insulator-ferromagnet magnetic tunnel junctions (MTJs) with reproducible characteristics, opening up the possibility of obtaining spin-resolved information on the tunneling density of states of band ferromagnets. We point out that, in an itinerant electron ferromagnet, a portion of the spectral weight is transferred [7] at finite temperatures from a majority- or minority-spin quasiparticle peak to a shadow-band peak [8] located near the opposite spin quasiparticle energy. The fraction of the spectral weight transferred is proportional, at low temperatures, to the saturation moment suppression. We propose that this effect is responsible for much [9] of the temperature dependence of MTJ magnetoresistance (MR).

Tunneling measurements are usually interpreted by assuming a weak link which can be modeled by a phenomenological tunneling Hamiltonian. This approach allows the tunneling current to be expressed quite generally in terms of electronic spectral functions [10]. Assuming only that the temperature is much smaller than the respective bandwidths, the tunneling conductance between two weakly linked ferromagnets is

$$G = \frac{2\pi e^2}{\hbar} \sum_{\sigma} \sum_{n_L,\vec{k}_L} \sum_{n_R,\vec{k}_R} |t(n_L,\vec{k}_L;n_R,\vec{k}_R)|^2 \times A^L_{n_L,\vec{k}_L,\sigma}(E_F) A^R_{n_R,\vec{k}_R,\sigma}(E_F)\,. \quad (1)$$

Here $A_{n,\vec{k}}(E)$ is the spectral weight function for band n at wave vector $\vec{k}$, L (left) and R (right) label ferromagnets on opposite sides of the MTJ, and $\sigma = \uparrow$ (majority spin on left side of junction), ($\downarrow$) (minority spin on left side of junction) labels spin. To establish notation we first discuss our view of the band theory interpretation of junction magnetoresistance.

In band theory, metallic ferromagnets are characterized by spin-split temperature-independent energy bands with infinite quasiparticle lifetimes: $A_{n,\vec{k},\sigma}(E) = \delta(E_{n,\vec{k},\sigma} - E)$. We assume that the tunneling amplitudes appearing in Eq. (1) can be approximately decoupled into factors depending separately on band wave functions on opposite sides of the barrier, i.e., that $|t(n_L,\vec{k}_L;n_R,\vec{k}_R)|^2 \approx |t(n_L,\vec{k}_L)|\,|t(n_R,\vec{k}_R)|$. This assumption is physically natural [11] and, as we comment below, is necessary to explain the common success of the Jullière [12] formula in interpreting MR data. The tunneling conductance is then proportional to a sum over spin directions of the product of factors depending separately on left and right ferromagnets:

$$G = \frac{2\pi e^2}{\hbar} \sum_{\sigma} t^L_\sigma N^L_\sigma t^R_\sigma N^R_\sigma . \quad (2)$$

Here N_σ is the Fermi level density of states and t_σ is a weighted average of tunneling amplitude factors defined by

$$t_\sigma N_\sigma = \sum_{n,\vec{k}} |t_{n,\vec{k}}| \delta(E_F - E_{n,\vec{k},\sigma})\,. \quad (3)$$

From Eq. (2) we can evaluate the parameter usually used to characterize the magnetoresistance of a MTJ:

$$\frac{G_P - G_A}{G_P} = \frac{2P^L P^R}{1 + P^L P^R}\,. \quad (4)$$

Here G_P and G_A are, respectively, the conductances when ordered moments on opposite sides of the junction have parallel and antiparallel orientations.

$$P = \frac{t_a N_a - t_i N_i}{t_a N_a + t_i N_i}, \tag{5}$$

where the indices a and i refer to m*a*jority and m*i*nority spins, respectively. Comparing Eqs. (5) and (2), P can be identified as the spin polarization of the tunneling current between a ferromagnet and a spin-unpolarized system. This quantity has been measured for most systems of interest [13]. The tunneling current is generally found to be dominated by the majority spins, even when their density of states is smaller, because tunneling amplitudes are larger [14] for states with a dominant s-wave character. Equation (4) is the Jullière [12] formula which is in good agreement with many experimental results; the present derivation demonstrates that its approximate validity rests on the factorizability of tunneling matrix elements.

We now address the importance for junction magnetoresistance of the modifications of band theory which are required at finite temperatures. Up to room temperature and beyond, the main effect of finite T on late transition element ferromagnets is to excite low-energy long-wavelength spin waves [1,2,15]. To a good approximation, the quasiparticle bands of the ferromagnet adiabatically follow the local instantaneous orientation of the magnetic moment. Although the quasiparticle spectrum in this approximation is rigid, its projection onto the time-averaged ordered moment direction is altered. A quasiparticle whose spin is aligned with the fluctuating bands will at finite temperature be a majority spin with probability $[1 + m(T)/m_0]/2$ and a minority spin with probability $[1 - m(T)/m_0]/2$. Here $m(T)/m_0$ is the factor by which the saturation moment is reduced at temperature T due to thermally excited spin waves. A *shadow-band* peak must appear in the minority-spin spectral function at the majority-spin quasiparticle energy. The effect on MR of shadow-band features in the majority- and minority-spin spectral functions is illustrated schematically in Fig. 1. Two terms contribute to $t_\uparrow N_\uparrow$ at finite temperatures, one arising from the majority-spin quasiparticle band, the other from the minority-spin shadow band. For example, in the left ferromagnet,

$$t_\uparrow^L N_\uparrow^L = \frac{1 + m(T)/m_0}{2} t_a^L N_a^L + \frac{1 - m(T)/m_0}{2} t_i^L N_i^L,$$
$$t_\downarrow^L N_\downarrow^L = \frac{1 + m(T)/m_0}{2} t_i^L N_i^L + \frac{1 - m(T)/m_0}{2} t_a^L N_a^L. \tag{6}$$

Corresponding expressions apply for the right ferromagnet. It follows that the Jullière formula continues to apply at finite temperatures with a reduced polarization factor $P(T) = [m(T)/m_0]P(0)$ for each ferromagnet. The saturation moments, $m(T)$, of bulk late transition element ferromagnets are reduced by $\sim 5\%$ between $T = 0$ and room temperature, and reduction factors near the surface can be larger by a factor of 2 [16] or more [17]. Reductions in MR of $\sim 20\%$ at room temperature, as seen in experiments, are readily accounted for by this mechanism. An experimentally testable prediction which follows from this assertion is that [18] MR should follow a $T^{3/2}$ law at low temperatures: $\mathrm{MR}(T) = \mathrm{MR}(T = 0)(1 - AT^{3/2} + \cdots)$, where A is $1 - \mathrm{MR}(T = 0)/2$ times the sum of the $T^{3/2}$ coefficients for the relative magnetization of the two ferromagnetic electrodes.

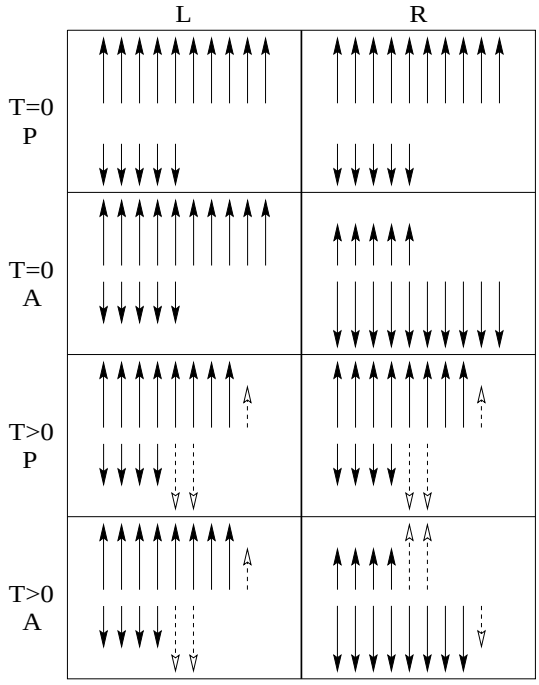

FIG. 1. Schematic illustration of spin-polarized tunneling between left (L) and right (R) ferromagnets with parallel (P) and antiparallel (A) magnetizations at zero and finite temperature. In each case long arrows represent quasiparticles whose spins are aligned with the fluctuating bands while short arrows represent quasiparticles with the opposing spin orientation. The number of large arrows for $T = 0$ is proportional to $t_a N_a$, and the number of small arrows proportional to $t_i N_i$. In this illustration, $t_a N_a = 10$ and $t_i N_i = 5$ in arbitrary units. At $T = 0$, $G = 10 \times 10 + 5 \times 5 = 125$ for parallel orientations, $G = 2 \times 10 \times 5 = 100$ for antiparallel orientations, and MR = 20%. The finite temperature panels correspond to $m(T)/m_0 = 0.6$, so that 80% of the spectral weight resides in quasiparticle peaks (solid lines) and 20% resides in shadow-band peaks (dashed lines). The parallel orientation conductance is then reduced to $G = 9 \times 9 + 6 \times 6 = 117$, the antiparallel orientation conductance increased to $G = 2 \times 9 \times 6 = 108$, and MR decreased to 7.7%.

We now turn to a more microscopic explanation of the shadow-band features in the electron spectral function. The abridged discussion presented here is intended to emphasize that the effect requires only that the ground state of the ferromagnet be a spontaneously spin-polarized Fermi liquid. It is compatible with strong local correlation features [5] being present in the spectral functions, compatible with strong band dependence for the quasiparticle energy spin splitting, and independent of the complexity and individuality of the quasiparticle bands of particular metallic ferromagnets. We assume that in the ground state of the ferromagnet, the one-particle Green's function is that of a spin-polarized Fermi liquid, with quasiparticle peaks for both $\uparrow$ and $\downarrow$ spins which become arbitrarily sharp as the Fermi energy is approached:

$$G_{n\sigma,n'\sigma'}(\vec{k},E) = [\delta_{n\sigma,n'\sigma'}E - H^{\rm QP}_{n\sigma,n'\sigma'}(\vec{k},E)]^{-1} = [\delta_{n\sigma,n'\sigma'}(E - E_{n,\sigma}(\vec{k},E)) + i\delta_{\sigma,\sigma'}\Gamma_{n\sigma,n'\sigma}(\vec{k},E)]^{-1}. \quad (7)$$

The real part of the electronic self-energy is included in $E_{n,\sigma}(\vec{k},E)$, and we use a representation where the Green's function is diagonal in the band index n. Invariance of the system under spin rotations about the moment direction guarantees that G is diagonal in spin indices. At the Fermi energy, chosen as $E = 0$, the imaginary part of the self-energy, $\Gamma_{n\sigma,n'\sigma'}$, vanishes. In the most naive version of ferromagnetic band theory the quasiparticle bands are rigidly spin split, $E_{n,\uparrow}(\vec{k},E) \to E_n(\vec{k}) - \Delta/2$ and $E_{n,\downarrow}(\vec{k},E) \to E_n(\vec{k}) + \Delta/2$. Modern spin-density functional ferromagnet quasiparticle bands are *not* rigidly spin split, and at $T = 0$, generally in qualitative [2,3] agreement with experiment.

In Fe, Ni, Co, and their alloys it is a good approximation, up to room temperature and beyond, to account for thermal fluctuations only in the ordered moment direction, to assume that these vary slowly on an atomic length scale, and to regard the quasiparticles as separate but coupled degrees of freedom. Keeping only the leading term in a gradient expansion, the excess energy density is $\rho_s|\nabla\vec{n}|^2/2$, where $\vec{n} = (n_x, n_y, n_z)$ is the unit vector which defines the local ordered moment orientation and ρ_s is the spin stiffness. For small tilts away from the $\hat{z}$ direction, the excess energy due to spin fluctuations, $H^{\rm SW}$, may be expressed in terms of transverse components of the moment orientation vector. Fourier transforming we find that

$$H^{\rm SW} = \frac{\rho_s}{2V}\sum_{\vec{q}} q^2[n_{x-\vec{q}}n_{x\vec{q}} + n_{y-\vec{q}}n_{y\vec{q}}]. \quad (8)$$

The quantum commutator between transverse spin components may be replaced by a c number as long as the saturation moment suppression is not large:

$$[n_{x-\vec{q}}, n_{y\vec{q}'}] = i\delta_{\vec{q},\vec{q}'}\frac{2V}{m_0}. \quad (9)$$

In Eq. (9), which results from coarse graining electron spin commutation relations, V is the system volume. This leads to a free boson spin-wave Hamiltonian:

$$H^{\rm SW} = E_0 + \sum_{\vec{q}} \epsilon_{\rm SW}(\vec{q})a^\dagger_{\vec{q}}a_{\vec{q}}, \quad (10)$$

where $[a_{\vec{q}}, a^\dagger_{\vec{q}'}] = \delta_{\vec{q},\vec{q}'}$, and $\epsilon_{\rm SW}(\vec{q}) = Dq^2 = 2\rho_s q^2/m_0$. The expression we use below for spin-wave quasiparticle coupling follows from the relationship between the spin-wave annihilation operator and the Fourier transforms of the transverse spin-orientation field:

$$a_{\vec{q}} = \left(\frac{m_0}{4V}\right)^{1/2}(n_{x\vec{q}} + in_{y\vec{q}}). \quad (11)$$

In the fluctuating band picture of itinerant electron ferromagnets, quasiparticle bands rotate in spin space along with a slow variation in the ordered moment direction. At the Fermi energy the imaginary part of the quasiparticle self-energy can be neglected and

$$H^{\rm QP}_{n\sigma,n'\sigma'}(\vec{k},E=0) \to \frac{\delta_{n,n'}}{2}\{[E_{n,\uparrow}(\vec{k}) + E_{n,\downarrow}(\vec{k})]\delta_{\sigma,\sigma'} - \Delta_n(\vec{k})(\vec{\tau}\cdot\vec{n})_{\sigma,\sigma'}\}, \quad (12)$$

where components of $\vec{\tau}$ are the Pauli matrices, $\Delta_n(\vec{k}) \equiv E_{n,\downarrow}(\vec{k}) - E_{n,\uparrow}(\vec{k})$ is the band and wave-vector dependent spin splitting, and all self-energies have been evaluated at $E = 0$. Expanding the right-hand side of Eq. (12) to leading order in n_x and n_y, the zeroth order term gives the ground state quasiparticle bands and the leading order correction gives the spin-wave quasiparticle interaction. Allowing the orientation to vary slowly [19] in space and Fourier transforming leads to the following interaction Hamiltonian between quasiparticles and spin waves, written in second quantized form:

$$H^{\rm SW-QP} = \sum_{n,\vec{k},\vec{q}} \frac{\Delta_n(\vec{k})}{\sqrt{V}m_0}[c^\dagger_{n,\vec{k}+\vec{q}/2,\uparrow}c_{n,\vec{k}-\vec{q}/2,\downarrow}a^\dagger_{\vec{q}} + \text{H.c.}]. \quad (13)$$

The evaluation of the single spin-wave-exchange self-energy is similar to the evaluation of the phonon-exchange [20] self-energy and leads to

$$\Sigma_{n\uparrow}(\vec{k},E) = \int \frac{d\vec{q}}{(2\pi)^3}\frac{\Delta_n^2(\vec{k}+\vec{q}/2)}{m_0}\frac{n_B(\epsilon_{\rm SW}(\vec{q})) + n_F(E_{n\downarrow}(\vec{k}+\vec{q}))}{[E + \epsilon_{\rm SW}(\vec{q}) - E_{n\downarrow}(\vec{k}+\vec{q})]}. \quad (14)$$

Because of the gapless spin-wave excitations, the Fermi occupation factor, n_F, in the numerator of the integrand can be neglected at finite temperatures in comparison with the Bose factor, n_B. The integration is dominated by the k-space volume satisfying $\epsilon_{\rm SW}(\vec{q}) < k_BT$. We assume that at temperatures of interest $q's$ satisfying this inequality are small compared to Brillouin-zone dimensions and set $\vec{q} \to 0$ on the right-hand side of Eq.(14). These approximations lead to

$$\Sigma_{n\uparrow}(\vec{k},E) \approx \frac{\Delta_n^2(\vec{k})}{2}\frac{1 - m(T)/m_0}{E - E_{n\downarrow}(\vec{k})}. \quad (15)$$

where

$$\frac{m(T)}{m_0} = 1 - \frac{2}{m_0} \int \frac{d\vec{q}}{(2\pi)^3} n_B(\epsilon_{\mathrm{SW}}(\vec{q})) \qquad (16)$$

is the relative magnetization suppression due to thermal spin-wave excitations. A similar calculation gives the contribution to the spin ↓ self-energy:

$$\Sigma_{n\downarrow}(\vec{k}, E) \approx \frac{\Delta_n^2(\vec{k})}{2} \frac{1 - m(T)/m_0}{E - E_{n\uparrow}(\vec{k})}. \qquad (17)$$

These simple self-energy expressions give Dyson equations which can be solved analytically. The spin ↑ Green's function has two simple poles, one at $E_{n\uparrow}(\vec{k})$ and one at $E_{n\downarrow}(\vec{k})$. When the magnetization suppression is small, the spectral weights of the two poles are $[1 + m(T)/m_0]/2$ and $[1 - m(T)/m_0]/2$, respectively, in agreement with the naive fluctuating band argument given above. Similarly the spin ↓ Green's function splits its spectral weight between poles at the $T = 0$ minority- and majority-band positions. Inserting these spectral functions in Eq. (1) leads to Eq. (6), as argued previously. When the magnetization suppression is large, the low-temperature approximations leading to this result begin to fail and alteration of the low-temperature spectral weights will become more complex and more material specific.

The authors acknowledge helpful interactions with W. H. Butler, J. F. Cooke, J. Freeland, J. S. Moodera, I. Schuller, R. S. Sooryakumar, and R. van de Veerdonk. This work was supported by the National Science Foundation under Grants No. DMR-9714055 and No. INT-9602140 and by the Ministry of Education of the Czech Republic under Grant No. ME-104.

Note added.—A recent experimental study [21] we learned of after this work was completed finds that the temperature dependence of MR for $Co/Al_2O_3/Ni_{80}Fe_{20}$ junctions is described by a $T^{3/2}$ law, as predicted here. The interpretation offered there also starts from the claim, based on indications from low-energy cascade electrons in spin-polarized photoemission experiments [17], that P is proportional to the T-dependent saturation moment. The theoretical framework presented here permits a simple and consistent interpretation of both experiments.

[1] H. Capellmann, J. Magn. Magn. Mater. **28**, 250 (1982).
[2] See, for example, G. G. Lonzarich, in *Electrons at the Fermi Surface* (Cambridge University Press, Cambridge, England, 1980); H. Ebert, P. Strange, and B. L. Gyorffy, J. Phys. F **18**, L135 (1988), and references therein.
[3] E. P. Wohlfarth, Rev. Mod. Phys. **25**, 211 (1953); D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).
[4] E. Dietz, U. Gerhardt, and C. J. Maetz, Phys. Rev. Lett. **40**, 892 (1978); D. E. Eastman, F. J. Himpsel, and J. A. Knapp, *ibid.* **40**, 1514 (1978).
[5] B. Sinkovic *et al.*, Phys. Rev. Lett. **79**, 3510 (1997).
[6] J. S. Moodera *et al.*, Phys. Rev. Lett. **74**, 3273 (1995); T. Miyazaki and N. Tezuka, J. Magn. Magn. Mater. **139**, L231 (1995); C. T. Tanaka, J. Nowak, and J. S. Moodera, J. Appl. Phys. **81**, 5515 (1997); W. J. Gallagher *et al.*, J. Appl. Phys. **81**, 3741 (1997).
[7] This property, although it has not usually been emphasized, is implicit in the fluctuating band theory of metallic ferromagnetism [V. Korenman, J. L. Murray, and R. E. Prange, Phys. Rev. B **16**, 4032 (1977); **16**, 4048 (1977); **16**, 4058 (1997)]; H. Capellmann, J. Phys. F **4**, 1466 (1974). For related more recent work, see B. L. Gyorffy, A. J. Pindor, J. Staunton, G. M. Stocks, and H. Winter, J. Phys. F **15**, 1337 (1985); L. M. Sandratskii and J. Kübler, Europhys. Lett. **23**, 661 (1993).
[8] We adopt this terminology in recognition of similarities between the microscopic physics, described later, which leads to the additional spectral peaks in ferromagnets and that responsible for the shadow-band peaks discussed in recent literature on antiferromagnetically correlated metals; A. M. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990); **42**, 7967 (1990); Y. M. Vilk, Phys. Rev. B **55**, 3870 (1997).
[9] Other effects can contribute to the T dependence of the junction magnetoresistance. See S. Zhang *et al.*, Phys. Rev. Lett. **79**, 3744 (1997); F. Guinea, e-print cond-mat/9709315. The present Letter shows that substantial temperature dependence is already present in the simplest-possible tunneling Hamiltonian description of a MTJ.
[10] E. L. Wolf, in *Principles of Electron Tunneling Spectroscopy* (Oxford University Press, New York, 1984).
[11] We assume that the tunneling barriers are sufficiently disordered that memory of the Bloch momentum parallel to the junction plane is lost upon tunneling, leaving a tunneling amplitude with independent dependence on initial and final states.
[12] M. Jullière, Phys. Lett. **54A**, 225 (1975).
[13] P. M. Tedrow and R. Meservey, Phys. Rev. Lett. **26**, 192 (1971); R. Meservey and P. M. Tedrow, Phys. Rep. **238**, 174 (1994).
[14] J. A. Hertz and Koya Aoi, Phys. Rev. B **8**, 3252 (1973); J. Mathon, *ibid.* **56**, 11 810 (1997); J. M. MacLaren, X.-G. Zhang, and W. H. Butler, *ibid.* **56**, 11 827 (1997).
[15] G. Lonzarich, in *Transition Metals 1977* (Institute of Physics, Bristol, 1978), p. 518; G. Lonzarich and A. V. Gold, Can. J. Phys. **52**, 694 (1974).
[16] D. L. Mills and A. A. Maradudin, J. Phys. Chem. Solids **28**, 1855 (1967).
[17] D. T. Pierce, R. J. Celota, J. Unguris, and H. C. Siegmann, Phys. Rev. B **26**, 2566 (1982); D. Mauri, D. Scholl, H. C. Siegmann, and E. Kay, Phys. Rev. Lett. **61**, 758 (1988).
[18] Below $T \sim 10$ K corrections due to the gap in the spin-wave spectrum created by anisotropy and internal fields can alter this result.
[19] For spatially constant $\vec{n}$ the interaction is diagonal in band indices and therefore nonlocal in space. For slowly varying $\vec{n}$ we evaluate the $\vec{n}$ at the midpoint of *bra* and *ket* position vectors. Spin-wave quasiparticle interactions which are off diagonal in band index vanish linearly with wave vector and are taken to be negligible here.
[20] See, for example, G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
[21] J. S. Moodera, J. Nowak, and R. J. M. van de Veerdonk, Phys. Rev. Lett. **80**, 2941 (1998); (unpublished).